ENUMATH 2023

LISBOA
PORTUGAL

04 - 08
SEPTEMBER

European Conference on Numerical Mathematics and Advanced Applications

BOOK OF ABSTRACTS

Full abstracts, including all authors, and references are available in electronic format at the conference webpage `https://enumath2023.com`.

A USB pen drive with the Book of Abstracts is included in the Conference Bag.

Contents

FOREWORD

The ENUMATH 2023 Conference to be held at the Instituto Superior Técnico (IST), Lisbon, Portugal, is the 14th of this series of conferences which started in Paris (1995), followed by Heidelberg (1997), Jyväskylä (1999), Ischia Porto (2001), Prague (2003), Santiago de Compostela (2005), Graz (2007), Uppsala (2009), Leicester (2011), Lausanne (2013), Ankara (2015), Bergen (2017) and Egmond aan Zee (2019).

It is a great pleasure to welcome you to this ENUMATH Conference and to the city of Lisbon. Our central goal in organizing the Conference is to fulfill the objectives of the ENUMATH conferences, namely to provide a forum for presenting and discussing novel and fundamental advances in numerical mathematics and challenging scientific and industrial applications on the highest level of international expertise. The conference includes 11 Plenary talks, 41 Minisymposia, some of them with several sessions, Contributed talks and Poster presentations, from 31 different countries.

The conference involves leading experts and young scientists, with special emphasis on contributions from Europe. We hope that you will find this meeting inspiring, both for scientific interactions and informal discussions.

The Local Organizing Committee

ORGANIZERS AND COMMITTEES

Local Organizing Committee

Adélia Sequeira (Chair) – IST and CEMAT, Universidade de Lisboa
Ana Silvestre (Co-Chair) – IST and CEMAT, Universidade de Lisboa
Jorge Tiago – IST and CEMAT, Universidade de Lisboa
Telma Guerra – IPSetúbal and CEMAT, Universidade de Lisboa
João Janela – CEMAPRE, ISEG, Universidade de Lisboa
Marília Pires – CIMA, Universidade de Évora
Svilen S. Valtchev – IPLeiria and CEMAT, Universidade de Lisboa

Programme Committee

Franco Brezzi - Università degli Studi di Pavia, Italy
Miloslav Feistauer - Universitas Carolina Pragensis, Czech Republic
Gunilla Kreiss - Uppsala Universitet, Sweden
Yuri Kuznetsov - University of Houston, USA
Pekka Neittaanmäki - University of Jyvaskula, Finland
Jacques Periaux - Dassault Aviation St. Cloud, France
Alfio Quarteroni - Politecnico di Milano, Italy
Rolf Rannacher - Ruprecht-Karls-Universität Heidelberg, Germany
Endre Süli - University of Oxford, UK
Barbara Wohlmuth (Chair) - Technische Universität München, Germany

Scientific Committee

Peter Benner – Max Planck Institute, Magdeburg, Germany
Jan Thije Boonkkamp – University of Technology, Eindhoven, The Netherlands
Malte Braack – Kiel University, Germany
Annalisa Buffa – CNR Imati, Pavia, Italy
Alexandre Ern – ENPC, Paris, France
Luca Formaggia – Politecnico di Milano, Italy
Martin Gander – Université de Genève, Switzerland
Francisco J. Gaspar – University of Zaragoza, Spain

Plenary Lectures

From condensed matter theory to sub-wavelength physics

Habib Ammari

Department of Mathematics, ETH Zürich, Switzerland
habib.ammari@math.ethz.ch

Abstract

The ability to manipulate and control waves at scales much smaller than their wavelengths is revolutionizing nanotechnology. The speaker will present a mathematical and numerical framework for this emerging field of physics and elucidate its duality with condensed matter theory.

Keywords: Subwavelength physics, Subwavelength resonances, Topological wave phenomena, Wave localization

References

[1] H. Ammari, B. Davies, E. Orvehed Hiltunen. *Spectral convergence in large finite resonator arrays: the essential spectrum and band structure.* arXiv: 2305.16788.

[2] H. Ammari, B. Davies, E. Orvehed Hiltunen. *Anderson localization in the subwavelength regime.* arXiv: 2205.13337.

[3] H. Ammari, B. Davies, E. Orvehed Hiltunen. *Functional analytic methods for discrete approximations of subwavelength resonator systems.* arXiv: 2106.12301.

Mathematical and numerical modeling of neurodegenerative diseases

Paola F. Antonietti

MOX - Laboratory for Modeling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano, Italy
paola.antonietti@polimi.it@polimi.it

Abstract

Neurodegenerative diseases (NDs) are complex disorders that primarily affect the neurons in the brain and nervous system, leading to progressive deterioration and loss of function over time. A common pathological hallmark among different NDs is the accumulation of disease–specific misfolded aggregated proteins in different areas of the brain (e.g., Aβ and tau in Alzheimer's disease, α–synuclein in Parkinson's disease). In this talk, we discuss the numerical modeling of the misfolding process of α–synuclein in Parkinson's disease. To characterize the progression of misfolded proteins across the brain we consider a suitable mathematical model (based on Fisher–Kolmogorov equations). For its numerical discretization, we propose and analyze a high-order discontinuous Galerkin method on polyhedral grids (PolyDG) for space discretization coupled with a Crank-Nicolson scheme to advance in time. Numerical simulations in patient-specific brain geometries reconstructed from magnetic resonance images are presented. In the second part of the talk, we introduce and analyze a PolyDG method for the semidiscrete numerical approximation of the equations of Multiple-Network Poroelastic Theory (MPET) in the dynamic formulation. The MPET model can comprehensively describe functional changes in the brain considering multiple scales of fluids and can be regarded as a preliminary attempt to model the perfusion in the brain. In this context, mechanisms for waste removal (clearance) from the brain play an important role in the onset and progress of NDs. We present and analyze the numerical approach and we present simulations in three dimensional patient-specific geometries.

Keywords: neurodegenerative diseases, discontinuous Galerkin methods, polygonal and polyhedral grids

Multithreaded Multilevel Spectral Domain Decomposition

Peter Bastian

Interdisciplinary Center for Scientific Computing, Heidelberg University, Germany
Peter.Bastian@iwr.uni-heidelberg.de

Abstract

Spectral domain decomposition methods are domain decomposition preconditioners where the coarse space is constructed from the solutions of certain generalized eigenproblems in the subdomains. An example is the GenEO method [4] which is a two-level method using overlapping subdomains. Its convergence can be shown to be independent of the mesh size, number of subdomains and coefficients of the underlying partial differential equation in the symmetric and coercive case (with extensions possible). Excellent results have been achieved for highly heterogeneous linear elasticity problems in [3].

The setup cost for the GenEO preconditioner is quite substantial although it can be very well parallelized. Since the cost for the local eigensolves scales superlinearly with subdomain size it is advantageous to choose smaller subdomains. However, this and the fact that todays supercomputers have a large number of cores, drives up the number of subdomains and thus the size of the necessary coarse problem. As a remedy, more than two levels can be employed [1, 2]. The resulting multilevel spectral domain decomposition method can be viewed as an algebraic multilevel method with aggressive coarsening based on spectral coarse spaces.

In this talk I will concentrate on the fast construction of the preconditioner exploiting SIMD vectorization in the eigensolver based on approximate orthogonal iteration as well as the shared memory parallelization of the setup phase which allows to decouple the number of subdomains and number of cores. Results will be presented for AMD and ARM-based (Apple) multicore CPUs.

Keywords: Finite elements, Domain decomposition, High-performance computing

References

[1] H. Al Daas, L. Grigori, P. Jolivet, P.-H. Tournier (2021). *A multilevel Schwarz preconditioner based on a hierarchy of robust coarse spaces*. SIAM Journal on Scientific Computing, 43, A1907 – A1928. https://doi.org/10.1137/19M1266964.

[2] P. Bastian, R. S. Scheichl, L. Seelinger, A. Strehlow (2022). *Multilevel Spectral Domain Decomposition*. SIAM Journal on Scientific Computing early access: https://doi.org/10.1137/21M1427231.

[3] R. Butler, T. Dodwell, A. Reinarz, A. Sandhu, R. Scheichl, L. Seelinger(2020). *High-performance dune modules for solving large-scale, strongly anisotropic elliptic problems with applications to aerospace composites*. Computer Physics Communications, 249, 106997. https://doi.org/10.1016/j.cpc.2019.106997.

[4] N. Spillane, V. Dolean, P. Hauret, F. Nataf, C. Pechstein, R. Scheichl (2014). *Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps*. Numerische Mathematik, 126, 741 – 770. https://doi.org/10.1007/s00211-013-0576-y.

Primal Dual methods for Wasserstein gradient flows

J.A. Carrillo

Mathematical Institute, University of Oxford, United Kingdom
carrillo@maths.ox.ac.uk

Abstract

Combining the classical theory of optimal transport with modern operator splitting techniques, I will present a new numerical method for nonlinear, nonlocal partial differential equations, arising in models of porous media,materials science, and biological swarming. Using the JKO scheme, along with the Benamou-Brenier dynamical characterization of the Wasserstein distance, we reduce computing the solution of these evolutionary PDEs to solving a sequence of fully discrete minimization problems, with strictly convex objective function and linear constraint. We compute the minimizer of these fully discrete problems by applying a recent, provably convergent primal dual splitting scheme for three operators. By leveraging the PDE's underlying variational structure, ourmethod overcomes traditional stability issues arising from the strong nonlinearity and degeneracy, and it is also naturally positivity preserving and entropy decreasing. Furthermore, by transforming the traditional linear equality constraint, as has appeared in previous work, into a linear inequality constraint, our method converges in fewer iterations without sacrificing any accuracy. Remarkably, our method is also massively parallelizable and thus very efficient in resolving high dimensional problems. We prove that minimizers of the fully discrete problem converge to minimizers of the continuum JKO problem as the discretization is refined, and in the process, we recover convergence results for existing numerical methods for computing Wasserstein geodesics. Finally, we conclude with simulations of nonlinear PDEs and Wasserstein geodesics in one and two dimensions that illustrate the key properties of our numerical method.

Keywords: Finite Volumes, Primal Dual, Optimal Transport

References

[1] J. A. Carrillo, K. Craig, L. Wang, C. Wei (2022). *Primal dual methods for Wasserstein gradient flows*. Found. Comput. Math. 22, 389 – 443.

What is a limit of numerical methods for compressible flows?

Mária Lukácová-Medvidová*

Institute of Mathematics, Johannes Gutenberg-University Mainz, Germany
lukacova@uni-mainz.de

Abstract

In this talk we introduce generalized solutions of compressible flows, the so-called dissipative solutions. We will concentrate on the inviscid flows, the Euler equations, and mention also the relevant results obtained for the viscous compressible flows, governed by the Navier-Stokes equations.

The dissipative solutions are obtained as a limit of suitable structure-preserving, consistent and stable finite volume schemes [1, 2, 3, 4]. In the case that the strong solution to the above equations exists, the dissipative weak solutions coincide with the strong solution on its life span [1].

Otherwise, we apply a newly developed concept of $\mathcal{K}$-convergence and prove the strong convergence of the empirical means of numerical solutions to a dissipative weak solution [5, 6]. The latter is the expected value of the dissipative measure-valued solutions and satisfies a weak formulation of the Euler equations modulo the Reynolds turbulent stress. If time permits, we will also derive error estimates for the corresponding finite volume method. The error analysis is realized by means of the relative energy which is a problem-suited "metric" [4]. Theoretical results will be illustrated by a series of numerical simulations.

Keywords: compressible fluid flows, Navier-Stokes equations, Euler equations, dissipative solutions, turbulence, Young measures, relative energy

References

[1] E. Feireisl, M. Lukáčová-Medvid'ová, H. Mizerová, B. She (2021). *Numerical analysis of compressible fluid flows*. Springer.

[2] E. Feireisl, M. Lukáčová-Medvid'ová, H. Mizerová (2020). *Convergence of finite volume schemes for the Euler equations via dissipative-measure valued solutions*. Found. Comput. Math., 20, 923 – 966.

[3] E. Feireisl, M. Lukáčová-Medvid'ová, H. Mizerová, B. She (2019). *Convergence of a finite volume scheme for the compressible Navier-Stokes system*. ESAIM: Math. Model. Num. 53, 1957 – 1979.

[4] M. Lukáčová-Medvid'ová, B. She, Y. Yuan (2022). *Error estimate of the Godunov method for multidimensional compressible Euler equations*, J. Sci. Comput. 91, 71.

[5] E. Feireisl, M. Lukáčová-Medvid'ová, H. Mizerová (2020). *$\mathcal{K}$-convergence as a new tool in numerical analysis*, IMA J. Numer. Anal. 40, 2227–2255.

[6] E. Feireisl, M. Lukáčová-Medvid'ová, B. She, Y. Wang (2021). *Computing oscillatory solutions of the Euler system via $\mathcal{K}$-convergence*, Math. Math. Models Methods Appl. Sci. 31, 537 – 576.

*The present research has been partially supported by TRR 146 Multiscale simulation methods for soft matter systems funded by the German Science Foundation and by the Gutenberg Research College.

Discretization of anisotropic PDEs using Voronoi's reduction of positive quadratic forms

Jean-Marie Mirebeau

Centre Borelli, ENS Paris-Saclay, University Paris-Saclay, France
jean-marie.mirebeau@ens-paris-saclay.fr

Abstract

Anisotropy, which refers to the existence of preferred direction in a domain, is a source of difficulty in the discretization of partial differential equations (PDEs). When the anisotropy is defined through symmetric positive definite matrices, such as a Riemannian metric, one can often leverage a matrix decomposition technique known as Voronoi's first reduction to design efficient finite difference schemes for a variety of PDEs. I will illustrate the strengths of this approach, but also some shortcomings of this decomposition, such as the low regularity of the coefficients, and the lack of uniqueness in dimension $d \geq 4$, and show how they can be addressed. Finally, we present an application to the numerical solution of a Finslerian eikonal PDE arising in seismic tomography.

Keywords: Adaptive finite differences, Anisotropic PDE, Hamilton-Jacobi equation, Voronoi's first reduction.

References

[1] F. Bonnans, G. Bonnet, J.-M. Mirebeau. *Monotone discretization of anisotropic differential operators using Voronoi's first reduction*. Submitted, 2023.

Numerical solution of nonlinear eigenvector problems

Daniel Peterseim*

Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences,
University of Augsburg
daniel.peterseim@uni-a.de

Abstract

Stationary states of Bose-Einstein condensates can be modelled by an eigenvalue problem for a nonlinear partial differential operator - the Gross-Pitaevskii equation or nonlinear Schrödinger equation. It is a representative of the larger class of nonlinear eigenvector problems arising in computational physics and chemistry, such as the Kohn-Sham model. The talk discusses their numerical solution by integrating techniques of Riemannian optimisation, computational PDEs and multiscale modelling and simulation. For the particular case of the Gross-Pitaevskii equation, numerical analysis and a series of numerical experiments demonstrate the ability of the resulting simulation methods to capture relevant physical effects of Bose-Einstein condensates, such as eigenstate localisation under disorder potentials and the formation of vortex lattices in rapidly rotating potential traps.

Keywords: Nonlinear Schrödinger equation, Riemannian optimisation, computational multiscale methods

References

[1] R. Altmann, D. Peterseim, T. Stykel (2022). *Energy-adaptive Riemannian optimization on the Stiefel manifold.* Math. Model. Numer. Anal. **56**, 1629 – 1653.

[2] R. Altmann, P. Henning, D. Peterseim (2022). *Localization and delocalization of ground states of Bose-Einstein condensates under disorder.* SIAM J. Appl. Math. **82(1)**, 330 – 358.

[3] R. Altmann, P. Henning, D. Peterseim (2021). *Numerical homogenization beyond scale separation.* Acta Numer. **30(1)**, 1 – 86.

[4] R. Altmann, D. Peterseim (2021). *The J-method for the Gross-Pitaevskii eigenvalue problem.* Numer. Math. **148(3)**, 575 – 610.

[5] P. Henning, D. Peterseim (2020). *Sobolev gradient flow for the Gross-Pitaevskii eigenvalue problem: global convergence and computational efficiency.* SIAM J. Numer. Anal. **58(3)**, 1744 – 1772.

[6] R. Altmann, P. Henning, D. Peterseim (2020). *Quantitative Anderson localization of Schrödinger eigenstates under disorder potentials.* Math. Models Methods Appl. Sci. **30(5)**, 917 – 955.

[7] R. Altmann, D. Peterseim (2019). *Localized computation of eigenstates of random Schrödinger operators.* SIAM J. Sci. Comput. **41**, B1211 – B1227.

[8] P. Henning, A. Målqvist, D. Peterseim (2014). *Two-level discretization techniques for ground state computations of Bose-Einstein condensates.* SIAM J. Numer. Anal. **52(4)**, 1525 – 1550.

*D. Peterseim's work is part of a project funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (*Computational Random Multiscale Problems*, Grant agreement No. 865751).

From differential equations to deep learning for image analysis

Carola–Bibiane Schönlieb

University of Cambridge, UK
cbs31@cam.ac.uk

Abstract

Images are a rich source of beautiful mathematical formalism and analysis. Associated mathematical problems arise in functional and non-smooth analysis, the theory and numerical analysis of partial differential equations, harmonic, stochastic and statistical analysis, and optimisation. Starting with a discussion on the intrinsic structure of images and their mathematical representation, in this talk we will learn about some of these mathematical problems, about variational models for image analysis and their connection to partial differential equations and deep learning. The talk is furnished with applications to art restoration, forest conservation and cancer research.

Challenges in numerical modeling of extreme plasma physics in the laboratory and in astrophysics

Luís O. Silva*

Department of Physics and GoLP/Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Portugal
luis.silva@tecnico.ulisboa.pt

Abstract

Ultra-intense lasers [1] and particle beams [2] hold the promise to reach novel physics regimes where the interplay between plasma dynamics and QED processes determines the system dynamics. Equivalent processes are also presented in some of the most extreme astrophysical objects such as neutron stars and black holes [3]. I will review some of these processes, and the associated key microphysics and I will provide a few examples, in the laboratory and in astrophysics, resorting to a combination of theory and numerical simulations where this interplay and these novel regimes are important, focusing on the numerical techniques underpinning the study of these regimes and the associated developments in state-of-the-art particle-in-cell numerical codes such as OSIRIS [4, 5].

Keywords: Plasma physics, particle-mesh, physics extensions, plasma physics, quantum electrodynamics

References

[1] A. Di Piazza, L. Willingale, J. D. Zuegel (2022). *Multi-Petawatt Physics Prioritization (MP3) Workshop Report*, arXiv:2211.13187.

[2] V. Yakimenko, S. Meuren, F. Del Gaudio, C. Baumann, A. Fedotov, F. Fiuza, T. Grismayer, M. J. Hogan, A. Pukhov, L. O. Silva, G. White (2019). *Prospect of Studying Nonperturbative QED with Beam-Beam Collisions*, Physical Review Letters 122, 190404.

[3] D. Uzdensky, M. Begelman, A. Beloborodov, R. Blandford, S. Boldyrev, B. Cerutti, F. Fiuza, D. Giannios, T. Grismayer, M. Kunz, N. Loureiro, M. Lyutikov, M. Medvedev, M. Petropoulou, A. Philippov, E. Quataert, A. Schekochihin, K. Schoeffler, L. Silva, L. Sironi, A. Spitkovsky, G. Werner, V. Zhdankin, J. Zrake, E. Zweibel (2019). *Extreme Plasma Astrophysics*, arXiV:1903.05328.

[4] R. A. Fonseca, L. O. Silva, F. S. Tsung, VK Decyk, W. Lu, C. Ren, W. B. Mori, S. Deng, S. Lee, TC KATSOULEAS, J. C. Adam (2002). *OSIRIS: A three-dimensional, fully relativistic particle in cell code for modeling plasma based accelerators*. In *Lecture Notes in Computer Science 2331*, eds.: P.M.A. Sloot et al. ICCS 2002, 342 – 351.

[5] R. A. Fonseca, S. f. Martins, L. O. Silva, J. W. Tonge, F. S. Tsung, W. B. Mori (2008). *One-to-one direct modeling of experiments and astrophysical scenarios: pushing the envelope on kinetic plasma simulations*. Plasma Physics and Controlled Fusion 50, 124034.

*The work of LOS has been partially supported by the European Research Council AdG grants 695088 and 267841, and the Portuguese Science Foundation grant 2022.02230.PTDC

The Role of Applied Mathematics in the Design of Coronary Stents

Alessandro Veneziani*[1,2]

[1]Department of Mathematics, Emory University, Atlanta, GA, USA
[2]Department of Computer Science, Emory University, Atlanta, GA, USA
avenez2@emory.edu

Abstract

Since their introduction in the Eighties, coronary stents have undergone significant design improvements, making them a critical tool for treating severe obstructions. From original Bare-Metal Stents (BMS) to Drug Eluting Stents (DES) to the most recent experience of Bioresorbable Stents, the design of these scaffolds was minimally supported by mathematical tools. The patient-specific quantitative analysis of stented coronaries is a difficult task for the variety of complex morphologies left by the stent deployment. Therefore, this type of analysis was limited to a minimal number of patients, not compatible with clinical trials. On the other hand, the development and the failure of Brioresorbable Stents clearly pointed out the importance of rigorous quantitative tools in the design of next-generation scaffolds. In this talk, we will present recent results in investigating coronary stents based on Applied Mathematics (as opposed to traditional animal models). We will consider in detail (i) the modeling of the elution in a multidomain problem solved by iterative substructuring methods involving simultaneously the lumen, the wall, and the struts of the stents; (2) the impact of the struts on the wall shear stress of a significant number of patients; (3) the consequent role of shape optimization and model order reduction in the design of scaffolds. This journey through a sophisticated combination of data and models will pinpoint the critical role of applied mathematics and scientific computing not only for a basic understanding of the biomechanics of stents but also for the clinical routine and the design of more performing prostheses.

See [1, 2, 3]

Keywords: Coronary Stents, Cardiovascular Mathematics, Model Order Reduction, Shape Optimization, Wall Shear Stress

References

[1] C. Lin, A. Veneziani, L. Ruthotto (2018). *Numerical methods for polyline-to-point-cloud registration with applications to patient-specific stent reconstruction.* International Journal For Numerical Methods In Biomedical Engineering. **34**, e2934.

[2] A. Lefieux, S. Bridio, D. Molony, M. Piccinelli, C. Chiastra, H. Samady, F. Migliavacca, A. Veneziani (2022). *Semi-Automatic Reconstruction of Patient-Specific Stented Coronaries based on Data Assimilation and Computer Aided Design.* Cardiovascular Engineering And Technology, 1 – 18.

[3] A. Irving Martinez. *Multi-Domain Modeling and Simulation of Blood Solutes and Elution in Stented Arteries via Iterative Substructuring Methods.* Submitted, 2023.

*AV thanks NIH R01EB031101 (PI L. Brooks), NSF DMS2012286 (PI A. Veneziani) and DMS2038118 (PI: J. Nagy).

Conservative Cut Finite Element Methods

Sara Zahedi*

Department of Mathematics, KTH Royal Institute of Technology, Sweden
sara.zahedi@math.kth.se

Abstract

I will discuss our recent development of unfitted finite element methods that are able to conserve quantities and obtain pointwise divergence-free approximations of solenoidal velocity fields. I will give an introduction to Cut Finite Element Methods (CutFEM) for interface problems and propose two corrections to the standard stabilization strategy in connection with CutFEM.

The first correction makes use of new stabilization terms in order to preserve the divergence-free property of $\mathbf{H}^{\text{div}}$-conforming elements in case of unfitted meshes. I will talk about a cut finite element discretization of a Darcy interface problem based on the mixed finite element pairs $\mathbf{RT}_k \times Q_k$ [1]. Here, Q_k is the space of discontinuous polynomial functions of degree k and $\mathbf{RT}_k$ is the Raviart-Thomas space. The proposed discretization has the following three properties: 1) optimal rates of convergence of the approximate velocity and pressure; 2) well-posed linear systems where the condition number of the system matrix scales as it does for fitted finite element discretizations; 3) optimal rates of convergence of the approximate divergence with pointwise divergence-free approximations of solenoidal velocity fields. All three properties hold independently of how the interface is positioned relative to the computational mesh.

The second correction makes use of a macro-element partition of the mesh so that cut finite element methods based on the Discontinuous Galerkin (DG) framework can inherit properties from the DG framework. We give criteria to categorize elements in an unfitted mesh as small or large. Macro-elements can then be constructed so that each small element is connected to a large element via a chain of face neighbours. The macro-elements behave as standard finite elements and inherit local conservation properties from the DG framework [2].

Keywords: cut elements, conservation, interface problems, unfitted finite elements

References

[1] T. Frachon, P. Hansbo, E. Nilsson, S. Zahedi (2023). *A divergence preserving cut finite element method for Darcy flow.* arXiv:2205.12023.

[2] M. G. Larson, S. Zahedi (2023). *Conservative cut finite element methods using macro-elements.* To appear in Comput. Methods Appl. Mech. Engrg.

*Thomas Frachon, Peter Hansbo, Mats Larson, Erik Nilsson

Minisymposia

MS01: Multilevel and Multiscale Methods for PDEs

MS02: Mixed Precision Computations in Theory and Practice

MS03: Numerical methods for fractional-derivative problems

MS04: Approximated boundary methods: modelling, mathematical analysis and simulations

MS05: Stable multiderivative time-integrators for Differential Equations

MS06: Theoretical and computational aspects of the discontinuous Galerkin method

MS07: Space-time methods for evolutionary PDEs

MS08: Problems in biomedical fluid mechanics

MS09: Non-homogeneous and multicomponent fluids for environmental applications

MS10: Entropy/energy-stable methods for time evolution problems

MS11: Reducing the irreducible: model reduction for transport-dominated problems

MS12: Structure-Preserving and Efficient Neural Networks for Scientific Machine Learning

MS13: Nonlinear problems in fluid mechanics and related problems

MS14: Goal-oriented Error Estimation and Adaptivity

MS15: Mathematical and computational models of cells, cell-populations, and applications thereof

MS16: Theoretical and numerical developments for high-dimensional parametric PDEs

MS17: Analysis and Numerics for Systems of Nonlinear PDEs in Mathematical Biology

MS18: Efficient numerical methods for direct or inverse wave propagation problems

MS19: Addressing Industrial Challenges in The Numerical Modeling of Flow and Geomechanics in Porous Media

MS20: Modern simulation & data science techniques for computational fluid dynamics problems in the exascale range

MS21: Surface geometry approximation and vector-valued PDEs

MS22: Model reduction and efficient linear algebra techniques for direct and inverse problems

MS23: Multiscale methods for wave propagation problems

MS24: Structure-preserving unfitted finite element discretizations

MS25: Transport at multiple scales in medical processes: from modelling to simulation

MS26: Multiscale and reduced-order modeling for poroelasticity

MS27: Novel numerical methods for the solution of nonlinear hyperbolic PDE's

MS28: Reduced-order modeling and learning of parameterized dynamical systems: state-of-the-art vs. avant-garde methods

MS29: Efficient numerical methods in computational biomechanics

MS30: Robust Numerical Methods for Nonlinear and Coupled Diffusion Problems in Biology

MS31: Advances in polytopal methods for multiphysics problems

MS32: Numerical methods for perturbed saddle-point formulations arising in coupled problems and applications to poromechanics

MS34: Efficient Solvers for Coupled Problems in Porous Media

MS35: Solving Multiphysics/Multiscale Problems: A Challenge between (Reduced) Model-Driven and Data-Driven approaches

MS36: Meshfree methods for direct and inverse problems in partial differential equations. In memoriam of Prof. Carlos J.S. Alves

MS37: Diseases, Diagnosis, Treatment: Mathematical Modeling and Numerical Analysis

MS38: Optimal control and parameter estimation problems with applications in biomedicine

MS39: Numerical methods for nonlinear and coupled processes (flow, reactive transport and deformation) in porous media

MS40: Multi-scale mathematical modeling of human diseases

MS41: Finite Element Methods for Constrained Problems

MS42: Nonsmooth and nonconvex optimization

MS01 - Multilevel and Multiscale Methods for PDEs

A mixed multiscale spectral generalized finite element method

Christian Alber[1], Chupeng Ma[2], and Robert Scheichl[1]

[1]Institute for Applied Mathematics and Interdisciplinary Center for Scientific Computing, Heidelberg University, Im Neuenheimer Feld 205, Heidelberg 69120, Germany
[2]Institute of Scientific Research, Great Bay University, Songshan Lake International Innovation Entrepreneurship A5, Dongguan 523000, China
{c.alber, r.scheichl}@uni-heidelberg.de; chupeng.ma@gbu.edu.cn

Abstract

In this talk, we present a mixed finite element method for solving second order elliptic multiscale problems based on the generalized finite element method (GFEM). This work is motivated by porous media flow applications with strongly heterogeneous rock permeabilities and aims to exploit the superior local mass conservation properties of mixed finite elements. Optimal local approximation spaces for the velocity component are built by solving local eigenvalue problems, which are posed on generalized harmonic spaces. Solving small local problems, the local spaces are used to construct a mixed finite element multiscale space, which is used to solve the global saddle point problem. The method is studied at continuous and discrete levels. Raviart-Thomas spaces are underlying the discrete method. At both continuous and discrete levels, the local approximation errors are proven to decay nearly exponentially and the multiscale space is shown to be inf-sup stable. Numerical results are presented to support the theory and validate the proposed method.

Keywords: mixed finite element method, generalized finite element method, multiscale method, local spectral basis, Raviart-Thomas spaces

Multi-scale Finite Element Method for incompressible flow in perforated domain

Loïc Balazi[1, 2], Grégoire Allaire[2], and Pascal Omnes[1]

[1]CEA/DES/ISAS/DM2S/SGLS/LCAN, CEA Saclay
[2]CMAP, Ecole Polytechnique
loic.balaziatchynillama@cea.fr

Abstract

Simulating the flow in a multi-scale media with many obstacles, such as nuclear reactor cores, is very challenging. Indeed, to capture the finest scales of the flow, one needs to use a very fine mesh, which often leads to intractable simulations due to the lack of computational resources. To overcome this limitation, various multi-scale methods have been developed in the literature to attempt to resolve scales below the coarse mesh scale. In this contribution, we focus on the Multi-scale Finite Element Method (MsFEM).

The MsFEM uses a coarse mesh on which one defines basis functions which are no longer the classical polynomial basis functions of finite elements, but which solve fluid mechanics equations on the elements of the coarse mesh. These functions are themselves numerically approximated on a fine mesh taking into account all the geometric details, which gives the multi-scale aspect of this method.

Based on the work of [1, 2], we develop an enriched non-conforming MsFEM to solve viscous incompressible flow in heterogeneous media. Our MsFEM is in the vein of the classical non-conforming Crouzeix-Raviart finite element method with high-order weighting functions. We perform a rigorous theoretical study of our MsFEM in two and three dimensions at both continuous and discrete levels. At the numerical level, we implement the MsFEM to solve the Stokes and the Oseen problems, in two and three dimensions, in a massively parallel framework in FreeFEM [3]. In order to solve the local problems in three dimensions, a new family of non-conforming finite elements had to be developed.

The perspective of this work is to be able to solve the Navier-Stokes equations in a perforated domain at high Reynolds number using MsFEM basis functions. Furthermore, to complete the study of our MsFEM, we are investigating on an a posteriori error estimate for MsFEM.

Keywords: Multi-scale Finite Element Method, Incompressible Flow, Stokes equations, Oseen equations, Parallel computing.

References

[1] G. Jankowiak, A. Lozinski (2018). *Non-Conforming Multiscale Finite Element Method for Stokes Flows in Heterogeneous Media. Part II : error estimates for periodic microstructure.* arXiv:1802.04389[math].

[2] Q. Feng, G. Allaire, P. Omnes (2022). *Enriched Nonconforming Multiscale Finite Element Method for Stokes Flows in Heterogeneous Media Based on High-order Weighting Functions.* Multiscale Model. Simul., 20(1):462–492.

[3] F. Hecht (2012). *New development in freefem++.* J. Numer. Math., 20(3-4), 251–265.

Homogenization of Foil Windings with Globally Supported Polynomials and Including Capacitive Effects

Jonas Bundschuh[1,2], Yvonne Späck-Leigsnering[2], and Herbert De Gersem[2]

[1]Institut für Teilchenbeschleunigung und Elektromagnetische Felder (TEMF), TU Darmstadt, 64293 Darmstadt, Germany
[2]Graduate School of Excellence Computational Engineering, 64293 Darmstadt, Germany
jonas.bundschuh@tu-darmstadt.de

Abstract

Foil windings are constructed by winding a thin, insulated metal foil. In a standard finite element procedure, the mesh would need to resolve each foil and each insulation layer separately. As a foil winding consists of hundreds of turns, this leads to extremely large meshes and, thus, to prohibitively long simulation times [1]. A high resolution in the foil winding domain can be avoided by homogenization approaches. The foil windings and the insulating layers are replaced by a homogenized material [2].

The derivation is based on the magnetoquasistatic approximation of Maxwell's equations, using the $\vec{A}$-ϕ-formulation, with the vector potential $\vec{A}$ and the scalar potential ϕ. The negative gradient of the scalar potential is approximated by $\Phi(u)\vec{\zeta}$, with the voltage function Φ that depends on u, the coordinate perpendicular to the foils, and the winding function for solid conductors $\vec{\zeta}$ from [3].

With the assumption of thin foils with respect to the skin depth, the current I through a foil can be approximated by $I \approx b \int_\Gamma \left(\sigma\left(\Phi(\alpha)\vec{\zeta} - \partial_t \vec{A}\right)\right) \cdot \vec{e}_w \mathrm{d}s$. Herein, b is the thickness of one foil, σ is the conductivity, Γ is a path between the foil tips and $\vec{e}_w$ is a unit vector pointing in the direction of the foils. The vector potential and the voltage function are discretized following the Galerkin procedure with the standard finite element edge functions and polynomials supported in the whole foil winding domain, respectively.

The formulation and the modeling of the homogenization take resistive and inductive effects into account. Capacitive effects are not considered in this model. However, when operating foil windings at elevated frequencies, they cannot be neglected anymore. Therefore, the talk will discuss the capacitive effects in foil windings as well.

The work is supported by the German Science Foundation (DFG project 436819664), the Graduate School CE within the Centre for Computational Engineering at the Technische Universität Darmstadt, and the Athene Young Investigator Fellowship of the Technische Universität Darmstadt.

Keywords: Foil windings, homogenization, eddy currents

References

[1] J. Gyselinck *et al.*, "Frequency-domain homogenization of bundles of wires in 2-D magnetodynamic FE calculations," *IEEE Trans. Magn.*, vol. 41, no. 5, pp. 1416–1419, May 2005.

[2] C. A. Valdivieso *et al.*, "Time-domain homogenization of foil windings in 2-D axisymmetric finite-element models," *IEEE Trans. Power Deliv.*, vol. 36, no. 3, pp. 1264–1269, Jun. 2021.

[3] S. Schöps *et al.*, "Winding functions in transient magnetoquasistatic field-circuit coupled simulations," *COMPEL*, vol. 32, no. 6, pp. 2063–2083, Nov. 2013.

A Super-Localized Generalized Finite Element Method

Philip Freese[1], Moritz Hauck[2], Tim Keil[3], and Daniel Peterseim[2]

[1]Institute of Mathematics, Hamburg University of Technology
[2]Institute of Mathematics, University of Augsburg
[3]Institute for Analysis and Numerics, University of Münster
philip.freese@tuhh.de; {moritz.hauck, daniel.peterseim}@uni-a.de; tim.keil@wwu.de

Abstract

In this talk, we present a novel multi-scale method for the solution of elliptic partial differential equations with arbitrarily rough coefficients. The method constructs operator-adapted solution spaces with uniform algebraic approximation rates. Localized basis functions having the same super-exponential localization properties as the recently proposed Super-Localized Orthogonal Decomposition [2] allow for efficient implementation. Stability of the basis is enforced by a partition of unity approach. We present a natural extension to higher order, resulting in higher approximation rates and enhanced localization properties. A rigorous a priori and a posteriori error analysis is performed, and we validate our theoretical findings in a series of numerical experiments. In particular, we demonstrate the method's applicability for challenging high-contrast channeled coefficients. For details, see [1].

Keywords: multiscale method, generalized finite element method, numerical homogenization, high-order method

References

[1] P. Freese, M. Hauck, T. Keil, D. Peterseim (2022). *A Super-Localized Generalized Finite Element Method*. arXiv:2211.09461.

[2] M. Hauck, D. Peterseim (2023). *Super-localization of elliptic multiscale problems*. Math. Comp., 92, 981-1003.

Multiscale Finite Element Methods for advection-diffusion problems

Frédéric LEGOLL[1]

[1]Ecole des Ponts and Inria
frederic.legoll@enpc.fr

Abstract

The Multiscale Finite Element Method (MsFEM) is a finite element (FE) approach that allows to solve partial differential equations (PDEs) with highly oscillatory coefficients on a coarse mesh, i.e. a mesh with elements of size much larger than the characteristic scale of the heterogeneities. To do so, MsFEMs use pre-computed basis functions, adapted to the differential operator, thereby taking into account the small scales of the problem [1].

When the PDE contains dominating advection terms, naive FE approximations lead to spurious oscillations, even in the absence of oscillatory coefficients. Stabilization techniques (such as SUPG) are to be adopted [2].

In this work, we consider multiscale advection-diffusion problems in the convection-dominated regime. We discuss different ways to define the MsFEM basis functions, and how to combine the approach with stabilization-type methods. In particular, we show that methods using suitable bubble functions and Crouzeix-Raviart type boundary conditions for the local problems turn out to be very effective.

Joint work with Rutger Biezemans, Claude Le Bris and Alexei Lozinski.

Keywords: Multiscale elliptic PDEs, advection-dominated problems, finite element methods

References

[1] Y. Efendiev, T. Hou (2009). *Multiscale Finite Element Methods*. Springer-Verlag.

[2] A. Quarteroni (2014). *Numerical Models for Differential Problems*. Springer-Verlag (second edition).

Homogeneous multigrid method for hybridizable discontinuous Galerkin methods

Peipei Lu[1], Andreas Rupp[2], and Guido Kanschat[3]

[1]Department of Mathematics Sciences, Soochow University
[2]School of Engineering Science, Lappeenranta–Lahti University of Technology
[3]Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University

Abstract

In this talk, we introduce a multigrid method that is homogeneous in the sense that it uses the same hybridizable discontinuous Galerkin (HDG) discretization scheme for Poisson's equation on all levels. Uniform convergence of the geometric multigrid V-cycle is proven for HDG methods with a new set of assumptions on the injection operators, and several possible injection operators are proposed to meet these assumptions. The analysis applies to the hybridized local discontinuous Galerkin method, hybridized Raviart-Thomas, and hybridized Brezzi-Douglas-Marini mixed element methods. Numerical experiments are provided to confirm the theoretical results.

Keywords: Multigrid, injection operator, Poisson equation, hybridized finite elements.

References

[1] P. Lu, A. Rupp, G. Kanschat, Homogeneous multigrid for HDG, IMA Journal of Numerical Analysis, 42 (2022), pp. 3135–3153.

[2] P. Lu, A. Rupp, G. Kanschat, Analysis of injection operators in geometric multigrid solvers for HDG methods, SIAM Journal on Numerical Analysis, 60 (2022), pp. 2293–2317,

Iterative solution of spatial network models by subspace decomposition

Axel Målqvist[1], Morgan Görtz[1], and Fredrik Hellman[1]

[1]Department of Mathematical Sciences, Chalmers University of Technology and University of Gothenburg
axel@chalmers.se; morgan.gortz@fcc.chalmers.se; fredrik.hellman@gmail.com

Abstract

We present and analyze a preconditioned conjugate gradient method (PCG) for solving spatial network problems. Primarily, we consider diffusion and structural mechanics simulations for fiber based materials, but the methodology can be applied to a wide range of models, fulfilling a set of abstract assumptions. The proposed method builds on a classical subspace decomposition into a coarse subspace, see [2], realized as the restriction of a finite element space to the nodes of the spatial network, and localized subspaces with support on mesh stars. The main contribution is the convergence analysis of the proposed method. The analysis translates results from finite element theory, including interpolation bounds, to the spatial network setting. A convergence rate of the PCG algorithm, only depending on global bounds of the operator and homogeneity, connectivity and locality constants of the network, is established. The theoretical results are confirmed by several numerical experiments. For more information see the preprint [1].

Keywords: Spatial network models, subspace decomposition, convergence analysis

References

[1] M. Görtz, F. Hellman, A. Målqvist, *Iterative solution of spatial network models by subspace decomposition,* arXiv:2207:07488

[2] R. Kornhuber, H. Yserentant, *Numerical homogenization of elliptic multiscale problems by subspace decomposition,* Multiscale Model. Simul., 14 (2016), 1017–1036.

Super-localized numerical stochastic homogenization

Moritz Hauck*[1], Hannah Mohr*[1], and Daniel Peterseim*[1,2]

[1]Institute of Mathematics, University of Augsburg
[2]Centre for Advanced Analytics and Predictive Sciences, University of Augsburg
{moritz.hauck, hannah.mohr, daniel.peterseim}@uni-a.de

Abstract

Numerical homogenization aims to effectively and accurately approximate the solution space of elliptic partial differential equations with arbitrarily rough coefficients by the choice of problem-adapted approximation spaces. However, in many physical settings, complete explicit knowledge of the underlying coefficient is unlikely. This raises the question of how this uncertainty on the fine scale changes the expected macroscopic response of the solution. In this talk, we derive a method to approximate the expected solution at a coarse scale, by combining the uncertainty quantification approach of [1, 2] with the Super-Localized Orthogonal Decomposition (SLOD) method of [3]. Due to the advantageous localization properties of SLOD, the uncertainty quantification only requires computations on particularly small subdomains.

Keywords: Numerical stochastic homogenization, Super-Localized Orthogonal Decomposition, Heterogeneous media, Multiscale method

References

[1] D. Gallistl, D. Peterseim (2019). *Numerical stochastic homogenization by quasilocal effective diffusion tensors.* Communications in Mathematical Sciences, 17, 637–651.

[2] J. Fischer, D. Gallistl, D. Peterseim (2021). *A priori error analysis of a numerical stochastic homogenization method.* SIAM Journal on Numerical Analysis, 59, 660–674.

[3] M. Hauck, D. Peterseim (2022). *Super-localization of elliptic multiscale problems.* Mathematics of Computation, 92, 981–1003.

*The work of all authors is part of a project that has received funding from the European Research Council ERC under the European Union's Horizon 2020 research and innovation program (Grant agreement No. 865751 - RandomMultiScales).

PDEs with Variable Coefficients on Locally Adaptive Sparse Grids

Riccarda Scherner-Grießhammer[1] and Christoph Pflaum[2]

[1]Department of Computer Science, Friedrich-Alexander-Universität Erlangen-Nürnberg
{riccarda.scherner, christoph.pflaum}@fau.de

Abstract

Elliptic partial differential equations with variable coefficients can be discretized on sparse grids. With prewavelets being L^2-orthogonal, one can apply the Ritz-Galerkin discretization to obtain a linear equation system with $O(N(\log N)^{d-1})$ unknowns [1], whereas the computing effort for classical full grids is $O(N^d)$.

However, for several applications like PDEs with corner singularities or the high-dimensional Schrödinger equation locally adaptive grids are needed to obtain optimal convergence. Therefore, we introduce a new kind of locally adaptive sparse grid and a corresponding algorithm that allows solving the resulting finite element discretization equation with optimal complexity.

Constructing such locally adaptive sparse grids comes with different requirements given by the optimality of the algorithm and basis transformations. One is the unidirectional approach, which can be maintained by using a local tensor-product structure. Another is the correct evaluation of the discretization mentioned above. Hence sparseness becomes a local criterion, which must be fulfilled when constructing such a grid.

Furthermore, these grids and the corresponding algorithm allow both MPI and OpenMP parallelization by making use of the grid structure and by splitting the algorithm by 2^d cases of restrictions and prolongations.

Keywords: Adaptive Sparse Grids, Variable Coefficients, Finite Element Method

References

[1] C. Pflaum, R. Hartmann. (2016) *A Sparse Grid Discretization of the Helmholtz Equation with Variable Coefficients in High Dimensions.* SIAM Journal On Numerical Analysis. **54**, 2707–2727.

Enhancing Wave Propagation Simulations with Deep Learning and the Parareal Algorithm

Richard Tsai[1]

[1]Department of Mathematics and Oden Institute, The University of Texas at Austin
ytsai@math.utexas.edu

Abstract

We present a deep learning approach for simulating wave propagation in media characterized by multi-scale wave speeds, utilizing a second-order linear wave equation model. Our approach employs neural networks to augment the precision of a low fidelity solver that under-resolves a specific category of multiscale wave media and associated wave fields. We generate training data by applying both the computationally efficient coarse solver and a more accurate solver to a range of wave media, characterized by their wave speed profiles, and initial wave fields.

We find that the trained neural networks can approximate the nonlinear dependence of wave propagation on wave speed, provided that causality is adequately represented in the training data. We integrate the neural-network-enhanced coarse solver with the parareal algorithm, showcasing the improved stability and accuracy.

Keywords: Wave Equation, Deep Learning, Parareal Methods

References

[1] Nguyen, H., & Tsai, R. (2020). *A stable parareal-like method for the second order wave equation.* Journal of Computational Physics, 405, 109156.

[2] Nguyen, H., & Tsai, R. (2023). *Numerical wave propagation aided by deep learning.* Journal of Computational Physics, 475, 111828.

The effect of approximate coarsest-level solves on the convergence of multilevel V-cycle methods

Petr Vacek*[1], Erin C. Carson *[1], and Kirk M. Soodhalter[2]

[1]Department of Numerical Mathematics, Faculty of Mathematics and Physics, Charles University
[2]School of Mathematics, Trinity College Dublin
{vacek, carson}@karlin.mff.cuni.cz, ksoodha@maths.tcd.ie;

Abstract

Multigrid methods are frequently used when solving systems of linear equations, applied either as standalone solvers or as preconditioners for iterative methods. Within each cycle, the approximation is computed using smoothing on fine levels and solving on the coarsest level.

With growth of the size of the problems that are being solved, the size of the problems on the coarsest level is also growing and their solution can become a computational bottleneck. In practice the problems on the coarsest level are often solved approximately, for example by Krylov subspace methods or direct methods based on low-rank approximation; see, e.g., [1]. The accuracy of the coarsest-level solver is typically determined experimentally in order to balance the cost of the solves and the total number of multigrid cycles required for convergence.

In this talk, we present an approach to analyzing the effect of approximate coarsest-level solves in the multigrid V-cycle method for symmetric positive definite problems. Based on these results, we discuss how the choice of the tolerance in relative residual stopping criterion for an iterative coarsest-level solver or the choice of the low-rank threshold parameter and finite precision arithmetic for the block low-rank direct coarsest-level solver may affect the convergence of the V-cycle method. We present new coarsest-level stopping criteria tailored to multigrid methods and a strategy for utilizing them in practice. The results are illustrated through numerical experiments.

Keywords: multigrid methods, approximate coarsest-level solver, coarsest-level stopping criteria

References

[1] A. Buttari et al. (2022), *Block Low Rank Single Precision Coarse Grid Solvers for Extreme Scale Multigrid Methods*. Numerical Linear Algebra with Applications, 29, e2407.

*We acknowledge funding from ERC Starting Grant No. 101075632, Charles University PRIMUS project no. PRIMUS/19/SCI/11, and the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

Optimal approximation of break-of-scale embeddings

Markus Weimar[1], Glenn Byrenheid[2], and Janina Hübner[3]

[1]Chair of Mathematics IX (Scientific Computing), University of Würzburg
[2]Institute of Mathematics, University of Jena
[3]Faculty of Mathematics, Ruhr University Bochum
markus.weimar@uni-wuerzburg.de; glenn.byrenheid@uni-jena.de;
janina.huebner@rub.de

Abstract

As a rule of thumb in approximation theory, the asymptotic speed of convergence of numerical methods is governed by the regularity of the objects we like to approximate. Besides classical isotropic Sobolev smoothness, the notion of dominating-mixed regularity of functions turned out to be an important concept in numerical analysis which arises in high-dimemsional real-world applications, e.g., related to the electronic Schrödinger equation. Although approximation rates of embeddings *within* the scales of isotropic or dominating-mixed L_p-Sobolev spaces are well-understood, not that much is known for embeddings *across* those scales (so-called *break-of-scale embeddings*).

In this talk we introduce particular instances of new hybrid smoothness spaces which simultaneously cover both scales as special cases. Moreover, we present (non-)adaptive wavelet-based multiscale algorithms that achieve optimal dimension-independent rates of convergence. Important special cases include the approximation of function having dominating mixed smoothness w.r.t. L_p in the norm of the (isotropic) energy space H^1.

The presented results are based on a recent paper [1] which represents the first part of a project in joint work with Janina Hübner (RUB), Glenn Byrenheid (FSU Jena), and Markus Hansen (PU Marburg).

Keywords: hyperbolic wavelets, tensor-product structures, best m-term approximation, (non-) linear multiscale approximation, function spaces, dominating-mixed smoothness, energy norm, break-of-scale

References

[1] G. Byrenheid, J. Hübner, M. Weimar (2023). *Rate-optimal sparse approximation of compact break-of-scale embeddings.*. Appl. Comput. Harmon. Anal., 65, 40–66. (arXiv:2203.10011).

MS02 - Mixed Precision Computations in Theory and Practice

Iterative refinement of Schur decompositions

Zvonimir Bujanović[1], Daniel Kressner[2], and Christian Schröder[3]

[1]University of Zagreb, Faculty of Science, Department of Mathematics, Croatia
[2]Institute of Mathematics, EPFL, Switzerland
[3]Freelancing numerical analyst, last academic position: Institut für Mathematik, TU Berlin, Germany
zbujanov@math.hr; daniel.kressner@epfl.ch; chris.schroeder@gmx.net

Abstract

The Schur decomposition of a square matrix A is an important intermediate step of state-of-the-art numerical algorithms for addressing eigenvalue problems, matrix functions, and matrix equations. This talk is concerned with the following task: Compute a (more) *accurate* Schur decomposition of A from a given *approximate* Schur decomposition. This task arises, for example, in the context of parameter-dependent eigenvalue problems and mixed precision computations. We have developed a Newton-like algorithm that requires the solution of a triangular matrix equation and an approximate orthogonalization step in every iteration. We prove local quadratic convergence for matrices with mutually distinct eigenvalues and observe fast convergence in practice. In a mixed low-high precision environment, our algorithm essentially reduces to only four high-precision matrix-matrix multiplications per iteration. When refining double to quadruple precision, it often needs only 3–4 iterations, which reduces the time of computing a quadruple precision Schur decomposition by up to a factor of 10–20.

Keywords: Schur decomposition, Eigenvalue computation, Mixed precision algorithm, Iterative refinement

References

[1] Z. Bujanović, D. Kressner, C. Schröder (2023). *Iterative refinement of Schur decompositions.* Numer. Algorithms, 92, 247–267.

[2] G. H. Golub, C. F. Van Loan (2013). *Matrix computations.* Johns Hopkins University Press.

[3] T. Ogita, K. Aishima (2018). *Iterative refinement for symmetric eigenvalue decomposition.* Jpn. J. Ind. Appl. Math., 35, 1007–1035.

Precision auto-tuning of high-performance neural networks

Quentin Ferro[1], Stef Graillat[1], Thibault Hilaire[1], Fabienne Jézéquel[1,2], and Basile Lewandowski[1]

[1]Sorbonne Université, CNRS, LIP6, Paris, F-75005, France
[2]Université Paris-Panthéon-Assas, Paris, F-75005, France
{quentin.ferro, stef.graillat, thibault.hilaire, fabienne.jezequel}@lip6.fr

Abstract

While often used in embedded systems with limited resource, neural networks can be costly in terms of memory and execution time. Reducing their cost has then become an objective. A possible solution consists in reducing the precision of their neurons parameters. In this presentation, we show how to lower the precision of the parameters while keeping an accurate output using an auto-tuning tool, PROMISE. We show that, to some extent, we can lower the precision of several neural network parameters without compromising the accuracy requirement.

Keywords: Precision, Neural networks, Auto-Tuning, Floating-Point, Stochastic arithmetic

References

[1] Q. Ferro, S. Graillat, T. Hilaire, F. Jézéquel, B. Lewandowski (2022). *Neural Network Precision Tuning Using Stochastic Arithmetic*, In *NSV'22, 15th International Workshop on Numerical Software Verification*, Haifa, Israel. ⟨hal-03682645v2⟩

[2] Q. Ferro, S., T. Hilaire, F. Jézéquel, B. Lewandowski (2022). *Neural Network Precision Tuning Using Stochastic Arithmetic*. In *Sparse Days Conference*, Saint-Girons, France. ⟨hal-03780505⟩

Mixed precision randomized preconditioners for regression problems on GPUs

Vasileios Georgiou[1] and Hartwig Anzt[2]

[1]Karlsruhe Institute of Technology
[2]University of Tennessee
vasileios.georgiou@kit.edu; hanzt@icl.utk.edu

Abstract

Randomization has emerged as a popular technique for tackling regression problems [2] over the past decade. At the same time, the introduction of native support for 16-bit precision formats on modern GPUs, has led to increased interest in mixed-precision implementations of various numerical methods [1]. The goal of this talk is to present experimental findings, regarding the performance improvement that is attainable from applying mixed precision techniques to randomized preconditioners. In order to achieve this, we implemented mixed precision randomized preconditioners for the LSQR and FGMRES methods on the GPU. We will present numerical experiments utilizing the half-precision and tensorcore units on the NVIDIA A100 GPU; to further test the effect of mixed precision arithmetic in solving regression problems, we combine the preconditioners with mixed precision versions of the above solvers.

References

[1] J. I. Aliaga, H. Anzt, T. Grützmacher, E. S. Quintana-Ortí, A. E. Tomás (2022). *Compressed basis GMRES on high-performance graphics processing units*. The International Journal of High Performance Computing Applications, 0(0).

[2] H. Avron, P. Maymounkov, S. Toledo (2010). *Blendenpik: Supercharging LAPACK's Least-Squares Solver*. SIAM Journal on Scientific Computing, 32(3) 1217-1236.

Keywords: Randomized preconditioners, Mixed precision, LSQR, FGMRES

Responsibly reckless matrix algorithms for HPC scientific applications

Hatem Ltaief[1], Marc G. Genton[1], Damien Gratadour[2], David E. Keyes[1], and Matteo Ravasi[1]

[1]King Abdullah University of Science and Technology
[2]Observatoire de Paris
hatem.ltaief@kaust.edu.sa; damien.gratadour@obspm.fr

Abstract

High-performance computing (HPC) achieved an astonishing three orders of magnitude performance improvement per decade for three decades, thanks to hardware technology scaling resulting in exponential improvement in the rate of floating point executions, though slowing in the most recent. Captured in the Top500 list, this hardware evolution cascaded through the software stack, triggering changes at all levels, including the redesign of numerical linear algebra libraries. HPC simulations on massively parallel systems are often driven by matrix computations, whose rate of execution depends on their floating point precision. Referred to by Jack Dongarra, the 2021 ACM A.M. Turing Award Laureate, as "responsibly reckless" matrix algorithms, we highlight the implications of mixed-precision (MP) computations for HPC applications. Introduced 75 years ago, long before the advent of HPC architectures, MP numerical methods turn out to be paramount for increasing the throughput of traditional and artificial intelligence (AI) workloads beyond riding the wave of the hardware alone. Reducing precision comes at the price of trading away some accuracy for performance (reckless behavior) but in noncritical segments of the workflow (responsible behavior) so that accuracy requirements of the application can still be satisfied. They offer a valuable performance/accuracy knob and, just as they are in AI, they are now indispensable in the pursuit of knowledge and discovery in simulations. In particular, we illustrate the MP impact on three representative HPC applications related to seismic imaging, climate/environment geospatial predictions, and computational astronomy.

Keywords: Mixed-precision computations, HPC applications,

References

[1] N. Doucet, H. Ltaief, D. Gratadour, D. Keyes (2019). *Mixed-Precision Tomographic Reconstructor Computations on Hardware Accelerators.* In *IEEE/ACM 9th Workshop on Irregular Applications: Architectures and Algorithms (IA3)*, Denver, CO, USA, pp. 31-38, doi: 10.1109/IA349570.2019.00011.

[2] S. Abdulah, Q. Cao, Y. Pei, G. Bosilca, J. Dongarra, M. G. Genton, D. E. Keyes, H. Ltaief, Y. Sun (2022). *Accelerating Geostatistical Modeling and Prediction With Mixed-Precision Computations: A High-Productivity Approach With PaRSEC.* IEEE Transactions on Parallel & Distributed Systems, vol. 33, no. 04, pp. 964-976, doi: 10.1109/TPDS.2021.3084071.

[3] H. Ltaief, M. G. Genton, D. Gratadour, D. E. Keyes, M. Ravasi (2022). *Responsibly Reckless Matrix Algorithms for HPC Scientific Applications.* Computing in Science & Engineering, vol. 24, no. 4, pp. 12-22, 1 July-Aug. 2022, doi: 10.1109/MCSE.2022.3215477.

Mixed precision Rayleigh quotient iteration for total least squares problems

Eda Oktay[1,2] and Erin Carson[1]

[1]Department of Numerical Mathematics, Charles University
[2]Department of Mathematics, Chemnitz University of Technology
{oktay, carson}@karlin.mff.cuni.cz

Abstract

With the recent emergence of mixed precision hardware, there has been a renewed interest in its use for solving numerical linear algebra problems fast and accurately. The solution of total least squares problems, i.e., solving $\min_{E,f} \|[E, f]\|_F$ subject to $(A + E)x = b + f$, arises in numerous application areas. The solution to this problem requires finding the smallest singular value and corresponding right singular vector of $[A, b]$, which is challenging when A is large and sparse. An efficient algorithm for this case due to Björck et al. [1] is based on Rayleigh quotient iteration coupled with the conjugate gradient method preconditioned via Cholesky factors, called RQI-PCGTLS. In this talk, we introduce a mixed precision variant of this algorithm, RQI-PCGTLS-MP, which aims to improve performance without affecting the level of attainable accuracy. In addition to numerical experiments, we discuss how to choose a suitable precision for the construction of a preconditioner, and develop a theoretical performance model.

Keywords: Mixed precision, Rayleigh quotient iteration, Total least squares problems

References

[1] Å. Björck, P. Heggernes, P. Matstoms (2000). *Methods for large scale total least squares problems.* SIAM Journal on Matrix Analysis and Applications 22(2), 413–429.

Algorithms for mixed precision recycling on GPUs

Eric de Sturler*[1] and Tim Warburton†[2]

[1]Department of Mathematics, Virginia Tech
[2]Department of Mathematics, Virginia Tech
{sturler, tcew}@vt.edu

Abstract

For hard problems, Krylov subspace recycling has proven highly effective, both improving the rate of convergence as well as providing good initial guesses. In GPU-based architectures, however, memory is often limited, and only a modest number of recycling basis vectors can be stored locally. On the other hand, computations involving local data are very fast. This leads to interesting trade-offs between the number of recycling vectors to store, the precision in which to store and use them, additional computations (very fast on the GPU), and algorithmic variations that improve accuracy/stability or using iterative refinement. We discuss a number of mixed precision algorithmic extensions as well as memory saving strategies to make recycling more effective on GPU-based architectures.

Keywords: Mixed precision algorithms, GPUs, Iterative Methods, Krylov subspace recycling

*This work is supported in part under NSF DMS 2208470.
†This work is supported in part under NSF DMS 2208470.

A backward error analysis framework for GMRES

Alfredo Buttari[2], Nicholas J. Higham[1], Théo Mary[3], and Bastien Vieublé[1]

[1]The University of Manchester, UK
[2]IRIT, France
[3]LIP6, France
alfredo.buttari@irit.fr; {nick.higham, bastien.vieuble}@manchester.ac.uk;
theo.mary@lip6.fr

Abstract

GMRES is a well-known iterative solver for the solution of linear systems $Ax = b$. Its combination with approximate computing techniques such as low precision or randomization has recently brought much attention. This is because these techniques can offer significant gains in speed and energy and enlarge the scale of problems we are able to solve. GMRES can employ approximate computing in many different ways: at the preconditioner level (e.g., [1]), at the restart level (e.g., [2]), at the orthogonalization level (e.g., [3]), etc. Moreover, considering the wide variety of preconditioners that can be used (e.g., ILU, polynomial, Jacobi, iterative solver, etc.) and the different orthogonalization algorithms and their variants (e.g., Householder, MGS, CGS2, etc.), the combinatory of possibilities is gigantic. Generally, existing backward error analyses of GMRES are specialized to one of these combinations and cannot be extended to others. For this reason, in this talk, we present a general framework for backward error analysis of GMRES that aims at gathering all these combinations inside a common and coherent analysis, in addition to give the proper tools to derive specialized bounds on the backward and forward errors of a given GMRES algorithm. We finally show how to apply these tools on a new mixed precision preconditioned restarted GMRES algorithm that uses six independent precision parameters and applies the preconditioner in a lower precision than the matrix-vector product with A. We cover both right- and left-preconditioned GMRES, and highlight the differences in convergence behavior between the two. We motivate this new mixed precision scheme by numerical experiments on real-life SuiteSparse matrices.

Keywords: GMRES, Linear systems, Mixed precision, Preconditioner, Restart

References

[1] M. Arioli, I. S. Duff (2008). *Using FGMRES to obtain backward stability in mixed precision.* ETNA. Electronic Transactions on Numerical Analysis.

[2] K. T., H. F. Walker (1992). *Efficient High Accuracy Solutions with GMRES(m).* SIAM Journal on Scientific and Statistical Computing.

[3] O. Balabanov, L. Grigori (2022). *Randomized Gram–Schmidt Process with Application to GMRES.* SIAM Journal on Scientific Computing.

MS03 - Numerical methods for fractional-derivative problems

Efficient and stable implementation of higher order methods for time-dependent fractional parabolic equations

Sebastian Franz[1] and Natalia Kopteva[2]

[1]Institute of Scientific Computing, TU Dresden
[2]Department of Mathematics and Statistics, University of Limerick
sebastian.franz@tu-dresden.de; natalia.kopteva@ul.ie

Abstract

In this talk we consider the fractional-order parabolic equation

$$D_t^\alpha u + Lu = f(x,t) \qquad \text{for } (x,t) \in \Omega \times (0,T]$$

with an initial condition $u(\cdot,0) = u_0$ in Ω and the boundary condition $u = 0$ on $\partial\Omega$ for $t > 0$, where $\alpha \in (0,1)$ and L is a spatial second-order elliptic operator. The fractional derivative is the Caputo fractional derivative in time, defined for $t > 0$ by

$$D_t^\alpha u := J_t^{1-\alpha}(\partial_t u), \qquad J_t^{1-\alpha} v(\cdot,t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha}\, v(\cdot,s)\, ds,$$

where $\Gamma(\cdot)$ is the Gamma function, and ∂_t denotes the partial derivative in t.

The fractional operator is by nature a non-local operator, which poses a major problem in the implementation of numerical methods for solving the equation. Typically, round-off errors and numerical instabilities cause the errors to grow so that the computed solutions can be far from the exact ones. This is especially true for higher order methods, which are more affected by these error sources.

We apply rewriting and adaptive quadrature techniques in order to obtain stable implementations for several different methods, starting with the classical L1-method and also for its generalisations in the form of collocation methods. We use the adaptive mesh-generation algorithm presented by Natalia Kopteva in a separate talk, which has the advantage of being able to deal with initial singularities and local irregularities in the solution. We present numerical simulations confirming stability and good convergence behaviour. Our results are reliable for α in the range of at least 0.1 and 0.999, and for meshes with mesh sizes that support a global error of 10^{-8} measured in the L^∞-norm.

Keywords: time-fractional, subdiffusion, adaptive time stepping algorithm, stable implementation, L1 method, L1-2 method, higher order collocation

References

[1] S. Franz and N. Kopteva (2023). *Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations*. J. Comp. Appl. Math. Accepted, arXiv:2211.06272.

Two kinds of numerical algorithms for ultra-slow diffusion equations

Min Cai*[1], Changpin Li†[1], and Yu Wang[1]

[1]Department of Mathematics, Shanghai University, Shanghai, China
{mcai, lcp, ywang_}@shu.edu.cn

Abstract

In this article, two kinds of numerical algorithms are derived for the ultra-slow (or superslow) diffusion equation in one and two space dimensions, where the ultra-slow diffusion is characterized by the Caputo-Hadamard fractional derivative of order $\alpha \in (0,1)$. To describe the spatial interaction, the Riesz fractional derivative and the fractional Laplacian are used in one and two space dimensions, respectively. The Caputo-Hadamard derivative is discretized by two typical approximate formulae, i.e., L2-1$_\sigma$ and L1-2 methods. The spatial fractional derivatives are discretized by the 2-nd order finite difference methods. When L2-1$_\sigma$ discretization is used, the derived numerical scheme is unconditionally stable with error estimate $\mathcal{O}(\tau^2 + h^2)$ for all $\alpha \in (0,1)$, in which τ and h are temporal and spatial stepsizes, respectively. When L1-2 discretization is used, the derived numerical scheme is stable with error estimate $\mathcal{O}(\tau^{3-\alpha} + h^2)$ for $\alpha \in (0, 0.3738)$. The illustrative examples displayed are in line with the theoretical analysis.

Keywords: Ultra-slow diffusion equation, Caputo-Hadamard derivative, Riesz derivative, Fractional Laplacian, L2-1$_\sigma$ formula, L1-2 formula

References

[1] M. Cai, C.P. Li, Y. Wang (2023). *Two kinds of numerical algorithms for ultra-slow diffusion equations*. Submited.

*MC was supported by the National Natural Science Foundation of China under grant no. 12201391.
†CL was supported by the National Natural Science Foundation of China under grant no. 12271339.

Generalized convolution quadrature for the fractional integral and fractional diffusion equations

Maria Lopez-Fernandez*[1] and Jing Guo †[2]

[1]Department of Mathematical Analysis, Statistics and O.R., and Applied Mathematics, University of Malaga
[2]School of Mathematics and Statistics, Hunan Normal University
maria.lopezf@uma.es; jingguo@smail.hunnu.edu.cn

Abstract

We consider the application of the generalized Convolution Quadrature (gCQ) of the first order to approximate fractional integrals and associated fractional diffusion equations. The gCQ is a generalization of Lubich's Convolution Quadrature (CQ) which allows for variable steps [1]. In this paper we analyze the application of the gCQ to fractional integrals, with a focus on the low regularity case. It is well known that in this situation the original CQ presents an order reduction close to the singularity. The available theory for the gCQ does not cover this situation. Here we use a different expression for the numerical approximation and the associated error, which allows us to significantly relax the regularity requirements for the application of the gCQ method. In particular we are able to eliminate the a priori regularization step required in the original derivation of the gCQ. We show first order of convergence for a general time mesh under much weaker regularity requirements than previous results in the literature [1, 2]. We also prove that uniform first order convergence is achievable for a graded time mesh, which is appropriately refined close to the singularity, according to the order of the fractional integral and the regularity of the data. Then we study how to obtain full order of convergence for the application to linear fractional diffusion equations. An important advantage of the gCQ method is that it allows for a fast and memory reduced implementation. We outline how this algorithm can be implemented and illustrate our theoretical results with several numerical experiments.

Keywords: fractional integral, fractional differential equations, generalized convolution quadrature, variable steps, graded meshes

References

[1] M. Lopez-Fernandez, S. Sauter (2013). *Generalized convolution quadrature with variable time stepping*. IMA J. Numer. Math, 33, 1156–1175.

[2] L. Banjai, F.J. Sayas (2022). *Integral Equation Methods for Evolutionary PDE: A Convolution Quadrature Approach*. Vol 59. Springer Nature.

*Maria Lopez-Fernandez thanks the support of a 2022 Leonardo Grant for Researchers and Cultural Creators, BBVA Foundation.

†Jing Guo thanks the China Scholarship Council (CSC) for its support with the scholarship number 202106720028.

Error analysis of finite difference schemes on non-uniform meshes for distributed-order differential equations

Maria Luísa Morgado*[1]

[1]Department of Mathematics, University of Trás-os-Montes e Alto Douro and Center of Stochastic and Computational Matematics, Instituto Superior Técnico, Portugal
luisam@utad.pt

Abstract

This work is focused on the numerical solution of distributed-order fractional differential equations, in which the fractional derivatives are given in terms of Caputo definition. Due to the potential presence of a singular behavior of the solution at the origin, a finite difference scheme on non-uniform meshes is presented and analysed in terms of stability and accuracy. We further explore and develop *a posteriori* error estimates, which will allow the construction of mesh adaptive algorithms. Altough such schemes based on *a posteriori* adapted mesh already exist for Caputo fractional differential equations ([1], [2]), to the best of our knowledge, these can not be found in the literature for distributed-order equations. Some numerical experiments and results are provided to illustrate the obtained theoretical results.

Keywords: Caputo fractional derivative, distributed-order derivative, finite difference scheme, a posteriori error estimate, adaptive mesh

References

[1] S. Franz, N. Kopteva (2023). *Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations.* Journal of Computational and Applied Mathematics 427 115122.

[2] N. Kopteva, M. Stynes (2022). *A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations.* J Sci Comput 92, 73.

*This work was supported by Fundação para a Ciência e Tecnologia within projects UIDB/04621/2020 and UIDP/04621/2020 and project 2022.06672.PTDC – Improving the Modelling of Anomalous Diffusion and Viscoelasticity.

Numerical methods for nonlocal and nonlinear parabolic equations with applications in hydrology and climatology

Łukasz Płociniczak[1]

[1]Faculty of Pure and Applied Mathematics, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland
lukasz.plociniczak@pwr.edu.pl

Abstract

Many natural and industrial phenomena exhibit nonlocal behaviour in temporal or spatial dimension. The former is responsible for processes for which its whole history influences the present state. The latter, on the other hand, indicates that faraway regions of the domain may have some impact on local points. This is useful in describing media of high heterogeneity.

Partial differential equations that are nonlocal involve one or several integral operators that encode this behaviour. For example, Riemann-Liouville or Caputo derivatives are used in temporal direction, while fractional Laplacian or its relatives describe spatial nonlocality. When it comes to numerical methods the discretization of these requires more care than their classical versions. Moreover, it is usually much more expensive, both on CPU and the memory, to conduct simulations involving nonlocal equations.

In this talk we will present several approaches to discretize nonlocal and nonlinear parabolic equations. These include: transformation into a pure integral equation for the time-fractional porous medium equation and Galerkin spectral methods for a general parabolic equation with temporal nonlocality. The talk is based on [2, 3, 1, 4].

Acknowledgement

Ł.P. has been supported by the National Science Centre, Poland (NCN) under the grant Sonata Bis with a number NCN 2020/38/E/ST1/00153.

Keywords: subdiffusion, numerical method, Caputo derivative, parabolic equations

References

[1] H. Okrasińska-Płociniczak, Ł. Płociniczak (2021). *Second order scheme for self-similar solutions of a time-fractional porous medium equation on the half-line*. Applied Mathematics and Computation 424, 127033.

[2] Ł. Płociniczak (2019). *Numerical method for the time-fractional porous medium equation*. SIAM Journal on Numerical Analysis, 57(2), 638–656.

[3] Ł. Płociniczak (2022). *Linear Galerkin-Legendre spectral scheme for a degenerate nonlinear and nonlocal parabolic equation arising in climatology*. Applied Numerical Mathematics 179, 105–124.

[4] Ł. Płociniczak (2023). *A linear Galerkin numerical method for a quasilinear subdiffusion equation*. Applied Numerical Mathematics 185, 203–220.

A generalised distributed-order Maxwell model

Magda Rebelo*[1], L. Ferrás †[2], and M.L. Morgado[3]

[1]NOVA MATH (CMA) and NOVA School of Science and Technology, Portugal.
[2]FEUP, University of Porto & CMAT - Centre of Mathematics, University of Minho, Portugal.
[3]CEMAT, Instituto Superior Técnico & University of Trás-os-Montes e Alto Douro, UTAD, Portugal.
msjr@fct.unl.pt; lferras@fe.up.pt; luisam@utad.pt

Abstract

In this talk we present a new model, based on distributed order derivative, that generalises the fractional viscoelastic model presented by Schiessel and Blumen [2]. The model consists of two distributed-order elements (distributed springpots) connected in series, as in the Maxwell model and allows for a more broad and accurate description of complex fluids when a proper weighting function that defines the distributed order derivative is chosen.

We discuss the connection between classical, fractional and viscoelastic models of distributed order and highlight the fundamental concepts that support these constitutive equations. We also derive the relaxation modulus, the storage and loss modulus and the creep compliance for specific weighting functions that distributes the weights through the different order derivatives.

Keywords: Maxwell model, Viscoelasticity, Distributed order fractional derivatives, Fractional calculus

References

[1] L.L. Ferrás, M.L. Morgado, M. Rebelo (2023). *Generalised distributed-order Maxwell model.* Mathematical Methods in the Applied Sciences 46 (1), 368-387

[2] H. Schiessel , A. Blumen, TF. Nonnenmacher (1995). *Generalized viscoelastic models: their fractional equations with solutions.* J Phys A: Math General. (28) 6567- 6584.

*This work was funded by national funds through the FCT-Fundação para a Ciência e a Tecnologia, I.P. (Portuguese Foundation for Science and Technology) under the scope of the projects UIDB/00297/2020 and UIDP/00297/2020 (Center for Mathematics and Applications).

†

Fractional diffusion problems with absorbing boundaries

Ercília Sousa [1]

[1]CMUC, Department of Mathematics, University of Coimbra
ecs@mat.uc.pt

Abstract

We consider a fractional partial differential equation that describes the diffusive motion of a particle, performing a random walk with Lévy distributed jump lengths, on one dimension, and subjected to an absorbing boundary condition. The equation has a spatial fractional operator based on the Riemann-Liouville fractional derivative. The main purpose of this talk is to show how the presence of the boundary can significantly change the properties of the problem and consequently the properties of a numerical method, namely its consistency and convergence.

Keywords: Fractional derivatives, Finite differences, Error bounds, Convergence analysis

References

[1] J.F. Kelly, H. Sankaranarayanan, M.M. Meerschaert (2019). *Boundary conditions for two-sided fractional diffusion.* J. Comput. Phys., 376, 1089–1107.

[2] E. Sousa (2022). *Convergence of consistent and inconsistent schemes for fractional diffusion problems with boundaries.* Adv. Comput. Math., 48, 68.

[3] G. Zumofen, J. Klafter (1995). *Absorbing boundary in one-dimensional anomalous transport.* Phys. Rev. E, 51, 2805.

Optimal long-time decay rate of solutions of complete monotonicity-preserving schemes for nonlinear time-fractional evolutionary equations

Martin Stynes[1] and Dongling Wang[2]

[1]Applied and Computational Math Division, Beijing CSRC, China
[2]School of Math and Computational Science, Xiangtan U., Hunan, China
m.stynes@csrc.ac.cn; wdymath@xtu.edu.cn

Abstract

The solution of the nonlinear initial-value problem $\mathcal{D}_t^\alpha y(t) = -\lambda y(t)^\gamma$ for $t > 0$ with $y(0) > 0$, where $\mathcal{D}_t^\alpha$ is the Caputo derivative of order $\alpha \in (0,1)$ and λ, γ are positive parameters, is known to exhibit $O(t^{-\alpha/\gamma})$ decay as $t \to \infty$. No corresponding result for any discretisation of this problem has previously been proved. We shall show that for the class of complete monotonicity-preserving schemes (which includes the L1 and Grünwald-Letnikov schemes) on uniform meshes $\{t_n := nh\}_{n=0}^\infty$, the discrete solution also has $O(t_n^{-\alpha/\gamma})$ decay as $t_n \to \infty$. For the L1 scheme, the $O(t_n^{-\alpha/\gamma})$ decay result is shown to remain valid on a very general class of nonuniform meshes. Our analysis uses a discrete comparison principle with discrete subsolutions and supersolutions that are carefully constructed to give tight bounds on the discrete solution. Numerical experiments are provided to confirm our theoretical analysis.

Full details are given in [1].

Keywords: Time-fractional evolutionary equations, Power nonlinear, $\mathcal{CM}$-preserving schemes, Polynomial decay rate

References

[1] D. Wang, M. Stynes. *Optimal long-time decay rate of solutions of complete monotonicity-preserving schemes for nonlinear time-fractional evolutionary equations.* SIAM J. Numer. Anal. (to appear).

Numerical approximation of the fractional material derivative and its link to Lévy walks

Marek Teuerle[1] and Łukasz Płociniczak[1]

[1]Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center,
Wroclaw University of Science and Technology
{marek.teuerle, lukasz.plociniczak}@pwr.edu.pl

Abstract

A Lévy walk process was proposed by Klafter, Blumen and Shlesinger in 1982 [1]. It was introduced as the microscopic description of dynamics within the continuous-time random-walk framework by including tight spatio-temporal coupling between heavy-tailed jumps and waiting times. The model has become a useful tool in modelling various anomalous diffusion processes that are characterised by finite-second moments. Namely, it has been applied in biological systems to describe the spatial collective behaviour of bacteria, bumblebees, seabirds, marine predators and humans, in statistical physics to describe the dynamics of cold atoms, blinking quantum dots, and random search strategies (see [2] for other examples).

Recently, the macroscopic characteristics of Lévy walks have been investigated. In particular, the scaling limits of their behaviour, as observed through Skorokhod's $\mathbb{J}_1$ convergence, were identified as α-stable processes that are subjected to strongly dependent inverse α-stable subordinators. This finding is a consequence of a strong interdependence between waiting times and jumps within the underlying microscopic scenario of the Lévy walk [3]. The results also show that the scaling limits' dynamics is governed by the so-called fractional material derivative [3, 4], which generalises the concept of the classical material derivative to fractional calculus.

In this work, we investigate the problem of numerical approximations of the fractional material derivative. We propose a numerical scheme that is based on spatiotemporal coupling and the known techniques proposed for fractional derivatives [5]. The stability of the scheme is established through rigorous analysis. Moreover, the accuracy of the introduced finite-volume upwind method is verified for the case of a one-sided probability problem related to Lévy walks and compared with the usual Monte Carlo approach.

Keywords: fractional material derivative, finite-volume upwind method, Lévy walk

References

[1] J. Klafter, A. Blumen, M.F. Shlesinger (1982) *Random walks with infinite spatial and temporal moments.*, J. Stat. Phys., 27, 499-–512.

[2] V. Zaburdaev, S. Denisov, J. Klafter (2015) *Lévy walks.* Rev. Mod. Phys., 87, 483–530.

[3] M. Magdziarz, M. Teuerle (2015) *Asymptotic properties and numerical simulation of multidimensional Lévy walks.* Commun. Nonlinear Sci. Numer. Simulat., 20, 489-–505.

[4] I.M. Sokolov, R. Metzler (2003) *Towards deterministic equations for Lévy walks: The fractional material derivative* Phys. Rev. E., 67, 010101(R).

[5] Ł. Płociniczak (2022) *Linear Galerkin-Legendre spectral scheme for a degenerate nonlinear and nonlocal parabolic equation arising in climatology.* Appl. Numer. Math., 179, 105–124.

MS04 - Approximated boundary methods: modelling, mathematical analysis and simulations

Elliptic Interface Problems with Jump Coefficients: A Fictitious Domain Approach with Distributed Lagrange Multiplier

Najwa Alshehri[1], Daniele Boffi[1,2], and Lucia Gastaldi[3]

[1]Computer, electrical and mathematical sciences and engineering division, King Abdullah University of Science and Technology (KAUST)
[2]Dipartimento di Matematica 'F. Casorati', University of Pavia
[3]Dipartimento di Ingegneria Civile, Architettura, Territorio, Ambiente e di Matematica, Università degli Studi di Brescia
{najwa.alshehri, daniele.boffi}@kaust.edu.sa; lucia.gastaldi@unibs.it

Abstract

Interface problems have gained significant attention in recent years due to their wide-ranging applications in various industries. The fictitious domain method with distributed Lagrange multiplier (FDDLM) is a popular approach for solving these problems, which involves the use of a fictitiously extended mesh of one domain into another domain. This technique has been shown to be effective in accurately modeling interface problems with complex geometries and large deformations. In this talk, we propose novel finite element methods for elliptic interface problems with jump coefficients, utilizing a fictitious domain formulation with piecewise constant distributed Lagrange multiplier. In particular, we present the derivation of the formulation and the a priori error estimate of the proposed scheme. Additionally, we introduce a residual-based a posteriori error estimator for these stable schemes, which provides both a global upper bound and a local lower bound for the exact error. Numerical experiments demonstrate the effectiveness of the schemes and confirm their theoretical convergence rate. Moreover, those experiments validate the reliability and efficiency of the a posteriori error estimator, which is used in implementing an adaptive refinement to enhance the accuracy and efficiency of the proposed finite element method.

Keywords: Interface problem, Fictitious domain approach, Lagrange multiplier, Mixed finite elements, A priori error estimate, A posteriori error estimate, Saddle point problem.

Numerical Analysis of Stefan Problems for Embedded Computation of Moving Internal Boundaries

T. Carlier[1], B. T. Helenbrook[2], H. Beaugendre[3], M.Colin[3], and L. Nouveau[4]

[1] Univ. Bordeaux, INRIA, CNRS, Bordeaux INP, IMB, UMR 5251, 33405, Talence, France
[2]Department of Mechanical and Aerospace Engineering, Clarkson University, Potsdam, NY 13699-5725, USA
[3]INRIA, Univ. Bordeaux, CNRS, Bordeaux INP, IMB, UMR 5251, 200 Avenue de la Vieille Tour, 33405 Talence, France
[4]Univ Rennes, INSA Rennes, CNRS, IRMAR - UMR 6625, 35000 Rennes, France
tiffanie.carlier@inria.fr

Abstract

Classical finite element methods used to model problems with internal boundaries rely on body fitted computational grids. However, those methods encounter computational challenges when the boundaries are deformed or moved substantially. In this direction, embedded methods do not require the use of boundary fitted grids in favor of immersing the boundary in a pre-existing fixed grid. In this talk we are interested in the shifted boundary method, where a surrogate boundary is added to the physical one. For simplicity, we focus on a Stefan Problem written in its mixed form. In the corresponding variational formulation, the moving boundary evolves at a speed determined by the normal flux jump. To obtain an accurate prediction of the temperature field on both sides of the discontinuity, as well as the position of the discontinuity itself, we propose an enhanced variant of the shifted boundary method based on an enriched stabilized mixed form (see [1], [2]). Note that, since the boundary is moving inside the domain, some instabilities can appear. It is then necessary to perform a linear stability analysis (see [3]). We also present some numerical computations, which confirm the expected overall second order accuracy of the method and its ability to properly simulate de-icing problems.

Keywords: Shifted Boundary Method, Moving Interface, Stefan Model, Phase-Change Problem

References

[1] L. Nouveau, M. Ricchiuto, G. Scovazzi (2019). *High-Order Gradients with the Shifted Boundary Method: An Embedded Enriched Mixed Formulation for Elliptic PDEs.* Journal of Computational Physics, 398.

[2] K. Li, N. Atallah, A. Main, G. Scovazzi (2019). *The Shifted Interface Method: A Flexible Approach to Embedded Interface Computations.* International Journal for Numerical Methods in Engineering, 121.

[3] B. Helenbrook, N. Barlowb (2016). *Spatial–temporal stability analysis of faceted growth with application to horizontal ribbon growth.* Journal of Crystal Growth, Volume 454.

ϕ-FEM: a immersed finite element method on domains defined by level-sets to solve elliptic PDEs

Michel Duprez*[1], Vanessa Lleras[2], and Alexei Lozinski[3]

[1]MIMESIS team, Inria Nancy-Grand Est, Université of Strasbourg, France
[2]IMAG, Université of Montpellier, France.
[3]Laboratoire de Mathématiques de Besançon, Université de Franche-Comté,
michel.duprez@inria.fr; vanessa.lleras@umontpellier.fr; alexei.lozinski@univ-fcomte.fr

Abstract

We present a new fictitious domain finite element method, well suited for elliptic problems posed in a domain given by a level-set function without requiring a mesh fitting the boundary. To impose the Dirichlet boundary conditions, we search the approximation to the solution as a product of a finite element function with the given level-set function, also approximated by finite elements (see [1]). The imposition of Neumann boundary conditions is less straightforward and requires the introduction of auxiliary variables near the boundary (see [2]). Unlike other recent fictitious domain-type methods (XFEM, CutFEM), our approach does not need any non-standard numerical integration, neither on the cut mesh elements nor on the actual boundary. We shall present the proofs of optimal convergence of our methods on the example of Poisson equation using Lagrange finite elements of any order. We will also give numerical tests illustrating the optimal convergence of our methods and discuss the conditionning of resulting linear systems and the robustness with respect to the geometry. In [3], we highlight the flexibility and efficiency of our method on elastic and dynamic problems. And more recently, in [4], we propose a ϕ-FEM formulation to solve particulate flows and Stokes equations.

Keywords: Fictitious finite element, elliptic PDEs, levelset

References

[1] M. Duprez, A. Lozinski (2020). *ϕ-FEM: a finite element method on domains defined by level-sets.* SIAM J. Numer. Anal., 58, 2, 1008–1028.

[2] M. Duprez, A. Lozinski, V. Lleras (2023). *A new ϕ-FEM approach for problems with natural boundary conditions.* Numer. Methods Partial Differ., Eq. 39, 1, 281–303.

[3] S. Cotin, M. Duprez, V. Lleras, A. Lozinski, K. Vuillemot (2022). *ϕ-FEM: an efficient simulation tool using simple meshes for problems in structure mechanics and heat transfer.* Partition of Unity Methods (Wiley Series in Computational Mechanics) 1st Edition, Wiley, 978-0470667088.

[4] Duprez, M. and Lozinski, A and Lleras, V. ϕ-FEM: an optimally convergent and easily implementable method for particulate flows and Stokes equations. Accepted in M2AN.

*These works was supported by the Agence Nationale de la Recherche, Project PhiFEM, under grant ANR-22- CE46-0003-01.

Local flux recovery for an elliptic interface problem using CutFEM

Aimene Gouasmi[1] and Daniela Capatina[1]

[1]LMAP & UMR CNRS 5142, Université de Pau et des Pays de l'Adour
{aimene.gouasmi, daniela.capatina}@univ-pau.fr

Abstract

In the literature, there is a recognized importance of the reconstruction of conservative local fluxes from primal discrete solutions. Such fluxes can be applied in *a posteriori* error analysis, where the difference between the numerical flux and a recovered equilibrated flux provides a reliable error indicator, which can be further used in adaptive mesh refinement procedures.

We consider a second order elliptic interface problem in 2D with discontinuous coefficients and with a jump in the normal flux on the interface. For the numerical approximation, we employ the Cut Finite Element Method of [2] where the mesh does not fit the interface. We are interested in recovering local conservative fluxes in the Raviart-Thomas space, by extending the approach introduced in [1] for the Poisson equation on fitted meshes. The construction is based on a mixed problem, with the primal solution coinciding with the original finite element solution and with the multiplier, which is defined on the sides of the mesh, being naturally used to define the degrees of freedom of the fluxes. It is important to note that the multiplier can be computed locally, by solving an explicit low-dimensional linear system for each vertex. Thus, the reconstruction method stands apart from the existing ones based on the partition of unity, which require solving local problems that are either constrained or in mixed form. In addition, this approach provides a uniform framework for several standard finite element methods and differential operators. It has recently been extended to a boundary problem with a unfitted mesh in [3].

In this talk, we treat the interface diffusion problem discretized by conforming finite elements. We show how to reconstruct a $H(div)$-flux on each sub-domain Ω_i, based on a hybrid mixed formulation with Lagrange multipliers associated to each sub-domain. On the cut elements, we use the whole edges to define the multipliers, leading to fluxes defined on the whole elements. In each Ω_i, the local conservation on a cut element is achieved with respect to an extension of the data f_i to the whole element. We thus obtain a robust reconstruction with respect to both the geometry of the interface and the diffusion coefficients. We next employ these fluxes to define a posteriori error indicators and to carry on the a posteriori error analysis, further used in adaptive mesh refinement.

Keywords: CutFEM, interface diffusion problem, flux recovery, *a posteriori* error analysis

References

[1] R. Becker, D. Capatina, R. Luce (2016). *Local flux reconstructions for standard finite element methods on triangular meshes.* SIAM J. Numer. Anal., 54, 2684–2706.

[2] E. Burman, P. Hansbo (2012). *Fictitious domain finite element methods using cut elements: II. A stabilized Nitsche method.* Appl. Numer. Math., 62, 328-341.

[3] D. Capatina, C. He (2021). *Flux recovery for Cut Finite Element Method and its application in a posteriori error estimation.* Math. Model. Numer. Anal., 55, 2759–2784.

Towards robust immersed interface methods for fluid-structure interaction

Ebrahim M. Kolahdouz[1], Michael Facci[2], Qi Sun[2], David R. Wells[2], and Boyce E. Griffith[2]

[1]Center for Computational Biology, Flatiron Institute, New York, NY USA
[2]Carolina Center for Interdisciplinary Applied Mathematics, University of North Carolina, Chapel Hill, NC USA
ekolahdouz@flatironinstitute.org; mfacci@live.unc.edu; qisun@unc.edu; {drwells, boyceg}@email.unc.edu

Abstract

This talk will provide an overview of ongoing work to develop accurate and efficient numerical methods for fluid-structure interaction based on the immersed interface method [1–3]. These numerical methods avoid using body-conforming discretizations of the moving fluid-structure interface. Instead, they use a structured discretization of the fluid equations along with a Lagrangian discretization of the structural dynamics. Kinematic matching conditions are imposed as a constraint on the motion, which is enforced through a Lagrange multiplier force imposed along the fluid-structure interface. Our numerical approach, which builds on an immersed interface method for discrete surfaces [1], integrates stress jump conditions that are generated by this surface force within the Cartesian discretization and allows us to capture accurate fluid traction forces up to the fluid-structure interface. The basic method can be extended to treat both rigid-body [2] and flexible-body [3] fluid-structure interaction using a simple Dirichlet-Neumann coupling scheme, and numerical tests suggest that the method does not suffer from artificial added mass instabilities. The talk will detail the numerical methodology along with extensions that are needed to treat the irregular interface discretizations that can occur in models involving complex geometries. It will also introduce and benchmark approaches to extending the method to geometries with sharp corners. The methodology will also be illustrated through selected biomedical applications.

Keywords: Fluid-structure interaction, Immersed interface method, Complex geometries

References

[1] E.M. Kolahdouz, A.P.S. Bhalla, B.A. Craven, B.E. Griffith (2020). *An immersed interface method for discrete surfaces.* J. Comput. Phys., 400, 108854.

[2] E.M. Kolahdouz, A.P.S. Bhalla, L.N. Scotten, B.A. Craven, B.E. Griffith (2021). *A sharp interface Lagrangian-Eulerian method for rigid-body fluid-structure interaction.* J Comput Phys., 443, 110442.

[3] E.M. Kolahdouz, D.R. Wells, S. Rossi, K.I. Aycock, B.A. Craven, B.E. Griffith (in press). *A sharp interface Lagrangian-Eulerian method for flexible-body fluid-structure interaction.* J Comput Phys.

Higher Order Unfitted Space-time Finite Element Methods for PDEs on Moving Domains

Fabian Heimann[1], Christoph Lehrenfeld[1], and Janosch Preuß[2]

[1]Institute for Numerical and Applied Mathematics, University of Göttingen
[2]University College London
{f.heimann, lehrenfeld}@math.uni-goettingen.de; j.preuss@ucl.ac.uk

Abstract

Unfitted finite element methods are interesting for applications in different areas of computational sciences because of their ability to cope with complicated geometries by means of an unaligned background mesh. The task of deriving numerical quadrature rules within these methods is particularly straightforward for geometry approximations which are elementwise linear or of second order in relevant norms. However, higher order finite element simulations can provide a desirable error scaling behaviour. Hence, we want to present a way to obtain unfitted higher order finite element simulations, in particular for a convection-diffusion problem on a moving domain. [1] We focus on a Discontinuous Galerkin in time space-time method, which comes in a very general formulation in regards to the discretisation order. Concerning the spatial discretisation, we generalise an isoparametric mapping known from merely spatial problems. [2] We briefly mention results from numerical analysis yielding inf-sup stability and optimal order convergence in reasonable norms, under certain assumptions. [3, 4] Moreover, we present numerical results confirming these higher order convergence properties in two and three spatial dimensions.

Keywords: Unfitted Finite Element methods, Space-Time methods, Convection-Diffusion problem, Higher order methods

References

[1] F. Heimann, C. Lehrenfeld, J. Preuß (2023). *Geometrically Higher Order Unfitted Space-Time Methods for PDEs on Moving Domains*. SIAM J. Sci. Comput., 45:2, B139-B165.

[2] C. Lehrenfeld (2016). *High Order Unfitted Finite Element Methods on Level Set Domains using Isoparametric Mappings*. Comput. Methods Appl. Mech. Eng., 300:716–733.

[3] J. Preuß (2018). *Higher Order Unfitted Isoparametric Space-Time FEM on Moving Domains*. Master's thesis, University of Göttingen, `http://cpde.math.uni-goettingen.de/data/Pre18_Ma.pdf`.

[4] F. Heimann (2020). *On Discontinuous- and Continuous-in-Time Unfitted Space-Time Methods for PDEs on Moving Domains*. Master's thesis, University of Göttingen, `https://cpde.math.uni-goettingen.de/data/Hei20_Ma.pdf`.

A ϕ-FEM approach with deep learning and varying geometry

Vanessa Lleras[1], Michel Duprez[2], Alexei Lozinski[3], Vincent Vigon[4], and Killian Vuillemot[1]

[1]IMAG, University of Montpellier
[2]INRIA MIMESIS, Strasbourg
[3]LMB, University of Franche Comté
[4]IRMA, University of Strasbourg
{vanessa.lleras, killian.vuillemot}@umontpellier.fr; michel.duprez@inria.fr;
alexei.lozinski@univ-fcomte.fr; vincent.vigon@math.unistra.fr

Abstract

ϕ-FEM is a recently proposed finite element method for the efficient numerical solution of partial differential equations posed in domains of complex shapes, using simple structured meshes, not necessarily fitted to the domain, and achieving the optimal accuracy [1, 2, 3]. The only geometrical input for this method is a level-set function of the domain. In this talk, we shall present a combination of ϕ-FEM with Fourier Neural Operators (FNO)[4]. FNO uses Fast Fourier Transform, so that the solution should be represented on a Cartesian grid. In this context, ϕ-FEM turns out to be a promising alternative for training a neural network to provide predictions under the varying applied forces and under the varying geometries, conveniently represented by level sets. The efficiency of this combination will be illustrated with some numerical results on the Poisson equation with Dirichlet boundary conditions and on varying shapes.

Keywords: Unfitted finite element method, Deep learning, Fast Fourier Transform, Level set.

References

[1] M. Duprez, A. Lozinski (2020). *ϕ-FEM: a finite element method on domains defined by level-sets.* SIAM J. Numer. Anal., 58(2):1008–1028.

[2] M. Duprez, V. Lleras, A. Lozinski (2023). *A new ϕ-FEM approach for problems with natural boundary conditions.* Numer. Methods Partial Differential Equations, 39(1):281–303.

[3] M. Duprez, V. Lleras, A. Lozinski (2023). *ϕ-FEM: an optimally convergent and easily implementable immersed boundary method for particulate flows and Stokes equations.* ESAIM: M2AN, accepted.

[4] Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, A. Anandkumar (2021). *Fourier neural operator for parametric partial differential equations*, paper ICLR.

A penalty-free Shifted Boundary Method of arbitrary order

J. Haydel Collins[1], Alexei Lozinski[2], and Guglielmo Scovazzi[1]

[1]Dept. of Civil and Environmental Engineering, Duke University, Durham, NC USA
[2]Laboratoire de Mathématiques, Université de Franche-Comté, Besançon, France
{haydel.collins, guglielmo.scovazzi}@duke.edu; alexei.lozinski@univ-fcomte.fr

Abstract

The Shifted Boundary Method (SBM), first introduced in [1] and fully analyzed in [2, 3], falls in the broader category of unfitted (or embedded) finite element methods. The SBM approach is aimed at avoiding integration over cut cells and all the implementation issues related with it, while providing the optimal approximation rates using finite elements of any order. The idea is to shift the location where boundary conditions are applied from the true boundary to an approximate (surrogate) one, and, at the same time, to modify the boundary conditions by means of Taylor expansions in order to avoid a reduction in the convergence rates of the overall formulation. The shifted boundary conditions are applied weakly, using a Nitsche strategy. This process yields a method which is simple, robust, accurate and efficient.

In the present talk, we propose a penalty-free version of SBM, inspired by [4], and based on an anti-symmetric variant of the Nitsche method. It avoids the tedious selection of a penalty parameter, needed in the previous variants of SBM. The theoretical analysis demonstrates that the penalty-free SBM is stable and convergent at any order of finite elements. The cornerstone of the proof is an inf-sup lemma for the bilinear form which replaces the coercivity of the more traditional variants. These theoretical results are confirmed by a series of numerical experiments for Poisson and Stokes equations.

We shall also compare SBM with an alternative ϕ-FEM approach [5] and discuss the relative merits of the two techniques.

Keywords: unfitted finite element methods; weak boundary conditions.

References

[1] A. Main, G. Scovazzi (2018), *The shifted boundary method for embedded domain computations. part I: Poisson and Stokes problems.* J. Comp. Phys., 372:972–995.

[2] N. Atallah, C. Canuto, G. Scovazzi (2021). *Analysis of the shifted boundary method for the poisson problem in domains with corners.* Math. of Comp., 90(331):2041–2069.

[3] N. Atallah, C. Canuto, G. Scovazzi (2022). *The high-order shifted boundary method and its analysis.* CMAME, 394:114885.

[4] E. Burman (2012). *A penalty-free nonsymmetric Nitsche-type method for the weak imposition of boundary conditions.* SIAM J. Num. Anal., 50(4):1959–1981.

[5] M. Duprez, A. Lozinski (2020). *ϕ-FEM: a finite element method on domains defined by level-sets.* SIAM J. Numer. Anal., 58(2):1008–1028.

An overview of the Transfer Path Method

Manuel Solano*[1]

[1]Department of Mathematical Engineering and Center for Research in Mathematical Engineering CI[2]MA, Universidad de Concepción, Chile
msolano@ing-mat.udec.cl

Abstract

In 2009, the authors in [1] presented a novel idea to numerically solve one dimensional boundary value problems by considering a computational domain Ω_h not necessarily fitting the true domain Ω. It was based on the fundamental theorem of calculus that provides an explicit representation of trace of the solution on $\partial\Omega_h$ in terms of two quantities: the prescribed boundary data on $\partial\Omega$ and the integral of the approximation of the derivative. This methodology was then extended to two and three dimensional problems [2, 3], where the Dirichlet boundary data is transferred from $\partial\Omega$ to $\partial\Omega_h$ along segments called *transfer paths*. Since then, the Transfer Path Method has been employed in a variety of problems, originating high order unfitted numerical methods to solve partial differential equations, mostly in the context of hybridizable discontinuous Galerkin methods (see [5] and the references therein) but also for mixed methods [4]. In addition, it has been recently considered in the context of dissimilar meshes [6], because it provides a way to tie two independently meshed regions.

This talk is devoted to provide an overview of the Transfer Path Method, from its origin in 2009 to current developments, by showing its features, capabilities and limitations.

Keywords: Unfitted method, transfer path, high order schemes

References

[1] B. Cockburn, D. Gupta, F. Reitich (2009). *Boundary-Conforming Discontinuous Galerkin Methods via extensions from subdomains.* J. Sci. Comput., 42, 144–164.

[2] B. Cockburn, W. Qiu, M. Solano (2014). *A priori error analysis for HDG methods using extensions from subdomains to achieve boundary conformity.* Math. Comput., 83 (286), 665–699.

[3] B. Cockburn, M. Solano (2012). *Solving Dirichlet Boundary-value Problems on Curved Domains by Extensions from Subdomains.* SIAM J Sci. Comput., 34, A497-A519.

[4] R. Oyarzúa, M. Solano, P. Zúñiga (2020). *A priori and a posteriori error analyses of a high order unfitted mixed-FEM for Stokes flow.* Comput. Methods Appl. Mech. Eng., 360, 112780.

[5] N. Sánchez, T. Sánchez-Vizuet, M. E. Solano (2021). *A priori and a posteriori error analysis of an unfitted HDG method for semi-linear elliptic problems.* Numer. Math., 148, 919–958.

[6] M. Solano, S. Terrana, N.-C. Nguyen, J. Peraire (2022). *An HDG method for dissimilar meshes.* IMA J. Numer. Anal., 42 (2), 1665–1699.

*The author thanks the financial support from ANID–Chile through Fondecyt 1200569 and BASAL funds for center of excellence FB210005.

Weak prescription of Dirichlet conditions in the finite element approximation of Maxwell's problem

Ramon Codina[1] and Önder Türk[2]

[1]Universitat Politècnica de Catalunya, 08034 Barcelona, Spain
[2]Institute of Applied Mathematics, Middle East Technical University, 06800 Ankara, Turkey
ramon.codina@upc.edu; onder.turk@yandex.com

Abstract

In this paper we consider the finite element approximation of Maxwell's problem and analyse the prescription of essential boundary conditions in a weak sense. To avoid indefiniteness of the problem, the original equations are augmented with the gradient of a scalar field that allows one to impose the zero divergence of the magnetic induction, even if the exact solution for this scalar field is zero. Two finite element approximations are considered, namely, one in which the approximation spaces are assumed to satisfy the appropriate inf-sup condition that render the standard Galerkin method stable, and another augmented and stabilised one that permits the use of finite element interpolations of arbitrary order. In both cases, two methods to prescribe Dirichlet type boundary conditions are analysed. The first one is the classical Nitsche's method, whereas the second one is what we call the linked Lagrange multiplier method; in the latter, boundary conditions are imposed through a Lagrange multiplier, but instead of considering it an independent variable it is related to the main unknowns through a least-squares term that allows one to condense the Lagrange multiplier. Stability and convergence results are provided for the two finite element formulations considered and for the two ways to prescribe essential boundary conditions, whose interest is also discussed. Numerical tests confirm the optimal performance of the methods proposed.

Keywords: Essential boundary conditions, Maxwell's problem, inf-sup stable elements, stabilised formulations, Nitsche's method, linked Lagrange multipliers

MS05 - Stable multiderivative time-integrators for Differential Equations

Jacobian-free implicit multiderivative Runge-Kutta methods

Jeremy Chouchoulis[1] and Jochen Schütz[1]

[1]Faculty of Sciences & Data Science Institute, Hasselt University, Belgium
{jeremy.chouchoulis, jochen.schuetz}@uhasselt.be

Abstract

In this presentation an approximate family of implicit multiderivative Runge-Kutta (MDRK) time integrators for stiff differential equations is introduced. The approximation procedure is based on the recent Approximate Implicit Taylor method [1], in which centered differences are applied for the recursive calculation of higher order derivatives. Given that any Taylor method can be written in MDRK format, the presented family constitutes a generalization.

Two different alternatives are investigated for the computation of the higher order derivatives: either directly as part of the stage equation, or either as separate formulas for each derivative added on top of the stage equation itself. From linearizing through Newton's method, it turns out that the conditioning of the Newton matrix behaves significantly different for both cases. Adding separate formulas has a more favorable behavior, the matrix conditioning being linearly dependent on the stiffness, regardless of the amount of derivatives.

Through various numerical testcases, stiff ODEs and 2D hyperbolic conservations laws, we will demonstrate that by means of the Jacobian-free procedure, multistage multiderivative methods are more tangible as a tool for solving differential equations up to high convergence orders.

Keywords: Multiderivative Runge-Kutta, Jacobian-free, Implicit methods

References

[1] A. Baeza, R. Búrger, M. d. C. Martí, P. Mulet, D. Zorío, (2020). *On approximate implicit Taylor methods for ordinary differential equations.* Comp. and. Appl. Math., 39, 304.

[2] J. Chouchoulis, J. Schütz, (2023) *Jacobian-free implicit MDRK methods for stiff systems of ODEs.* submitted.

Compact implicit numerical methods for conservation laws

Peter Frolkovič*[1], Michal Žeravý[1], and Dagmar Žáková[1]

[1]Department of Mathematics and Descriptive Geometry, Slovak University of Technology in Bratislava
peter.frolkovic@stuba.sk

Abstract

We present novel compact implicit schemes for numerical solution of conservation laws. In the spirit of multi-derivative methods, we use approximations by finite Taylor series where the time derivatives are replaced using the (partial) Cauchy-Kovalevskaya procedure allowing for mixed temporal and spatial derivatives. Suggesting different approximations for each term with mixed derivatives in the Taylor series expressed in an implicit (backward) manner, one can obtain algebraic systems with compact stencils opposite to fully implicit schemes obtained by standard Cauchy-Kovalevskaya procedure. Consequently, using fast sweeping iterative solvers and, eventually, fractional time step methods, one can solve the resulting algebraic systems in much more efficient way.

Keywords: compact schemes, implicit methods, conservation laws

References

[1] P. Frolkovič, M. Žeravý, (2023). *High resolution compact implicit numerical scheme for conservation laws.* Applied Mathematics and Computation, 442, 127720.

[2] D. Žáková, P. Frolkovič, (2023). *Higher order compact implicit finite volume schemes for scalar conservation laws.* submitted.

*The work was supported by the grant VEGA 1/0314/23 and APVV-19-0460.

High order strong stability preserving multi-derivative implicit and IMEX Runge–Kutta methods with asymptotic preserving properties

Zachary Grant[1], Sigal Gottlieb[2], Jingwei Hu[3], and Ruiwen Shu[4]

[1]CMSE, Michigan State University, zack.j.grant@gmail.com
[2]Center for Scientific Computing and Data Science Research, UMass Dartmouth, sgottlieb@umassd.edu
[3]Department of Applied Mathematics, University of Washington, hujw@uw.edu
[4]Department of Mathematics, University of Georgia, ruiwen.shu@uga.edu

Abstract

In this talk we present a class of high order unconditionally strong stability preserving (SSP) implicit multi-derivative Runge–Kutta schemes, and SSP implicit-explicit (IMEX) multi-derivative Runge–Kutta schemes where the time-step restriction is independent of the stiff term. The unconditional SSP property for a method of order $p > 2$ is unique among SSP methods, and depends on a backward-in-time assumption on the derivative of the operator. We show that this backward derivative condition is satisfied in many relevant cases where SSP IMEX schemes are desired. We devise unconditionally SSP implicit Runge–Kutta schemes of order up to p=4, and IMEX Runge–Kutta schemes of order up to p=3. For the multi-derivative IMEX schemes, we also derive and present the order conditions, which have not appeared previously. The unconditional SSP condition ensures that these methods are positivity preserving, and we present sufficient conditions under which such methods are also asymptotic preserving when applied to a range of problems, including a hyperbolic relaxation system, the Broadwell model, and the Bhatnagar-Gross-Krook (BGK) kinetic equation. We present numerical results to support the theoretical results, on a variety of problems.

Keywords: strong stability preserving, implicit Runge–Kutta, IMEX, asymtotic preserving, multiderivative

New efficient IMEX using two derivative method for solving ordinary and partial differential equations

Eleni Theodosiou*[1], Jochen Schütz[1], and David Seal[2]

[1]Faculty of Sciences & Data Science Institute, Hasselt University, Belgium
{eleni.theodosiou, jochen.schuetz}@uhasselt.be; seal.david@gmail.com

Abstract

Ordinary and partial differential equations were always at the center of attention in computational mathematics. Regarding high-order methods in time, one most often considers the Runge Kutta (RK) methods. More specifically, achieving higher accuracy for RK methods happens by calculating intermediate stages between two time steps. For example, in explicit RK schemes, seven stages are required for a 6th-order accurate method. So going to high-order methods using RK schemes, there is a tremendous need for increased storage, time and high computational cost. A more generalized group of methods for temporal discretization that can help with this is the multi-derivative, multistage methods combined with a predictor-corrector approach. In this case, higher-order derivatives can be calculated to achieve higher-order accurate schemes and simultaneously decrease the number of stages. The predictor-corrector methods can increase the order to match the order of the underlying quadrature rule and reduce the computational cost by providing a suitable initial value.
In the case of nonlinear and stiff differential equations, usually, there is a need for implicit-explicit (IMEX) schemes. Differential equations that can be put in IMEX form often result from the discretization of singularly perturbed differential equations. However, there is a pitfall when one uses implicit-explicit in combination with multi-derivative methods. It has been noticed that because of the need to calculate higher-order temporal derivatives, the explicit part is also involved in implicit calculations [1]. More specifically, consider the ordinary differential equation $w'(t) = Q(w(t))$ and assume that the operator can be written in an IMEX form $Q(w) = Q_E(w) + Q_I(w)$. Considering the calculation of the implicit part $\dot{Q}_I(w) = \frac{\partial Q_I(w)}{\partial w} w'(t) = \frac{\partial Q_I(w)}{\partial w} (Q_E(w) + Q_I(w))$ so, from here, it is clear that the explicit part is involved in calculating the implicit part $\dot{Q}_I(w)$. This means that the inversion of the explicit part $Q_E(w)$ is necessary.
This presentation will discuss a more efficient way to use the IMEX scheme using the multi-derivative method. This method is derived by integrating a Hermite-Birkhoff polynomial through the stages. More specifically, we will present a new IMEX scheme using two derivative methods, and numerical results for ordinary and partial differential equations will be presented.

Keywords: Multi-derivative methods, IMEX, Predictor-corrector methods, Hermite-Birkhoff polynomial

References

[1] E. Theodosiou, J. Schütz, D. C. Seal (2023). *An explicitness-preserving IMEX-split multiderivative method.* UHasselt Preprint UP2301 (2023). URL: https://www.uhasselt.be/media/zvvbnhh0/up2301.pdf.

*E. Theodosiou was funded by the Fonds voor Wetenschappelijk Onderzoek (FWO, Belgium) - project no. G052419N.

MS06 - Theoretical and computational aspects of the discontinuous Galerkin method

Parameter free adaptivity indicator for a p-adaptive discontinuous Galerkin method for the shallow water equations

Vadym Aizinger[1] and Sara Faghih-Naini[1]

[1]Chair of Scientific Computing, University of Bayreuth
{vadym.aizinger, sara.faghih-naini}@uni-bayreuth.de

Abstract

In this talk, we present a new adaptivity indicator [2] for a quadrature-free discontinuous Galerkin discretization of the shallow water equations [1]. The proposed indicator automatically detects the high- and low-regularity solution regions, incorporates a slope limiting procedure, and does not need and problem-dependent parameters. By relying on a reconstruction scheme, the indicator also works for the lowest order (piecewise constant) discretization spaces. Based on this indicator, we introduce a special type of p-adaptive method which separates the non-adaptive (lower order) from the adaptive (higher order) parts of the solution algorithm allowing to execute them on separate hardware [3].

Keywords: discontinuous Galerkin method, shallow water equations, p-adaptivity

References

[1] S. Faghih-Naini, S. Kuckuk, V. Aizinger, D. Zint, R. Grosso, H. Köstler (2020). *Quadrature-free discontinuous Galerkin method with code generation features for shallow water equations on automatically generated block-structured meshes.* Advances in Water Resources, 138, 103552.

[2] S. Faghih-Naini, V. Aizinger (2022). *p-adaptive discontinuous Galerkin method for the shallow water equations with a parameter-free error indicator.* GEM: International Journal on Geomathematics, 13.

[3] S. Faghih-Naini, V. Aizinger, S. Kuckuk, R. Angersbach H. Köstler. *p-adaptive discontinuous Galerkin method for the shallow water equations on heterogeneous computing architectures.* Submitted to Transactions on Mathematical Software.

Discrete hybrid finite elements on hypergraphs

Hanz Martin Cheng[1], Guido Kanschat[2], and Andreas Rupp[1]

[1]School of Engineering Science, Lappeenranta–Lahti University of Technology, P.O. Box 20, 53851 Lappeenranta, Finland
[2]Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University, Mathematikon, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany.
{hanz.cheng, andreas.rupp@lut.fi}@lut.fi; kanschat@uni-heidelberg.de

Abstract

In this talk, we present a framework for discretizing partial differential equations on hypergraphs, i.e., networks of lines, surfaces, volumes, etc., based upon the work in [1]. In particular, we remark that mixed and hybrid formulations are the natural setting for posing PDEs on hypergraphs. The numerical discretizations that will be presented are thus based upon hybrid discontinuous Galerkin methods.

Keywords: hybrid finite element methods, hybrid discontinous Galerkin methods, hypergraphs

References

[1] A. Rupp, M. Gahn, G. Kanschat (2022). *Partial differential equations on hypergraphs and networks of surfaces: Derivation and hybrid discretizations.* ESAIM: M2AN, 56, 505–528.

On Slope Limiters in Discontinuous Galerkin Discretizations of Convection-Diffusion Problems

Volker John[1], Derk Frerichs-Mihov[2], and Linus Henning[3]

[1]Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Mohrenstr. 39, 10117 Berlin, Germany and Freie Universität Berlin, Department of Mathematics and Computer Science, Arnimallee 6, 14195 Berlin, Germany
[2]Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Mohrenstr. 39, 10117 Berlin, Germany
[3]Freie Universität Berlin, Department of Mathematics and Computer Science, 14195 Berlin, Germany
{john, frerichs-mihov}@wias-berlin.de; linus.henning@fu-berlin.de

Abstract

Many stabilized discretizations of steady-state convection-diffusion equations lead to numerical solutions with notable spurious oscillations in a vicinity of layers. Using discontinuous Galerkin methods offers the possibility to reduce such oscillations effectively with post-processing techniques, so-called slope limiters. In the first part of the talk, several of these techniques from the literature and improvements proposed in [1, 2] will be discussed and numerical assessments will be presented. The second part of the talk studies the question whether a feed forward neural network (multilayer perceptrons), which is trained on the basis of these techniques, is likewise able to limit spurious oscillations, see [3].

Keywords: Convection-diffusion equations, Discontinuous Galerkin methods, Spurious oscillations, Slope Limiters, Deep neural networks

References

[1] D. Frerichs, V. John (2021). *On reducing spurious oscillations in discontinuous Galerkin (DG) methods for steady-state convection–diffusion equations.* Journal of Computational and Applied Mathematics, 393, 113487. doi.org/10.1016/j.cam.2021.113487.

[2] D. Frerichs-Mihov, V. John (2022). *On a technique for reducing spurious oscillations in DG solutions of convection–diffusion equations.* Applied Mathematics Letters, 129, 107969. doi:10.1016/j.aml.2022.107969.

[3] D. Frerichs-Mihov, L. Henning, V. John (2022). *Using deep neural networks for detecting spurious oscillations in discontinuous Galerkin solutions of convection-dominated convection-diffusion equations.* WIAS Preprint 2986, submitted. doi.org/10.20347/WIAS.PREPRINT.2986.

Dissipation-based WENO stabilization of high-order discontinuous Galerkin methods for hyperbolic problems

Joshua Vedral[1] and Dmitri Kuzmin[1]

[1]Department of Mathematics, TU Dortmund University
joshua.vedral@math.tu-dortmund.de; kuzmin@math.uni-dortmund.de

Abstract

We extend a new kind of weighted essentially nonoscillatory (WENO) schemes to high-order discontinuous Galerkin (DG) discretizations of scalar hyperbolic conservation laws. The proposed methodology was introduced in [1] in the context of continuous Galerkin methods. In contrast to WENO-based limiters for DG approximations [2, 3, 4], our approach uses a reconstruction-based smoothness sensor to blend the numerical viscosity operators of high- and low-order stabilization terms. The so-defined hybrid approximation introduces low-order nonlinear diffusion in the vicinity of shocks, while preserving the high-order accuracy of the baseline DG discretization in regions where the exact solution is smooth. The underlying reconstruction procedure performs Hermite interpolation on stencils consisting of a mesh cell and its neighbors. The amount of numerical dissipation depends on the relative differences between partial derivatives of reconstructed candidate polynomials and those of the consistent finite element approximation. All derivatives are taken into account by the employed smoothness sensor. To assess the accuracy of our DG-WENO scheme, we derive error estimates and perform numerical experiments. In particular, we prove that the consistency error of the nonlinear stabilization is of the order $p + 1/2$, where p is the polynomial degree. This estimate is optimal for general meshes. For uniform meshes and smooth exact solutions, the experimentally observed rate of convergence is as high as $p + 1$.

Keywords: Hyperbolic problems, DG methods, Shock capturing, WENO reconstruction, Smoothness indicator

References

[1] D. Kuzmin, J. Vedral (2022). *Dissipation-based WENO stabilization of high-order finite element methods for scalar conservation laws.* Preprint arXiv:2212.14224 [math.NA].

[2] H. Luo, J. D. Baum, R. Löhner (2007). *A Hermite WENO-based limiter for discontinuous Galerkin method on unstructured grids.* J. Comput. Phys., 225, 686–713.

[3] J. Qiu, C.-W. Shu (2005). *Runge–Kutta discontinuous Galerkin method using WENO limiters.* SIAM J. Sci. Comput., 26, 907–929.

[4] J. Zhu, X. Zhong, C.-W. Shu, J. Qiu (2017). *Runge–Kutta discontinuous Galerkin method with a simple and compact Hermite WENO limiter on unstructured meshes.* Commun. Comput. Phys., 21, 623–649.

A filtering monotonization technique for DG discretizations of hyperbolic problems

Giuseppe Orlando[1]

[1]Department of Mathematics, Politecnico di Milano
giuseppe.orlando@polimi.it

Abstract

In this talk, we will introduce a filtering monotonization technique for Discontinuous Galerkin (DG) approximations of hyperbolic problems. In particular, we will present an approach to reduce the spurious oscillations that naturally arise in presence of discontinuities when high order spatial discretizations are employed. This goal is achieved using a filter function that keeps the high order scheme when the solution is regular and switches to a monotone low order approximation if it is not, following an approach already proposed for the Hamilton-Jacobi equations by other authors. The method has been implemented in the framework of the *deal.II* numerical library, whose mesh adaptation capabilities are also employed to reduce the region in which the low order approximation is used. The potentialities of the proposed filtering technique are shown in a number of numerical experiments. Ongoing work on the application of such techniques to global atmosphere dynamics benchmarks will be also discussed.

Keywords: Discontinuous Galerkin method, Monotone schemes, Conservation laws, Filtering methods

References

[1] G.Orlando (2023). *A filtering monotonization approach for DG discretizations of hyperbolic problems*. Computers & Mathematics with Applications, 129, 113-125.

[2] O. Bokanowski, M. Falcone, S. Sahu (2016). *An efficient filtered scheme for some first order time-dependent Hamilton–Jacobi equations*. SIAM Journal on Scientific Computing, 38, A171–A195.

Discontinuous Galerkin Methods for Modeling Hurricane Storm Surge

Jennifer Proft[1] and Clint Dawson[2]

[1]Oden Institute, The University of Texas at Austin
[2]Aerospace Engineering Department, Oden Institute, The University of Texas at Austin

Abstract

Storm surge due to hurricanes and tropical storms can result in significant loss of life, property damage, and long-term damage to coastal ecosystems and landscapes. Computer modeling of storm surge can be used for two primary purposes: forecasting of surge as storms approach land for emergency planning and evacuation of coastal populations, and hindcasting of storms for determining risk, development of mitigation strategies, coastal restoration and sustainability.

Storm surge is modeled using the depth-averaged shallow water equations coupled with wind forcing. Tides, riverine forcing, atmospheric pressure, bottom friction, the Coriolis effect and wind stress are all important for characterizing the inundation due to surge. The problem is inherently multi-scale, both in space and time. To model these problems accurately requires significant investments in acquiring high-fidelity input, accurate discretization of the computational domain using unstructured finite element meshes, and numerical methods capable of capturing highly advective flows, wetting and drying, and multi-scale features of the solution.

The discontinuous Galerkin method appears to allow for many of the features necessary to accurately capture storm surge physics. We describe the application of the method to hurricane storm surge and focus on applications of the model to recent events around the Gulf of Mexico.

Keywords: Hurricane storm surge, Discontinuous Galerkin

Convergence Analysis of DG for Time-Dependent Navier-Stokes Equations

Beatrice Riviere*[1], Rami Masri[2], and Chen Liu[3]

[1]Rice University
[2]Simula
[3]Purdue University
riviere@rice.edu; rami@simula.no; liu3373@purdue.edu

Abstract

Splitting schemes for the solution of the time-dependent incompressible Navier-Stokes equations are popular because they are computationally efficient. By decoupling the nonlinearity in the convection term from the pressure term in the momentum equation, the schemes result in smaller and better-conditioned systems to be solved. There are several variants of the splitting method; a good review is the paper by Guermond, Minev and Shen in 2006. In this talk, we formulate and analyze an interior penalty discontinuous Galerkin method coupled with a pressure correction splitting algorithm. The particular splitting approach we consider was first introduced by Timmermans, Minev and Van De Vosse in 1996. We derive a priori error estimates to show convergence of the scheme. Rates are verified by numerical experiments.

Keywords: Incompressible Navier-Stokes equations, splitting scheme, error estimates

References

[1] R. Masri, C. Liu, B. Riviere (2022). *A discontinuous Galerkin pressure correction scheme for the incompressible Navier-Stokes equations: stability and convergence.* Mathematics of Computation, 91, 1625–1654.

[2] R. Masri, C. Liu, B. Riviere (2023). *Improved a priori error estimates for a discontinuous Galerkin pressure correction scheme for the Navier-Stokes equations.* Numerical Methods for Partial Differential Equations.

[3] L.J.P. Timmermans, P.D. Minev, F.N. Van de Vosse (1996). *An approximate projection scheme for incompressible flow using spectral elements.* International Journal for Numerical Methods in Fluids, 22, 673–388.

[4] J.L. Guermond, P. Minev, J. Shen (2006). *An overview of projection methods for incompressible flows.* Computer Methods in Applied Mechanics and Engineering, 195, 6011–6045.

*Research partially funded by NSF.

Quasi-Monte Carlo and discontinuous Galerkin

Andreas Rupp[1] and Vesa Kaarnioja[2]

[1]School of Engineering Science, LUT University, P.O. Box 20, FI-53851 Lappeenranta
[2]Department of Mathematics and Computer Science, Free University of Berlin, Arnimallee 6, D-14195 Berlin
andreas.rupp@fau.de; vesa.kaarnioja@fu-berlin.de

Abstract

In this talk, we consider the development of tailored quasi-Monte Carlo (QMC) cubatures for non-conforming discontinuous Galerkin (DG) approximations of elliptic partial differential equations (PDEs) with random coefficients. We consider both the affine and uniform and the lognormal models for the input random field, and investigate the use of QMC cubatures to approximate the expected value of the PDE response subject to input uncertainty. In particular, we prove that the resulting QMC convergence rate for DG approximations behaves in the same way as if continuous finite elements were chosen. Notably, the parametric regularity bounds for DG, which are developed in this work, are also useful for other methods such as sparse grids. Numerical results underline our analytical findings.

Keywords: discontinuous Galerkin, quasi-Monte Carlo, uncertainty quantification

A priori error analysis of a Local Discontinuous Galerkin time-continuous scheme for a nonlinear degenerate parabolic equation modeling porous media flows

Sunčica Sakić[1], Vít Dolejší[1], and Scott Congreve[1]

[1]Department of Numerical Mathematics, Charles University
{sakic, dolejsi, congreve}@karlin.mff.cuni.cz

Abstract

We study an error analysis of a semidiscrete scheme for a doubly nonlinear parabolic partial differential equation, which can admit the fast-diffusion type of degeneracy. Consequently, the solution to this problem is not regular. Moreover, its existence, uniqueness, and regularity have been studied in [1, 4]. A typical example of this class of problems is Richards' equation, widely used in the modeling of flows in porous media.

Many numerical methods have been suggested to solve such problems. In [5], the higher-order space-time discontinuous Galerkin finite element method has been applied and shown great performance in the sense of efficiency, accuracy, and robustness. However, the corresponding rigorous mathematical theory has not been provided yet.

This talk presents the a priori error analysis for the time-continuous scheme. Due to the presence of nonlinearities for the spatial discretization, we choose the Local Discontinuous Galerkin method [2]. Thus, instead of the original problem, we consider the expanded mixed formulation [3] and define the method. Moreover, since the considered problem has an additional nonlinearity, special techniques are applied to derive the a priori error bounds. In particular, we give error estimates in L^2-norm and the jump form with respect to the spatial discretization parameter and the Hölder coefficient of the nonlinear term derivative. Numerical examples accompany the proposed theory.

Keywords: Error estimates, Local Discontinuous Galerkin method, Degenerate parabolic equation, Fast-diffusion, Richards' equation

References

[1] H. W. Alt, S. Luckhaus (1983). *Quasilinear elliptic-parabolic differential equations.* Math. Z., 183, 311–342.

[2] D.N. Arnold, F. Brezzi, B. Cockburn L.D. Marini (2002). *Unified analysis of discontinuous Galerkin methods for elliptic problems.* SIAM J. Numer. Anal., 39 (5), 1749–1779.

[3] T. Gudi, N. Nataraj, A. Pani (2008). *An hp-local discontinuous Galerkin method for some quasilinear elliptic boundary value problems of nonmonotone type.* Math. Comput., 77 (262), 731–756.

[4] F. Otto (1996). *L^1-contraction and uniqueness for quasilinear elliptic-parabolic equations.* J. Differ. Equ., 131 (1), 20–38.

[5] V. Dolejší, M. Kuraz, P. Solin (2019). *Adaptive higher-order space-time discontinuous Galerkin method for the computer simulation of variably-saturated porous media flows.* Appl. Math. Model., 276–305.

A local dG-method for composite finite elements applied to convection-dominated problems

Friedhelm Schieweck[1]

[1]Department of Mathematics, University Magdeburg, Germany
schiewec@ovgu.de

Abstract

The discontinuous Galerkin (dG) method applied to convection-dominated problems has the big advantage that it delivers with its upwind version for convective terms a parameter-free stabilization of higher order. On the other hand, it has compared to continuous finite element methods the disadvantage that it needs much more unknowns as well as much more couplings between the unknowns and that a static condensation for higher order elements is not possible.

In this talk, we propose a modification of the underlying finite element space that keeps the advantage and removes the disadvantages of the usual dG-method. The idea is to use composite finite elements (macro-elements), i.e., for instance, quadrilateral or hexahedral elements each of which is composed of a fixed number of triangular or tetrahedral sub-elements. Then, discontinuities in the discrete functions of our dG-method are allowed only locally in the interior of macro-elements, i.e., the discrete functions are required to be continuous at the boundaries of the macro-elements. Thus, the number of couplings as well as the number of unknowns in the corresponding dG-method is reduced essentially compared to the classical dG-method applied on the fine triangular or tetrahedral mesh. Moreover, a static condensation is now possible within the new approach.

We show that the additional continuity requirements along the macro-element boundaries do not destroy the good stabilization properties of the corresponding dG-method. In particular, for a scalar convection-diffusion model problem, we prove a quasi-optimal error estimate in a suitable dG-norm including the streamline derivative of the error.

We present some numerical examples for the convection dominated case which confirm the theoretical results of our new approach.

Keywords: dG-method, composite finite elements, convection-diffusion equation, error estimates

Spectrally deferred time integration for compressible flows

Jochen Schütz[1], Arjun Thenery Manikantan[1], and Jonas Zeifang[1]

[1]Faculty of Sciences and Data Science Institute, UHasselt, Hasselt, Belgium
jochen.schuetz@uhasselt.be

Abstract

In this talk, we consider the discretization of the time-dependent compressible Navier-Stokes equations. We show how a recently developed two-derivative spectrally deferred correction scheme [1] can be used for implicit time integration in the context of a discontinuous Galerkin spectral element (DGSEM) discretization of the equations. After a short introduction of the methodology, we focus both on an efficient implementation - including the use of an adaptive Newton solver - and the extension of the methodology to cope with parallelism in time. Numerical results are shown, highlighting both strenghts and weaknesses of the discretization. The presentation follows the lines of [2] and further recent developments.

Keywords: compressible Navier-Stokes equations, implicit time integration, multiderivatives

References

[1] J. Zeifang, J. Schütz (2022). *Implicit two-derivative deferred correction time discretization for the discontinuous Galerkin method.* Journal of Computational Physics, 464, 111353.

[2] J. Zeifang, A. Thenery Manikantan, J. Schütz (2022). *Time parallelism and Newton-adaptivity of the two-derivative deferred correction discontinuous Galerkin method.* UHasselt Preprint UP2201, https://www.uhasselt.be/media/3snkyq1s/up2201.pdf

A Discontinuous Galerkin Approach for Moist Air and Rain with Implicit Condensation

Henry von Wahl[*†1], Sabine Hittmeir[*1], Philip L. Lederer[2], and Joachim Schöberl[*3]

[1]Faculty of Mathematics, University of Vienna
[2]Department of Applied Mathematics, University of Twente
[3]Institute of Analysis and Scientific Computing, TU Wien
henry.wahl@univie.ac.at

Abstract

Precipitation still causes one of the most significant uncertainties in weather forecasting and climate models, and the equations governing cloudy air are still actively debated. Therefore, the numerical simulation of cloudy air models is a critical tool to help investigate the importance of individual thermodynamic components.

The equations of a detailed model governing air with warm rain can be formulated as a non-linear hyperbolic conservation law with source terms governing the phase changes of water, i.e., condensation, auto-conversion of cloud water into rainwater, rain accretion and evaporation [1]. Unfortunately, the source term modelling condensation is not given explicitly. To avoid this problematic source term, we combine the densities of water vapour and cloud water into a single density to obtain a set of equations with modellable source terms. In particular, we consider the micro-physics parametrisation from the COSMO model [2].

We use a discontinuous Galerkin (DG) discretisation to solve the resulting hyperbolic conservation law system. In the context of DG, explicit time-stepping allows efficient use of high-performance computing hardware through matrix-free routines. The ability to utilise HPC hardware is vital to solving the huge systems resulting from the large domains of interest. To evaluate the flux in every time step, we must recover the water vapour density, cloud water density and temperature from our set of primary variables in the hyperbolic conservation law. However, due to our formulation, these variables are now the solution to a non-linear algebraic problem. We use a novel approach to recover these variables by solving the non-linear algebraic problem in every quadrature point and reconstructing the polynomial solution through an L^2-projection. Consequently, we have a highly parallelisable scheme and include the process of water condensation implicitly in our scheme. Furthermore, we do not require sub-iterations to enforce the saturation threshold in each time step. We illustrate the potential of this approach using numerical examples based on several established problems. This includes optimal high-order convergence rates for the case of smooth solutions.

Keywords: Atmospheric flow, Discontinuous Galerkin, Implicit condensation, Compressible Euler, Matrix free.

References

[1] W. Cotton, G. Bryan, S. van den Heever (2011). eds. *Storm and Cloud Dynamics. The Dynamics of Clouds and Precipitating Mesoscale Systems.* 2nd ed. Vol. 99. International Geophysics.

[2] G. Doms et al. (2021) *COSMO-Model Version 6.00: A Description of the Non-hydrostatic Regional COSMO-Model - Part II: Physical Parametrizations.* Tech. rep. COSMO Consortium for Small-Scale Modelling.

*HvW, SH and JS acknowledge support through the Austrian Science Fund (FWF) project F65.
†The computational results presented have been achieved in part using the Vienna Scientific Cluster (VSC)

MS07 - Space-time methods for evolutionary PDEs

Space-time continuous and coercive formulation for the wave equation

Paolo Bignardi[1] and Andrea Moiola[1]

[1]Department of Mathematics, University of Pavia, Italy
[1]paolo.bignardi01@universitadipavia.it; andrea.moiola@unipv.it

Abstract

Space-time methods for evolution PDEs regard time as an additional dimension, compared to semidiscretisation techniques, such as the method of lines where the equation is discretised in the space component and only then the resulting ODE system is solved. For the second-order wave equation, a stable general space-time variational formulation that allows the use of general discretisations is not available.

To derive such a formulation, we use integration by parts testing against a Morawetz multiplier (i.e. specially crafted test functions) and obtain a bilinear form that is continuous and coercive (sign-definite) as required by the Lax-Milgram theorem. This strategy follows the approach previously adopted for Helmholtz problems in [1]. The formulation is set in a function space endowed with a norm that is stronger than the usual one on $H^1(\Omega \times (0,T))$, and because of this any conforming discretisation is required to be $C^1(\overline{(0,T)\times\Omega})$. This approach is valid for problems where impedance boundary condition $\partial_t u + \theta \partial_{\boldsymbol{n}} u$ are imposed on $\partial\Omega \times (0,T)$ when Ω is star-shaped with respect to a ball and also in scattering problems with a star-shaped scatterer with Dirichlet boundary conditions. The Lax-Milgram theorem implies the well-posednes of the variational formulation on any discrete space $V_h \subset C^1(\overline{(0,T)\times\Omega})$, and by Céa's lemma explicit error bounds can be computed. Numerical experiments confirm the theoretical results.

Keywords: Wave equation, Space-time methods, Sign-definite formulation, Lax-Milgram theorem, High-order discretisations

References

[1] A. Moiola, E. A. Spence (2014). *Is the Helmholtz equation really sign-indefinite?*. In: *SIAM Review*, 56.2., 274–312.

On a space-time first-order system least-squares formulation of parabolic PDEs

Gregor Gantner*[1,2] and Rob Stevenson†[3]

[1]SERENA project-team, Inria Paris, France
[2]CEREMICS research center, École des Ponts ParisTech, France
[3]Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Netherlands
gregor.gantner@inria.fr; r.p.stevenson@uva.nl

Abstract

While the common space-time variational formulation of a parabolic PDE results in a bilinear form that is non-coercive, [1] recently proved well-posedness of a space-time first-order system least-squares (FOSLS) formulation of the heat equation. Least-squares formulations always correspond to a symmetric and coercive bilinear form. In particular, the Galerkin approximation from any conforming trial space exists and is a quasi-optimal approximation. Additionally, the least-squares functional automatically provides a reliable and efficient error estimator.

In this talk, we present our generalization [2] of the least-squares method of [1] to general second-order parabolic PDEs with possibly inhomogenoeus Dirichlet or Neumann boundary conditions. For homogeneous Dirichlet conditions, we have further proved convergence of a standard adaptive finite element method driven by the least-squares estimator. As the convergence rates can still be slow for highly singular solutions, we have constructed a trial space with enhanced approximation properties in [3]. Finally, we present our generalization [4] of [1] to the instationary Stokes equations with slip boundary conditions.

Keywords: Parabolic PDEs, Space-time FOSLS, Instationary Stokes equations

References

[1] T. Führer, M. Karkulik (2021). *Space–time least-squares finite elements for parabolic equations*, Comput. Math. Appl., 92, 27–36.

[2] G. Gantner, R. Stevenson (2021). *Further results on a space-time FOSLS formulation of parabolic PDEs*, ESAIM Math. Model. Numer. Anal., 55.1, 283–299.

[3] G. Gantner, R. Stevenson (2022). *Improved rates for a space-time FOSLS of parabolic PDEs.* arXiv:2208.09616 [math.NA].

[4] Gregor Gantner, Rob Stevenson (2022). *A well-posed first order system least squares formulation of the instationary Stokes equations.* SIAM J. Numer. Anal., 60(3):1607-1629.

*The author's research has been supported by the Austrian Science Fund (FWF) under grant J4379-N.
†The author's research has been supported by NSF Grant DMS 172029.

Shape optimization for parabolic problems on time-dependent domains

Rahel Brügger[1], Helmut Harbrecht[2], and Johannes Tausch[3]

[1]Fraunhofer Institute for Algorithms and Scientific Computing (SCAI), Germany
[2]Department of Mathematics and Computer Science, University of Basel, Switzerland
[3]Department of Mathematics, Southern Methodist University, Texas
rahel.bruegger@scai.fraunhofer.de; helmut.harbrecht@unibas.ch; tausch@smu.edu

Abstract

This talk is concerned with the solution of time-dependent shape optimization problems. Specifically, we consider the heat equation in a domain which might change over time. We compute Hadamard's shape gradient in case of both, domain integrals and boundary integrals. As particular examples, we consider the one-phase Stefan problem and the detection of a time-dependent inclusion. We discuss the numerical solution of these problems and present respective results.

Keywords: Shape optimization, Heat equation, Space-time tubes

References

[1] R. Brügger, H. Harbrecht (2022). *On the reformulation of the classical Stefan problem as a shape optimization problem.* SIAM J. Control Optim., 60, 310–329.

[2] R. Brügger, H. Harbrecht, J. Tausch (2021). *On the numerical solution of a time-dependent shape optimization problem for the heat equation.* SIAM J. Control Optim., 59, 931–953.

Towards space-time finite elements for the wave equation

Thomas Führer*[1], Roberto González[2], and Michael Karkulik†[2]

[1]Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Chile
[2]Departamento de Matemática, Universidad Técnica Federico Santa María, Chile
tofuhrer@mat.uc.cl; robert.gonzalezf@sansano.usm.cl; michael.karkulik@usm.cl

Abstract

Recently in [1], we presented a space-time finite element method for the heat equation, cf. [2] for general parabolic equations. Our method is robust on locally refined space-time meshes and easy to implement. In this talk, we share our latest findings in our attempt to carry over our ideas to the wave equation

$$\begin{aligned} u'' - \Delta u &= f \text{ in } \Omega \times (0,T), \\ u(0) &= u_0 \text{ in } \Omega, \\ u'(0) &= u_1 \text{ in } \Omega. \end{aligned}$$

We discuss a variety of approaches to obtain space-time discretizations and present the inherent difficulties when trying obtain robustness on locally refined space-time meshes.

Keywords: Wave equation, space-time discretizations, finite element method

References

[1] T. Führer, M. Karkulik (2021). *Space-time least-squares finite elements for parabolic equations.* Comput. Math. Appl., 92, 27–36.

[2] G. Gantner, R. Stevenson (2021). *Further results on a space-time FOSLS formulation of parabolic PDEs.* ESAIM Math. Model. Numer. Anal., 55.1, 283–299.

*The author's research has been supported by ANID Chile, Fondecyt Regular No. 1210391.
†The author's research has been supported by ANID Chile, Fondecyt Regular No. 1210579.

A space-time fast boundary element method for the heat equation with temporal nearfield compression

Günther Of[1] and Raphael Watschinger*[1]

[1]Institute of Applied Mathematics, Graz University of Technology, Austria
of@tugraz.at

Abstract

We consider a space-time boundary element method for the solution of initial boundary value problems of the heat equation in three spatial dimensions. In particular we deal with tensor product meshes with adaptive decompositions of the considered time interval and adaptive spatial meshes. We apply a space-time fast multipole method as well as shared and distributed memory parallelization with respect to space and time.

We present a novel temporal nearfield compression technique which enables efficient computations for fine spatial mesh resolutions related to the considered adaptive tensor product meshes. In particular, we introduce a version of the adaptive cross approximation tailored to the nature of the considered heat kernel. Finally, we present numerical experiments that demonstrate the great benefits of the new method for tensor product meshes with spatially fine meshes and adaptive spatial meshes.

Keywords: Heat equation, Fast boundary element methods, Space-time method, Adaptive cross approximation

*The authors acknowledge support provided by the Austrian Science Fund (FWF) under the project I 4033-N32 in a joint project with the Czech Science Foundation (project 17-22615S).

Space-time virtual elements for the heat equation

Ilaria Perugia[1], Sergio Gómez[2], Lorenzo Mascotto[3], and Andrea Moiola[3]

[1]Faculty of Mathematics, University of Vienna, Austria
[2]Department of Mathematics, University of Pavia, Italy
[3]Department of Mathematics and its Applications, University of Milano-Bicocca, Italy
ilaria.perugia@unvie.ac.at; sergio.gomez01@universitadipavia.it;
lorenzo.mascotto@unimib.it; andrea.moiola@unipv.it

Abstract

Space-time methods, as opposed to time-marching schemes, are based on variational formulations of the considered time-dependent problems in both space and time. Advantages of this monolithic approach are that high-order approximations both in space and time are simple to obtain, simultaneous local refinement in space and time is possible, and the numerical solution is available at all times. For a survey of space-time discretizations of parabolic problems, we refer to [4]. Recent developments include [1, 2].

In this talk, we present a space-time virtual element method for the approximation of the heat equation [3], which generalizes the Petrov-Galerkin finite element method of [5]. The considered meshes are tensor products of polytopic meshes in space and interval partitions in time. Local test and trial functions are defined as solutions to a heat problem with polynomial data. Global approximation spaces are constructed by approximating continuity across time-like facets in a nonconforming way. This allows for an analysis setting and an implementation strategy, which are independent of the spatial dimension. Approximation functions are allowed to be discontinuous in time, and the information across space-like facets is transmitted through upwinding. As typical of the virtual element framework, the basis functions are not known in closed form. The method is therefore defined in terms of degrees of freedom only, with the help of suitable local projections onto underlying space-time polynomial spaces. Theoretical results, as well as their numerical validation, will be discussed.

Keywords: Space-time methods; Virtual element methods; Heat equation; Polytopic meshes.

References

[1] T. Führer, M. Karkulik (2021). *Space-time least-squares finite elements for parabolic equations.* Comput. Math. Appl., 92, 27–36.

[2] G. Gantner, R. Stevenson (2021). *Further results on a space-time FOSLS formulation of parabolic PDEs.* ESAIM Math. Model. Numer. Anal., 55, 283–299.

[3] S. Gómez, L. Mascotto, A. Moiola, I. Perugia (2022). *Space-time virtual elements for the heat equation.* arXiv:2212.05343 [math.NA].

[4] U. Langer, O. Steinbach eds. (2019). *Space-Time Methods: Applications to Partial Differential Equations.* Volume 25 of Radon Series on Computational and Applied Mathematics, De Gruyter.

[5] O. Steinbach (2015). *Space-time finite element methods for parabolic problems.* Comput. Methods Appl. Math., 15, 551–566.

Thermo-elastic coupling with finite elements in space-time: modeling and simulation for multiphysics systems

Michael Reichelt[1] and Olaf Steinbach[1]

[1]Institute of Applied Mathematics, Graz University of Technology, Austria
{michael.reichel, o.steinbach}@tugraz.at

Abstract

We present a novel approach for the thermo-elastic coupling using space-time finite elements. This method enables the simultaneous simulation of heat transfer and structural mechanics in a fully coupled manner. We will discuss the mathematical formulation of this approach, highlight its advantages, and present numerical examples that demonstrate its accuracy and computational efficiency in analyzing multiphysics systems. We will also cover recent developments, challenges, and future directions in this area.

Keywords: Space-Time finite elements, Multiphysics, Thermo-Elasticity

References

[1] O. Steinbach, M. Zank (2020). *Coercive space-time finite element methods for initial boundary value problems*. Electron. Trans. Numer. Anal., 52, 154–194.

[2] O. Steinbach, M. Zank (2019). *A stabilized space-time finite element method for the wave equation*. In: *Advanced Finite Element Methods with Applications. Selected papers from the 30th Chemnitz FEM Symposium 2017*, eds.: T. Apel, U. Langer, A. Meyer, and O. Steinbach, Lecture Notes in Computational Science and Engineering, vol. 128, Springer, 341–370.

ENUMATH 2023, September 4 – 8, Lisbon, Portugal

Interpolation operators for parabolic problems

Rob Stevenson*[1] and Johannes Storn†[2]

[1]Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Netherlands
[2]Department of Mathematics, Bielefeld University, Germany
r.p.stevenson@uva.nl; jstorn@math.uni-bielefeld.de

Abstract

This talk introduces interpolation operators with approximation and stability properties suited for parabolic problems in primal and mixed formulations. We derive localized error estimates for tensor product meshes (occurring in classical time-marching schemes) as well as for locally in space-time refined meshes.

Keywords: Interpolation operator, Parabolic problems, Heat equation

*The author's research has been supported by the Netherlands Organization for Scientific Research (NWO) under contract. no. SH-208-11 and by the NSF Grant DMS ID 1720297.

†The author's research has been supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – SFB 1283/2 2021 – 317210226.

MS08 - Problems in biomedical fluid mechanics

On the strain based hemolysis models in the context of viscoelastic fluids flows

Tomáš Bodnár*[1]

[1]Institute of Mathematics, Czech Academy of Sciences, Czech Republic
bodnar@math.cas.cz

Abstract

The recent advances in in the development and application of ventricular assist devices and other mechanical aids in human circulatory system revealed the need for better understanding and estimation of mechanically introduced blood damage. Several models were developed and are currently in use, based on either Eulerian or Lagrangian [1] formulations of empiric stress dependent correlations. Some of the most recent models are however exploring the possibility to use certain intermediate variable (instead of stress) to estimate blood damage [2], [3]. These are typically based on some scalar measure of local strain (deformation). Interestingly, the strain tensor equations are very similar to rheological models describing the viscoelastic stress tensor [4], [5]. In the present work we are are exploring the possibility to use some of the advanced rheological models of blood for direct estimate of blood damage. The present work can be seen as a continuation of development and application of the viscoelastic fluids models presented in [4], [6] in the context of strain based blood damage models described in [3].

The numerical experiments testing different mathematical models were performed using an in-house developed finite-volume code previously used e.g. in. [5] and [4].

Keywords: blood damage, strain, viscoelastic fluid, hemolysis, blood coagulation.

References

[1] H. Yu, S. Engel, G. Janiga, D. Thevenin (2017). *A Review of Hemolysis Prediction Models for Computational Fluid Dynamics*. Artificial Organs, 41(7):603–621.

[2] P.L. Maffettone, M. Minale (1998). *Equation of change for ellipsoidal drops in viscous flow*. Journal of Non-Newtonian Fluid Mechanics, 78, 227–241.

[3] D. Arora, M. Behr, M. Pasquali (2004). *A Tensor-based Measure for Estimating Blood Damage*. Artificial Organs 28(11):1002–1015.

[4] A. Sequeira, T. Bodnár (2022). *Analysis of the Shear-Thinning Viscosity Behavior of the Johnson-Segalman Viscoelastic Fluids*. Fluids 7(1), 1–24.

[5] T. Bodnár, K.R. Rajagopal, A. Sequeira (2011) *Simulation of the Three - Dimensional Flow of Blood Using a Shear - Thinning Viscoelastic Fluid Model*. Mathematical Modelling of Natural Phenomena. 6(5), 1–24.

[6] T. Bodnár, A. Sequeira (2014) *Blood Coagulation Simulations using a Viscoelastic Model*. Mathematical Modelling of Natural Phenomena. 9(6), 34-45.

*The financial support for the present work was partly provided by the Praemium Academiae of prof. Š. Nečasová and by the Research Plan *RVO 67985840*.

Numerical simulation of multiphase flows with multiple rheologies: from visco-elastic flows to elastic solids

Alexandre Caboussat[1], Léo Diserens[1,2], and Marco Picasso[2]

[1]Geneva School of Business Administration (HEG), University of Applied Sciences and Arts Western Switzerland (HES-SO)
[2]Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL)
{alexandre.caboussat,leo.diserens}@hesge.ch; {leo.diserens, marco.picasso}@epfl.ch

Abstract

A unified numerical model for the simulation of multiphase flows with free surfaces and involving multiple rheologies is presented. The several phases range from incompressible Newtonian flows, Olroyd-B viscoelastic flows to neo-Hookean elastic solids. The interactions between these various phases are strongly nonlinear and with potentially large deformations and topology changes.

We advocate an Eulerian modeling of the multiphase flows, relying on a volume-of-fluid (VOF) method in order to track the various phases. The numerical framework relies on an operator splitting strategy to decouple advection and diffusion phenomena, and a two-grid method relying on a structured Cartesian grid and an unstructured finite element mesh. On the one hand, transport equations are solved with a method of forward characteristics on the Cartesian grid. On the other hand, the space discretization relies on conforming, low-order, finite elements. A novel semi-implicit discretized scheme allows to jointly solve a Stokes problem, and an Oldroyd-B problem without advection terms.

The numerical model is validated with several numerical experiments. We focus on interactions between elastic solids and Newtonian or visco-elastic fluids, and present results ranging from collisions between elastic solids, shock absorption or the immersion of an elastic ball in a fluid.

Keywords: multiphase flows, visco-elastic flows, elastic solids, Eulerian model, free surfaces, operator splitting

References

[1] A. Bonito, M. Picasso, M. Laso (2006). *Numerical simulation of 3D viscoelastic flows with free surfaces*. J. Comput. Phys., 215(2), 691–716.

[2] N. James, S. Boyaval, A. Caboussat, M. Picasso (2014). *Numerical simulation of 3D free surface flows, with multiple incompressible immiscible phases. Applications to impulse waves*. Int. J. Num. Meth. Fluids, 42(7), 1004–1024.

[3] M. Picasso (2016). *From the free surface flow of a viscoelastic fluid towards the elastic deformation of a solid*. C. R. Math., 354(5), 543–548.

Numerical study of generalized Newtonian fluids flow in bypass

Radka Keslerová[1] and Anna Lancmanová*[1]

[1]Department of Technical Mathematics, Czech Technical University in Prague
{Radka.Keslerova, Anna.Lancmanova}@fs.cvut.cz

Abstract

This paper deals with the numerical solution of the blood flow in the channel with narrowing and bypass. The optimal value of the angle of the bypass anastomosis to the main channel is the subject of the numerical study in this paper. The focus is on values between 30 and 60 degrees. The mathematical model is based on the three-dimensional generalized Navier-Stokes equations, where either a Newtonian model or a non-Newtonian rheological model is considered. In the case of non-Newtonian models, the Carreau and the Power law models are used to address the shear thinning character of the blood flow. The numerical results are compared using wall shear stress measurement.

The numerical tests are performed in order to test whether and how much such a variation depends on the connection angle or the applied generalized Newtonian model. Numerical results are obtained using OpenFOAM and are compared for all values of the bypass connection angle and selected rheological viscosity models.

Keywords: Generalized Navier-Stokes equations, bypass geometry, Newtonian model, Carreau model, Power law model

References

[1] R. Dutra, F. Zinani, L. Rocha, C. Biserni (2021). *Effect of non-newtonian fluid rheology on an arterial bypass graft: A numerical investigation guided by constructal design.* Computer methods and programs in biomedicine 201 105944.

[2] R. Keslerová (2023). *Numerical modeling of generalized Newtonian fluids flow in S-type geometry of bypass.* Journal of Computational and Applied Mathematics, 429 115237.

[3] D. Lee, J. Su, H. Liang (2001). *A numerical simulation of steady flow fields in a bypass tube.* Journal of Biomechanics, 34 (11) 1407–1416.

[4] B. Thomas, K. Sumam, N. Sajikumar (2021). *Patient specific modelling of blood flow in coronary artery.* Journal of Applied Fluid Mechanics, 14 (5) 1469–1482.

*The financial support for the present work was provided by the Czech Technical University, Faculty of Mechanical Engineering, under the Grant No. SGS22/148/OHK2/3T/12.

On the development of a numerical model for the simulation of air flow in the human airways

Anna Lancmanová[*1,2] and Tomáš Bodnár[†1,2]

[1]Department of Technical Mathematics, Faculty of Mechanical Engineering,
Czech Technical University in Prague, Czech Republic
[2]Institute of Mathematics, Czech Academy of Sciences, Czech Republic
{Anna.Lancmanova, Tomas.Bodnar}@fs.cvut.cz

Abstract

This work is motivated by the air flow in the human respiratory system, although similar problems are also common in other areas of biomedical, environmental or industrial fluid mechanics. The air flow in the respiratory system as well as the blood flow in the circulatory system share some physical similarities. From the mathematical modelling point of view both problems can be seen (with certain level of simplification) as flow of an incompressible viscous fluid in a system of branching channels. The fluid is flowing through channels that are characterized by a multilevel (almost fractal like) branching with secondary branches of different size and orientation with respect to the main channel. The complicated configuration of the channels leads to numerous problems related to geometry description, its discretization and mathematical formulation of the associated problems including suitable boundary conditions. In this work we focus on the implementation and interconnection (coupling) of different numerical codes solving 3D (or 2D) and 1D models using finite-difference and finite-volume techniques.

Keywords: incompressible Navier-Stokes equations, air flow, human respiratory system, channel flow, coupling

References

[1] K. Ahookhosh, O. Pourmehran, H. Aminfar, M. Mohammadpourfard, M.M Sarafraz, H. Hamishehkar (2020). *Development of human respiratory airway models: A review.* European Journal of Pharmaceutical Sciences. 145:105233.

[2] Y. Shang, J. Dong, L. Tian, K. Inthavong, J. Tu (2019). *Detailed computational analysis of flow dynamics in an extended respiratory airway model.* Clinical Biomechanics, 61:105–111.

[3] C.J. Roth, (2017). *Multi-dimensional Coupled Computational Modeling in Respiratory Biomechanics.* Dissertation. Technische Universität München.

[4] Y. Liu, R.M.C. So, C.H. Zhang (2003). *Modeling the bifurcating flow in an asymmetric human lung airway.* Journal of Biomechanics, 36(7):951–959.

[5] P. Koullapis, F. Lizal, J. Jedelsky, L. Nicolaou, K. Bauer, O. Sgrott, M. Jicha, M. Sommerfeld, S. C. Kassinos. *Aerosol deposition in the human upper airways: Application Challenge AC7-01.* KBwiki - ERCOFTAC [online]:2019 [cit. 2023]. Available from: www.kbwiki.ercoftac.org

*We acknowledge the financial support provided by the Czech Technical University, Faculty of Mechanical Engineering, under the Grant No. SGS22/148/OHK2/3T/12.

†The financial support for the present work was partly provided by the Praemium Academiae of prof. Š. Nečasová and by the Research Plan *RVO 67985840*.

Application of artificial diffusion in simulations of Oldroyd-B type viscoelastic fluids for biomedical flows

Marília Pires[*1,2] and Tomáš Bodnár[†3,4]

[1]Department of Mathematics, Technology Sciences School, CIMA-UE, University of Évora, Portugal
[2]CEMAT- Instituto Superior Técnico, Lisboa, Portugal
[3]Institute of Mathematics, Czech Academy of Sciences, Czech Republic
[4]Department of Technical Mathematics, Faculty of Mechanical Engineering, Czech Technical University in Prague, Czech Republic
marilia@uevora.pt, Tomas.Bodnar@fs.cvut.cz

Abstract

Breakdown of numerical solutions of non-Newtonian viscoelastic fluids flows at higher values of the Weissenberg number, known as the High Weissenberg Number Problem (HWNP), remains an extremely challenging issue. In particular, in simulations using the finite elements method this problem has been extensively studied. It was shown recently that in some cases, HWNP can be avoided (or at least delayed) by adding a stress diffusion term to the transport equations for viscoelastic tensors [1], [3]. In this work the summary of known and tested forms of artificial diffusion is presented based on our most recent works. Several numerical tests are presented and solved using finite element code employing the FreeFem++ library [5]. The benefits and added robustness due to artificial diffusion are evaluated and discussed. The most recent developments are reported together with an outlook towards more advanced diffusive terms employing the spectral analysis of the conformation tensor.

Keywords: Finite Element Method, Oldroyd-B fluid, numerical stabilization, artificial stress diffusion.

References

[1] M. Pires, T. Bodnár. (2023) *Application of vanishing diffusion stabilization in Oldroyd-B fluid flow simulations.*. SN Applied Sciences, 5:135.

[2] M. Pires, T. Bodnár. (2022) *Artificial stress diffusion in numerical simulations of viscoelastic fluid flows.* In Carapau and Vaidya [4], chapter 9.

[3] M. Pires, T. Bodnár. (2022) *Temporal artificial stress diffusion for numerical simulations of Oldroyd-B fluid flow.*. Mathematics, 10(3).

[4] F. Carapau, A. Vaidya, editors. (2022) *Recent Advances in Mechanics and Fluid-Structure Interaction with Applications.* Advances in Mathematical Fluid Mechanics. Birkhäuser Cham.

[5] F. Hecht. (2012) *New development in FreeFem++.* Journal of Numerical Mathematics, 20(3-4):251–265.

[*]The work of M.P. This funded by National Funds through FCT – Foundation for Science and Technology within the scope of the UIDB/04674/2020 project.
[†]Both authors acknowledge the financial support provided by the Praemium Academiae of prof. Š. Nečasová and by the Research Plan *RVO 67985840*.

Application of finite element method for approximation of fluid-structure-acoustic interactions related to human phonation process

Petr Sváček*[1]

[1]Department of Technical Mathematics, Faculty of Mechanical Engineering,
Czech Technical University in Prague, Czech Republic
Petr.Svacek@fs.cvut.cz

Abstract

In this paper the problem of human phonation is addressed. Human voice is created by a complex process consisting of mutual interactions of flowing air, vibrating vocal folds and the sound propagation through the vocal tract. The fundamental sound is created by the mutual interaction of the flowing air with vibrations of vocal folds(VFs), where the underlying mechanism of the vibrations is the flutter type of aeroelastic instability. The arising fundamental sound is enriched by aeroacoustic sound sources and propagated through the vocal tract, where it is further articulated in mouth and influenced by resonances of e.g. nasal acoustic cavities.

In this paper the problem is mathematically described as a fluid-structure-acoustic interaction (FSAI) problem, where one needs to take into an account the deformation of an elastic body, the complex fluid flow and the acoustics together with all mutual couplings, see [1]. For the sound propagation aeroacoustic models are used. The attention is further paid to the inclusion of the model of the VFs contact in the model based on several ingredients as suitable boundary conditions (see [2]), modification of the flow model (see [3]) and robust mesh deformation algorithm. The role of pre-stressed vocal fold is disscussed. The numerical approximation of the problem is presented and numerical results are shown.

Keywords: Navier-Stokes equations, aeroelasticity, acoustics, human phonation.

References

[1] J. Valášek, M. Kaltenbacher, P. Sváček (2019). *On the application of acoustic analogies in the numerical simulation of human phonation process.* Flow, Turbulence and Combustion, 102:129—143.

[2] J. Valášek, P. Sváček, J. Horáček (2019). *On suitable inlet boundary conditions for fluid-structure interaction problems in a channel.* Applications of Mathematics, 64(2):225–251, 2019.

[3] P. Sváček, J. Horáček (2021). *FE numerical simulation of incompressible airflow in the glottal channel periodically closed by self-sustained vocal folds vibration.* Journal of Computational and Applied Mathematics, Volume 393, 2021, 113529.

*Authors acknowledge the financial support provided by the Czech Technical University, Faculty of Mechanical Engineering, under the Grant No. SGS22/148/OHK2/3T/12.

On interpolation between finite element meshes in simulation of human vocal fold vibrations

Jan Valášek*[1] and Petr Sváček[2]

[1]Institute of Mathematics, Czech Academy of Sciences, Czech Republic
[2]Department of Technical Mathematics, Faculty of Mechanical Engineering,
Czech Technical University in Prague, Czech Republic
valasek@math.cas.cz, Petr.Svacek@fs.cvut.cz

Abstract

The numerical simulation of the human phonation process is an interesting and still ongoing research topic, see e.g. [1]. The healthy vocal folds vibration is characterized by a complete closure of the airflow channel. It is very challenging to reproduce such a phenomenon numerically since numerical solver needs to address topological change of the computational domain and a suitable boundary condition needs to be used in the here considered case of incompressible fluid flow simulation interacting with compliant elastic structure, [3]. In this talk, we pay a special attention to the interpolation procedure between two FE meshes along many possible solutions within finite element (FE) framework.

The approach of [2] based on combination of a computationally cheap interpolation method together with constraints enforcing conservation of desired quantities, like e.g. total mass, kinetic energy or potential energy, is followed. Its advantage is global conservation of chosen quantities, however this is not generally valid locally. The numerical results consist of the test case and the application of the interpolation method to the FSI problem without a priori known position of elastic structure.

Keywords: Human phonation simulation, Fluid structure interaction, Penalization boundary condition, Interpolation with restrictions.

References

[1] M. Lasota, P. Šidlof, M. Kaltenbacher, S. Schoder (2021). *Impact of the sub-grid scale model in aeroacoustic simulation of human voice*, Applied Sciences 11:4.

[2] A. Pont, R. Codina, J. Baiges (2017). *Interpolation with restrictions between finite element meshes for flow problems in an ale setting*, International Journal for Numerical Methods in Engineering 110:13, 1203–1226.

[3] J. Valášek, P. Sváček, J. Horáček (2019). *On suitable inlet boundary conditions for fluid-structure interaction problems in a channel*, Applications of Mathematics 64:2, 225–251.

*This work was partially supported by the Praemium Academiae of prof. Š. Nečasová and by the Research Plan *RVO 67985840* provided by the Czech Academy of Sciences.

Study of blood flows in the aortic root by means of direct three-dimensional numerical simulations

K. Tůma[1], J. Fara[1], J. Hron[1], A. Jarolímová[1], and J. Málek[1]

[1]Mathematical Institute, Faculty of Mathematics and Physics, Charles University, Prague, Czechia
{ktuma, fara, hron, jarolimova, malek}@karlin.mff.cuni.cz

Abstract

We develop a robust and reliable three-dimensional finite element code to systematically study how various effects, such as chosen slip boundary conditions, influence blood flow in the aortic root. We start with the simulation of the Poiseuille flow in the straight tube for which the analytic solution is known for different slip conditions [1]. Next, we extend the tube with the sinusoidal profile (see [2]) for which the analytical solution is not known anymore. To check that our 3D code works fine, we compare it with the finite element solution of the axi-symmetric 2D-like problem computed with a very fine resolution. Finally, we replace the rigid boundary with the elastic aortic wall, enable the interaction between blood and wall, and compare the results to those for the rigid boundary.

Keywords: Navier-Stokes, Slip boundary condition, Fluid-structure Interaction, Finite Element Simulation

References

[1] R. Chabiniok, J. Hron, A. Jarolímová, J. Málek, K.R. Rajagopal, K. Rajagopal, H. Švihlová, K. Tůma: *A benchmark problem to evaluate implementational issues for three-dimensional flows of incompressible fluids subject to slip boundary conditions.* Appl. Eng. Sci., 6, 100038, 2021.

[2] R. Chabiniok, J. Hron, A. Jarolímová, J. Málek, K.R. Rajagopal, K. Rajagopal, H. Švihlová, K. Tůma: *Three-dimensional flows of incompressible Navier–Stokes fluids in tubes containing a sinus, with varying slip conditions at the wall.* Int. J. Eng. Sci., 180, 103749, 2022.

MS09 - Non-homogeneous and multicomponent fluids for environmental applications

Numerical analysis of flow phenomane in discharge objects with siphon using Smoothed Particle Hydrodynamcis Method

Luděk Beneš[1], Ondřej Krejčí*[1], and Tomáš Halada[1]

[1]Department of Mathematics, Faculty of Mechanical Engineering, Czech technical university in Prague
{ludek.benes, onrej.krejci, tomas.halada}@fs.cvut.cz

Abstract

We present numerical simulation of flow in a discharge object with the welded siphon with presence of free surface using meshfree particle method Smoootdhed Pariticle Hydrodynamics (SPH). For the solution, we use open source code DualSPHysics version 4.4. and 5.0. We focus on influence of numerical parameters on the solutions. Namely we investigated the influence of kernel size, smoothing length, viscous term formulation, coefficient of artificial viscosity and usage of particle shifting techniques. Key parameters are set and highlighted. Moreover, we compared solutions obtained with two time integration schemes, Verlet scheme and Symplectic Position Verlet scheme and investigated the differences in the solution using the Cubic spline and Wendland kernel. In addition, we discuss the problems associated with the inlet boundary condition, which turned out to be one of the most significant problems in the realization of the simulations. The input boundary condition implemented in DualSPHysics uses a so-called buffer zone and suffers from a number of instabilities in the case of inflow to the back pressure and is very sensitive to the simulation parameters. We compare the obtained results of flow field with provided PIV measurement in several longitudinal and horizontal trough the channel.

Keywords: Smoothed Particle Hydrodynamics, Free surface flow, DualSPHysics

References

[1] J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Goméz-Gesteira (2022). *DualSPHysics: from fluid dynamics to multiphysics problems.* Computational Particle Mechanics, 9(5), 867–895.

[2] J. Fürst, T. Halada, M. Sedlář, T. Krátký, P. Procházka, M. Komárek (2021). *Numerical Analysis of Flow Phenomena in Discharge Object with Siphon Using Lattice Boltzmann Method and CFD.* Mathematics, 9(15), 1–20.

[3] D. Violeau (2012). *Fluid Mechanics and the SPH Method: Theory and Applications.* Oxford University Press.

*Author to whom correspondence should be addressed.

Weak solutions to the heat conducting compressible self-gravitating flows in time dependent domains

Kuntal Bhandari[1], Binkang Huang[2], and Šárka Nečasová[3]

[1,3]Institute of Mathematics, Czech Academy of Sciences, Czech Republic
[2]School of Mathematics, Hefei University of Technology, China
{bhandari, matus}@math.cas.cz; bkhuang92@hotmail.com

Abstract

We consider a flow of heat conducting self-gravitating compressible fluid (often referred as "flow of a gaseous star") inside a moving domain whose shape in time is prescribed. The flow is governed by the 3d Navier–Stokes–Fourier-Poisson system where the velocity is supposed to fulfill the full-slip boundary condition and fluid temperature on the boundary is given by *non-homogeneous Dirichlet condition*. The idea is to first extend this system to a reference domain (by means of several penalization parameters) which now consists of a fluid part and an artificial solid part. Then our goal is to find the uniform energy bounds w.r.t. the parameters and pass to the limit to get rid of the density-dependent solid part.

The presence of non-homogeneous temparature and heat flux on the boundary gives more interests to our work. Indeed, to handle the boundary heat flux, we need to introduce here the concept of *ballistic energy inequality* and this gives some additional technical difficulties to obtain the uniform energy estimates w.r.t. the penalization parameters. And, in the presented article we show the existence of a variational solution for our system.

Keywords: Compressible Navier-Stokes-Fourier-Poisson equations, non-homogeneous boundary heat flux, time dependent domain, Ballistic energy.

References

[1] N. Chaudhuri, E. Feireisl (2022). *Navier-Stokes-Fourier system with Dirichlet boundary conditions.* Appl. Anal., 101(12), 4076–4094.

[2] E. Feireisl, O. Kreml, Š. Nečasová, J. Neustupa, J. Stebel (2013). *Weak solutions to the barotropic Navier-Stokes system with slip boundary conditions in time dependent domains. J. Differential Equations*, 254(1), 125–140.

[3] O. Kreml, V. Mácha, Š. Nečasová, A. Wróblewska-Kamińska (2018). *Weak solutions to the full Navier-Stokes-Fourier system with slip boundary conditions in time dependent domains.* J. Math. Pures Appl. (9), 109, 67–92.

[4] O. Kreml, V. Mácha, Š. Nečasová, A. Wróblewska-Kamińska (2018). *Flow of heat conducting fluid in a time-dependent domain.* Z. Angew. Math. Phys., 69(5), 119, 27.

Stably stratified turbulence: second-order closure scheme without critical Richardson number

Matteo Caggio [1], Mario Schiavon[2], Francesco Tampieri[3], and Tomáš Bodnár[4]

[1]Institute of Mathematics, Czech Academy of Sciences, Žitná 25, 115 67 Prague 1, Czech Republic.
[2]Independent, Bologna, Italy.
[3]National Research Council of Italy, Institute of Atmospheric Sciences and Climate (CNR-ISAC), Via P. Gobetti 101, Bologna, 40129, Italy
[4]Faculty of Mechanical Engineering, Czech Technical University in Prague, Karlovo N aměstí 13, 121 35 Prague 2, Czech Republic.
caggio@math.cas.cz; mario.skiavon@gmail.com; F.Tampieri@isac.cnr.it; Tomas.Bodnar@fs.cvut.cz

Abstract

We present a modification of the second-order turbulence closure that removes the critical gradient Richardson number limitation. The mean wind speed and potential temperature profiles are derived for the modified model in terms of similarity and structure functions depending on the gradient Richardson number. Some recent closure assumptions for pressure-temperature and heat flux are considered. Variances and co-variances of the turbulent fluctuations are also investigated with respect to the gradient Richardson number. The new model predictions are confronted with some well known models. Potential future research directions will be also discussed.

Keywords: Atmospheric boundary layer · Second-order closure model · Turbulence parameterizations · Strong stratification · Critical Richardson number

References

[1] M. Caggio, M. Schiavon, F. Tampieri, T. Bodnár (2022). *Closure scheme for stably stratified turbulence without critical Richardson number.* SN Applied Sciences 4(8), 214.

Numerical investigation of turbulent stratified flows in ocean and atmosphere

Philippe Fraunié[1] and Tomáš Bodnár*[2]

[1]Mediterranean Institute of Oceanography, Université de Toulon, France
[2]Department of Technical Mathematics, Faculty of Mechanical Engineering,
Czech Technical University in Prague, Czech Republic
Philippe.Fraunie@univ-tln.fr; Tomas.Bodnar@fs.cvut.cz

Abstract

In stable conditions, stratified flows in ocean and atmosphere play a significant role in mixing and exchanges of mass, matter and energy, especially through retention mechanisms and internal waves formation. The competition between turbulent fluxes and buoyancy damping when rated by the Richardson number is still identified as a challenging bottleneck for numerical models from local to climatic global scales [1], [2]. Moreover, fine grid "wave permitting" models poorly recover observations when the wavelengths are locked on the grid size.

The generation of internal waves in the 3D computational domain requires specific treatment of discretization and especially boundary conditions [3]. Here we report recent investigations in environmental flows with high order numerical discretization and adapted boundary conditions [4] with applications to laboratory experiments and realistic situations in atmosphere and ocean by resolving lee and internal waves.

A critical overview of the tested numerical methods is presented when restricted in finite volume approach.

Keywords: stratified flow, Bousinesq approximation, Richardson number, finite-volume, finite-difference

References

[1] F. Tampieri (2017). *Turbulence and Dispersion in the Planetary Boundary Layer*. Springer.

[2] M. Caggio, M. Schiavon, F. Tampieri, T. Bodnár (2022). *Closure scheme for stably stratified turbulence without critical Richardson number*. SN Applied Sciences, vol. 4, 214 .

[3] T. Bodnár T., Fraunié P. (2020). *Numerical simulation of three-dimensional lee waves behind an isolated hill*. Applied Mathematical Modelling, 78, 648-664.

[4] T. Bodnár, P. Fraunié, P. Knobloch, H. Řezníček (2021). *Numerical evaluation of artificial boundary condition for wall-bounded stably stratified flows*. Discrete and Continuous Dynamical Systems. Series S, 14(3), 785-801. ISSN 1937-1632.

*The financial support for the present work was provided by the Czech Science Foundation under the grant No. *P201-22-01591S* and by the Research Plan *RVO 67985840*.

Existence of weak solution for a compressible multicomponent fluid structure interaction problem

Šárka Nečasová*[1], Martin Kalousek †[1], and Sourav Mitra ‡[1]

[1]Institute of Mathematics, Czech Academy of Sciences, Žitná 25, 11567 Prague, Czech Republic
{matus, kalousek, sourav}@math.cas.cz

Abstract

We analyze a system of PDEs governing the interaction between two compressible mutually noninteracting fluids and a shell of Koiter type encompassing a time dependent 3D domain filled by the fluids. The dynamics of the fluids is modelled by a system resembling compressible Navier-Stokes equations with a physically realistic pressure depending on densities of both the fluids. The shell possesses a non-linear, non-convex Koiter energy. Considering that the densities are comparable initially we prove the existence of a weak solution until the degeneracy of the energy or the self-intersection of the structure occurs for two cases. In the first case the adiabatic exponents are assumed to solve $\max\{\gamma, \beta\} > 2$, $\min\{\gamma, \beta\} > 0$, and the structure involved is assumed to be non-dissipative. For the second case we assume the critical case $\max\{\gamma, \beta\} \geq 2$ and $\min\{\gamma, \beta\} > 0$ and the dissipativity of the structure. The result is achieved in several steps involving, extension of the physical domain, penalization of the interface condition, artificial regularization of the shell energy and the pressure, the almost compactness argument, added structural dissipation and suitable limit passages depending on uniform estimates.

Keywords: multicomponent compressible fluids, shell of Koiter type, weak solutions

References

[1] M. Kalousek, S. Mitra, Š. Nečasová (2023) *Existence of weak solution for a compressible multicomponent fluid structure interaction problem*, arXiv:2301.11216

*The financial support for the present work was provided by the Czech Science Foundation under the grant No. *P201-22-01591S*, by Praemium Academiæ of Š. Nečasová and by the Research Plan *RVO 67985840*

†The financial support for the present work was provided by the Czech Science Foundation under the grant No. *P201-22-01591S*, by Praemium Academiæ of Š. Nečasová and by the Research Plan *RVO 67985840*

‡The financial support for the present work was provided by Praemium Academiæ of Š. Nečasová and by the Research Plan *RVO 67985840*

Influence of city trees on dustiness inside urban boundary layer computed by LES model PALM for different stratifications

Hynek Řezníček[1,2], Jan Geletič[2], Martin Bureš[2], Pavel Krč[2], Jaroslav Resler[2], Vladimír Fuka[3], and Luděk Beneš[1]

[1]Faculty of Mechanical Engineering, Czech Technical Uni. in Prague
[2]Institute of Computer Science, Czech Academy of Sciences, Prague
[3]Faculty of Mathematics and Physics, Charles University, Prague
hynek.reznicek@fs.cvut.cz

Abstract

City trees are usually planted as a protective measure against overheating of inhabitants on the streets, unfortunately they also influence the dustiness and ventilation inside the urban-canyon. The investigation of these phenomena is the main idea of this contribution.

Model PALM is an advanced and state-of-the-art meteorological modeling system for atmospheric boundary layer flows specialized for urban sublayer. It was developed as a turbulence-resolving Large-Eddy Simulation (LES) model with dynamical core based on Navier-Stokes equations solver in Bussinesq approximation.

The simulations are conducted over Prague quarter Dejvice, similar domain as was used earlier for the latest model validation campaign. The Particulate Matter (PM) line source is placed in the middle of the road and values of a real car-traffic pollution is prescribed (as a dust source).

The effect of different tree cover on the ventilation of the street is numerically examined. Line of the trees is planted at both street sides and the planting density is varied during the simulation scenarios by changing the amount of trees in each line. The influence of the thermal stratification is also considered because different stratification plays important role in the character of the flow inside the urban-canyon (different patterns of turbulent coherent structures). Therefore an influence of two parameters (total amount of trees in the street canyon and thermal stratification) on the PM concentration at the pedestrian level is studied.

Keywords: Navier-Stokes equations, atmospheric boundary layer, large eddy simulation, thermal stratification

References

[1] B. Maronga et al. (2020) *Overview of the PALM model system 6.0* Geosci. Model Devel. 13(3).

[2] J. Resler et al. (2021) *Validation of the palm model system 6.0 in a real urban environment: A case study in Dejvice, Prague, the Czech Republic.* Geosci. Model Devel. 14(8).

[3] V. Sessa, Z.T. Xie, S. Herring (2020). *Thermal stratification effects on turbulence and dispersion in internal and external boundary layers,* Boundary-Layer Meteorology, 176(1).

Nematic liquid crystal-colloidal interaction model

Arnab Roy[1], Zhiyuan Geng[2], and Arghir Dani Zarnescu[2]

[1]Technische Universität Darmstadt
[2]Basque Center for Applied Mathematics
royarnab244@gmail.com; {zgeng, azarnescu}@bcamath.org

Abstract

We consider a mathematical model describing the movement of colloidal particles in a nematic-fluid flow. We model colloidal particle as a rigid body which is closed, bounded, simply connected. The colloidal particle is moving inside a bounded smooth domain $\Omega \subset \mathbb{R}^3$ which is filled with a viscous incompressible fluid with active liquid crystals. In the case of nematic fluid flow, there is the additional stress tensor and the Navier-Stokes equations are coupled with the equation describing the orientation of the anisotropic liquid crystal molecules. Moreover, there is a competition between elasticity and the interaction between liquid crystal molecules and surfaces (known as "anchoring") in the nematic fluid-colloid interaction. This makes this interaction problem qualitatively different from the incompressible Newtonian fluid-rigid body interaction. In this talk, we want to discuss about existence of a weak solution of this coupled system.

Keywords: Liquid crystals, Fluid-structure interaction, Navier-Stokes equations, Q-tensor, Weak Solutions.

MS10 - Entropy/energy-stable methods for time evolution problems

Variational modeling and structure-preserving approximation of a non-isothermal phase-field model for sintering

Aaron Brunk[1], Herbert Egger[2], Timileyin David Oyedeji[3], and Bai-Xiang Xu[3]

[1]Institute of Mathematics, Johannes Gutenberg University, Mainz, Germany
[2]Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria
[2]Institute for Numerical Mathematics, Johannes Kepler University Linz, Austria
[3]Mechanics of Functional Materials Division, Technical University Darmstadt, Germany
abrunk@uni-mainz.de; herbert.egger@jku.at; timileyin.oyedeji@tu-darmstadt.de;
xu@mfm.tu-darmstadt.de

Abstract

In this talk, we consider a thermodynamic consistent variational phase-field model for the non-isothermal sintering process with cross-kinetic coupling. Sintering is an essential part of the industrial process of additive manufacturing via powder bed fusion, such that further understanding and modeling is necessary to increase the efficiency and applicability in industrial applications. The cross-kinetic coupling accounts for strongly asymmetric material properties like heat conductivity or mass diffusivity across the interface. Such cross-kinetic coupling leads to cross-diffusion systems, where mathematical analysis and numerical approximation are more involved. In order to develop mathematical theory and suitable numerical approximations, we first rephrase the model in a more natural formulation by introducing the inverse temperature as a new variable. For the new formulation, we will discuss thermodynamic consistency and introduce a fully discrete numerical approximation by conforming finite elements in space and backward differences in time. We show that the numerical method is unconditionally entropy-stable and mass- and energy-conservative. This enables us to consider relative entropy methods based on the *exergy* to prove the stability of discrete solutions with respect to a perturbed system. We illustrate the theoretical finding by suitable numerical experiments.

Keywords: relative entropy, entropy-stable, cross-diffusion system, structure-preserving, complex pde system

Lax equivalence principle in the context of problems in fluid dynamics

Eduard Feireisl[1]

[1]Institute of Mathematics, Czech Academy of Science, Praha Czech Republic

Abstract

We generalize the celebrated Lax equivalence principle valid for linear problems, namely stability + consistency yields convergence, to nonlinear equations of compressible fluid dynamics. The key points are conditional regularity results in the class of bounded solutions and the concept of very weak (measure-valued) solution with the associated weak-strong uniqueness principle.

Keywords: weak-strong uniqueness, fluid dynamics, structure-preserving, complex pde system

Approximation of Classical Two-Phase Flows by a Navier-Stokes/Allen-Cahn System

Maximilian Moser[1], Helmut Abels[2], and Julian Fischer[1]

[1]Institute of Science and Technology Austria
[2]Faculty of Mathematics, University of Regensburg
{maximilian.moser, julian.fischer}@ist.ac.at;
helmut.abels@mathematik.uni-regensburg.de

Abstract

In this talk we consider the sharp interface limit of a Navier-Stokes/Allen Cahn equation in a bounded smooth domain in two or three space dimensions, for the case of vanishing mobility $m_\varepsilon = c\varepsilon^\alpha$, where $c > 0$ and $\alpha \in (0, 2)$, when the small parameter $\varepsilon > 0$ related to the thickness of the diffuse interface is sent to zero. The limit problem is given by the classical two-phase Navier-Stokes-system with surface tension and we show convergence for well-prepared initial data and for small times such that a strong solution to the limit problem exists. The approach is via the relative entropy method, i.e. one shows Gronwall-type estimates for suitable energy functionals that control the error between the solution to the diffuse and sharp interface systems in a suitable way.

In Hensel, Liu [1] the same method was applied for constant mobility, i.e. $\alpha = 0$. In this case the limit problem is given by a two-phase Navier-Stokes system coupled to mean curvature flow. Compared to the latter work we have to use a similar but more sophisticated choice for the energy functionals. This leads to a complicated remainder term in the Gronwall estimates which we estimate in a novel way.

This is joint work with H. Abels (Univ. of Regensburg) and J. Fischer (IST Austria).

Keywords: Navier-Stokes equations, Allen-Cahn equation, sharp interface limit, relative entropy method

References

[1] S. Hensel, Y. Liu (2022). *The sharp interface limit of a Navier–Stokes/Allen–Cahn system with constant mobility: Convergence rates by a relative energy approach.* Preprint arXiv:2201.09423.

Lagrangian particle schemes for porous media flows using semi-discrete optimal transport

Thomas O. Gallouët[1], Quentin Mérigot[2], and Andrea Natale[3]

[1]Team Mokaplan, Inria Paris 75012 Paris, CEREMADE, CNRS, UMR 7534, Université Paris-Dauphine, PSL University, 75016 Paris, France
[2]Université Paris-Saclay, CNRS, Laboratoire de mathmatiques dOrsay, 91405, Orsay, France and Institut universitaire de France (IUF)
[3]Inria, Univ. Lille, CNRS, UMR 8524 - Laboratoire Paul Painlev, F-59000 Lille, France
{thomas.gallouet, andrea.natale}@inria.fr@inria.fr;
quentin.merigot@universite-paris-saclay.fr

Abstract

The Wasserstein gradient flow structure of nonlinear diffusion models, such as the classical porous medium equations, allows one to define a natural notion of Lagrangian flow associated with their solutions, describing the trajectories of mass particles in the domain. At least formally, such Lagrangian flow also follows a gradient flow dynamics, but with respect to a simple L^2-metric. In this talk, I will describe a class of particle discretizations that reproduce this structure, and in which the energy is regularised variationally via a semi-discrete optimal transport problem. For these methods, I will show how the convexity of the energy in the Eulerian variables can be exploited in the non-convex Lagrangian setting to prove quantitative convergence estimates towards smooth solutions of the continuous models, using an appropriately constructed relative entropy. Finally, I will describe how our approach can be generalized to compressible fluids (in particular, the barotropic Euler equations) by simply replacing the L 2 gradient flow structure with a Hamiltonian one.

Keywords: Particle methods, Porous medium equations, Semi-discrete optimal transport

References

[1] T.O. Gallouët, Q. Mérigot, A. Natale (2022). *Convergence of a Lagrangian discretization for barotropic fluids and porous media flow.* SIAM Journal on Mathematical Analysis 54.3, 2990–3018.

[2] A. Natale (2023). *Gradient flows of interacting Laguerre cells as discrete porous media flows.* arXiv preprint arXiv:2304.05069.

Approximating dynamic phase-field fracture with a first-order formulation for velocity and stress

Marita Thomas[1], Sven Tornquist[2], and Christian Wieners[3]

[1]Department of Mathematics and Computer Science, Freie Universität Berlin, and Weierstraß Institute for Applied Analysis and Stochastics, Berlin
[2]Department of Mathematics and Computer Science, Freie Universität Berlin
[3]Department of Mathematics, Karlsruhe Institute of Technology
{marita.thomas, sven.tornquist}@fu-berlin.de; christian.wieners@kit.edu

Abstract

We investigate a model for dynamic fracture at small strains. The sharp crack interface is regularized with a phase-field approximation. For the phase-field variable a viscous evolution with a quadratic dissipation potential is employed and a non-smooth penalization prevents material healing. For the solid material both the case of a visco-elastic and of a purely elastic constitutive law is considered. The momentum balance is formulated as a first order system and coupled in a nonlinear way to the non-smooth evolution equation of the phase-field variable. We introduce a full discretization in time and space, using a discontinuous Galerkin method for the first order system. Based on this, we show the existence of discrete solutions. We discuss their convergence to a suitable notion of weak solution of the system as the step size in space and time tends to zero and give a comparison to other formulations existing in literature. Simulation results are presented.

This is joint work with Sven Tornquist (Berlin) and Christian Wieners (Karlsruhe) and also based upon collaboration with Kerstin Weinberg and Kai Friebertshäuser (both Siegen) within the priority programme "Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials" (SPP 2256), project "Nonlinear Fracture Dynamics: Modeling, Analysis, Approximation, and Applications", financially supported by the German Research Foundation (DFG).

Keywords: Dynamic phase-field fracture, Discontinuous Galerkin method, First-order formulation of momentum balance, Elastic waves in solids

References

[1] M. Thomas, S. Tornquist, C. Wieners (2023). *Approximating dynamic phase-field fracture in viscoelastic materials with a first-order formulation for velocity and stress.* WIAS-Preprint 3002.

[2] K. Friebertshäuser, M. Thomas, S. Tornquist, K. Weinberg, C. Wieners (2023). *Dynamic Phase-Field Fracture in Viscoelastic Materials using a First-Order Formulation.* Proceedings in Applied Mathematics and Mechanics, 22(1), e202200249.

[3] K. Weinberg, C. Wieners (2022). *Dynamic phase-field fracture with a first-order discontinuous Galerkin method for elastic waves.* Computer Methods in Applied Mechanics and Engineering (CMAME), 389, 114330.

MS11 - Reducing the irreducible: model reduction for transport-dominated problems

Non-intrusive model order reduction of a 2D wildland fire model with topological changes

Shubhaditya Burela[1] and Philipp Krah[2]

[1]Institute of Mathematics, Technische Universität Berlin
[2]Institut de Mathématiques de Marseille (I2M), Aix-Marseille Université
burela@tnt.tu-berlin.de; philipp.krah@univ-amu.fr

Abstract

Civil protection has made forecasting forest fires a crucial task [1]. To predict forest fires the wildland fire model [2] can be simulated over a range of different scenarios. However, numerical simulations can be computationally time-consuming, for which model order reduction (MOR) is unavoidable. Unfortunately, traditional MOR methods like proper orthogonal decomposition (POD) cannot capture the moving flame fronts of the wildland fire model in a linear subspace. As a solution, shifted proper orthogonal decomposition (sPOD) proposed in [4] was used in [3], which decomposes transport fields using co-moving frames and a few spatial basis functions computed with the help of POD. In this work, we combine the sPOD method with neural networks to learn the spread of forest fires in a non-intrusive fashion. First, a low-dimensional description of the wildland fire model is created using snapshot data from a representative set of input parameters. Then, neural networks are trained to predict the spread of forest fires for any new parameter set. This approach closely follows and builds upon [5] and is tested on one- and two-dimensional wildland fires with varying reaction rates and topology-changing fronts due to wind. The preliminary results indicate that the proposed approach yields highly accurate results within the percent range, while also enabling rapid prediction of system states within seconds.

Keywords: Model order reduction, shifted proper orthogonal decomposition, deep learning, wildland fires

References

[1] G. DaCosta, D. Derigo, G. Liberta, T. Durrant, J. San-miguel-ayanz (2020). *European wildfire danger and vulnerability in a changing climate: towards integrating risk dimensions.* Publications Office of the European Union.

[2] J. Mandel, Bennethum, S. Lynn, Beezley, D. Jonathan, Coen, L. Janice, Douglas, C. Craig, Kim, Minjeong, Vodacek, Anthony (2008). *A wildland fire model with data assimilation.* Mathematics and Computers in Simulation, Vol.79, 3, 584-606.

[3] Black, Felix, Schulze, Philipp, Unger, Benjamin (2021). *Efficient Wildland Fire Simulation via Nonlinear Model Order Reduction.* Fluids, Vol.6, 8, 280.

[4] J. Reiss, P. Schulze, J. Sesterhenn, V. Mehrmann (2018). *The Shifted Proper Orthogonal Decomposition: A Mode Decomposition for Multiple Transport Phenomena.* SIAM Journal on Scientific Computing Vol.40, 3, A1322-A1344.

[5] Fresca, Stefania, Manzoni, Andrea. *POD-DL-ROM: Enhancing deep learning-based reduced order models for nonlinear parametrized PDEs by proper orthogonal decomposition.* Computer Methods in Applied Mechanics and Engineering, Vol.388, 114-181.

Dynamical low-rank approximation for Burgers' equation with uncertainty

Jonas Kusch[1], Gianluca Ceruti[2], Lukas Einkemmer[1], and Martin Frank[3]

[1]University of Innsbruck, Innsbruck, Austria
[2]École Polytechnique Fédérale de Lausanne, Switzerland
[3]Karlsruhe Institute of Technology, Karlsruhe, Germany
{jonas.kusch, lukas.einkemmer}@uibk.ac.at; gianluca.ceruti@epfl.ch;
martin.frank@kit.edu

Abstract

Quantifying uncertainties in hyperbolic equations is a source of several challenges. The solution forms shocks leading to an oscillatory behavior in the numerical approximation of the solution, and the numerical approximation itself is observed to suffer from the so-called curse of dimensionality - the number of unknowns required for an effective discretization of the solution grows exponentially with the dimension of the uncertainties. The unknowns can be reduced using the generalized polynomial chaos expansion, allowing for an efficient representation of the distribution for the known uncertainties e.g., the initial conditions. However, the proposed ansatz is not capable to properly catch the long-time propagation, despite reducing the dimensionality of the original problem. In this contribution, dynamical low-rank approximation (DLRA) is introduced [6, 4], and a memory-wise efficient approximation of the solution on a lower dimensional manifold for Burgers' equation is obtained. Efficiently implementable robust numerical integrators for DLRA together with their properties are introduced [5, 3], and the time evolution equations for the spatial and uncertain basis functions are derived [2]. It is illustrated that these integrators possess the ability to guarantee an accurate approximation of the solution even if the underlying probability distributions change over time [1]. The proposed methodology is analyzed for Burgers' equation equipped with uncertain initial values.

Keywords: uncertainty quantification, conservation laws, hyperbolic, intrusive UQ methods, dynamical low-rank approximation, matrix projector-splitting integrator, unconventional integrator

References

[1] J. Kusch, L. Einkemmer, G. Ceruti (2023). *On the stability of robust dynamical low-rank approximations for hyperbolic problems*. SIAM Journal on Scientific Computing 45 (1), A1-A24.

[2] J. Kusch, G. Ceruti, L. Einkemmer, M Frank (2022). *Dynamical low-rank approximation for Burgers' equation with uncertainty*. International Journal for Uncertainty Quantification 12 (5).

[3] G. Ceruti, C. Lubich (2022). *An unconventional robust integrator for dynamical low-rank approximation*. BIT Numerical Mathematics 62 (1), 23-44.

[4] L. Einkemmer, C. Lubich (2018). *A low-rank projector-splitting integrator for the Vlasov–Poisson equation*. SIAM Journal on Scientific Computing, 40(5), B1330-B1360.

[5] C. Lubich, I. Oseledets (2014). *A projector-splitting integrator for dynamical low-rank approximation*. BIT Numerical Mathematics 54.1 (2014): 171-188.

[6] O. Koch, C. Lubich (2007). *Dynamical low-rank approximation*. SIAM Journal on Matrix Analysis and Applications, 29(2), 434-454.

Model Reduction on Polynomially Mapped Manifolds

Patrick Buchfink[2], Silke Glas[1], Bernard Haasdonk[2], and Hongliang Mu[1]

[1]Department of Applied Mathematics, University of Twente
[2]Institute of Applied Analysis and Numerical Simulation, University of Stuttgart
{s.m.glas, h.l.mu}@utwente.nl; {patrick.buchfink,
haasdonk}@mathematik.uni-stuttgart.de

Abstract

For advection-dominated or wave-like problems, the decay of the Kolmogorov n-widths can be slow, see e.g., [1, 2]. Recent advances in projection-based model reduction utilize autoencoders to build a nonlinear embedding from reduced-order space to full-order space. Those methods can achieve good accuracy for ROMs of low dimension, but the online evaluation (without employing hyper-reduction) scales with the size of the full-order models (FOMs). In this talk we consider ROMs on polynomially mapped manifolds. This bridges the aforementioned approaches in terms that we can achieve higher accuracy than the linear-subspace ROMs and the online evaluation of the ROMs is independent of the size of the FOMs. We extend recent approached in e.g., [3, 4] to structure-preserving model reduction of Hamiltonian systems, such that the reduced model is again a Hamiltonian system, where in particular make use of quadratic polynomial embeddings. In order to do so, we choose a particular quadratic polynomial embedding as the symplectic decoder function in [5]. We perform numerical experiments for a 1D wave equation.

Keywords: Model reduction, polynomially mapped manifolds, nonlinear approximation methods

References

[1] M. Ohlberger, S. Rave (2016). *Reduced basis methods: Success, limitations and future challenges.* Proceedings of ALGORITMY, 1–12.

[2] C. Greif, K. Urban (2019). *Decay of the Kolmogorov n-width for wave problems.* Applied Mathematics Letters 96, 216–222.

[3] J. Barnett, C. Farhat (2022). *Quadratic Approximation Manifold for Mitigating the Kolmogorov Barrier in Nonlinear Projection-Based Model Order Reduction.* Journal of Computational Physics 464, 111348.

[4] R. Geleen, S. Wright, K. Wilcox (2023). *Operator inference for non-intrusive model reduction with nonlinear manifolds.* Computer Methods in Applied Mechanics and Engineering 403, 115717.

[5] P. Buchfink, S. Glas, B. Haasdonk (2023). *Symplectic model reduction of Hamiltonian systems on nonlinear manifolds and approximation with weakly symplectic autoencoder.* SIAM Journal on Scientific Computing, 45(2), A289–A311.

Registration-based nonlinear model order reduction for transport-dominated problems using geodesic shooting

Hendrik Kleikamp*[1], Mario Ohlberger[1], and Stephan Rave[1]

[1]Institute for Analysis and Numerics, Mathematics Münster, University of Münster, Einsteinstrasse 62, 48149 Münster, Germany
{hendrik.kleikamp, mario.ohlberger, stephan.rave}@uni-muenster.de

Abstract

Model order reduction for parametrized hyperbolic or transport dominated problems typically suffers from a slowly decaying Kolmogorov N-width of the corresponding solution manifold [1, 3]. In this contribution we introduce a new approach for model order reduction of such problems based on techniques from diffeomorphic *image registration*. The *geodesic shooting* algorithm [2] computes diffeomorphic transformations of an underlying domain to match functions over the domain by integrating vector fields over time. The vector fields are determined in such a way that the time evolution of the diffeomorphism follows a geodesic in the diffeomorphism group. Therefore, the time evolution of the vector fields is already determined by the initial vector field. In our setting, the diffeomorphisms act on snapshot data of the considered problem. Due to the smoothness of the vector fields, it is possible to obtain efficient reduced order models in the space of vector fields [4]. In turn, the reduced space of vector fields (obtained via *proper orthogonal decomposition*) induces a set of diffeomorphisms which can be used to transform reference snapshots. The main idea of our approach is therefore to construct a reduced basis of vector fields that generates a set of diffeomorphisms using the geodesic shooting approach, and to finally transform reference snapshots using these diffeomorphisms. During the online phase, for a new parameter, a vector field in the reduced subspace is computed and the diffeomorphism is generated accordingly that transforms a reference snapshot into an approximation of the solution. The potential of the proposed method is shown by numerical examples such as a parametrized Burgers' equation.

Keywords: Nonlinear model order reduction, Parametrized hyperbolic equations, Diffeomorphic registration

References

[1] C. Greif, K. Urban (2019). *Decay of the Kolmogorov N-width for wave problems.* In *Applied Mathematics Letters*, 96:216–222.

[2] M. I. Miller, A. Trouvé, L. Younes (2006). *Geodesic shooting for computational anatomy.* In *Journal of Mathematical Imaging and Vision*, 24(2):209–228.

[3] M. Ohlberger, S. Rave (2016). *Reduced basis methods: Success, limitations and future challenges.* In *Proceedings of the Conference Algoritmy*, pages 1–12.

[4] J. Wang, W. Xing, R. M. Kirby, M. Zhang (2019). *Data-driven model order reduction for diffeomorphic image registration.* In *Information Processing in Medical Imaging*, pages 694–705, Cham. Springer International Publishing.

*The authors acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy EXC 2044 –390685587, Mathematics Münster: Dynamics–Geometry–Structure.

Gradient-preserving adaptive model order reduction of parametric conservative dynamical systems

Cecilia Pagliantini[1] and Federico Vismara[2]

[1]University of Pisa, Italy
[2]Eindhoven University of Technology, Netherlands
cecilia.pagliantini@unipi.it; f.vismara@tue.nl

Abstract

Model order reduction of parametric differential equations aims at constructing low-complexity high-fidelity surrogate models that allow rapid and accurate solutions under parameter variation. The development of reduced order models for conservative dynamical systems is challenged by several factors: (i) failing to preserve the geometric structure encoding the physical properties of the dynamics might lead to instabilities and unphysical behaviors of the resulting approximate solutions; (ii) the slowly decaying Kolmogorov n-width of transport-dominated and non-dissipative phenomena demands large reduced spaces to achieve sufficiently accurate approximations; and (iii) nonlinear operators require hyper-reduction techniques that preserve the gradient structure of the flow velocity. We will discuss how to address these aspects via structure-preserving nonlinear model order reduction. The gist of the proposed method is to adapt in time an approximate low-dimensional phase space endowed with the geometric structure of the full model and to ensure that the reduced flow retains the physical properties of the original model.

Keywords: Model order reduction, Structure-preserving numerical methods, Adaptive Discrete Empirical Interpolation

References

[1] C. Pagliantini, F. Vismara (2022). *Gradient-preserving hyper-reduction of nonlinear dynamical systems via discrete empirical interpolation.* arXiv e-print: arXiv:2206.01792.

Registration of coherent structures in bounded domains: mathematical analysis and application to model reduction

Tommaso Taddei* [1]

[1]IMB, UMR 5251, University of Bordeaux; Inria Bordeaux Sud-Ouest, Team MEMPHIS; 33400, Talence, France
tommaso.taddei@inria.fr

Abstract

We present a nonlinear registration-based model reduction procedure for rapid and reliable solution of parameterized two-dimensional steady conservation laws. This class of problems is challenging for model reduction techniques due to the presence of nonlinear terms in the equations and also due to the presence of parameter-dependent sharp gradient regions that cannot be adequately represented through linear approximation spaces.

Our approach builds on the following ingredients: (i) a general (i.e., independent of the underlying equation) registration procedure [1, 2] for the computation of a parametric mapping that tracks moving features of the solution field; (ii) an hyper-reduced least-squares Petrov-Galerkin reduced-order model for the rapid and reliable estimation of the solution field; (iii) a greedy procedure driven by a residual-based error indicator for efficient exploration of the parameter domain; and (iv) an adaptive mesh refinement technique for the definition of an accurate discretization for all parameter values.

We present results for a representative nonlinear problem in steady aerodynamics to demonstrate the effectiveness and the mathematical soundness of our methodology.

Keywords: model order reduction; parameterized hyperbolic conservation laws; nonlinear approximations.

References

[1] A. Ferrero, T. Taddei, L. Zhang (2022). *Registration-based model reduction of parameterized two-dimensional conservation laws*, Journal of Computational Physics, vol. 457.

[2] T. Taddei (2020). *A registration method for model order reduction: data compression and geometry reduction*, SIAM Journal on Scientific Computing, vol. 42(2).

*Work in collaboration with Nicolas Barral, Angelo Iollo and Ishak Tifouti (Inria Bordeaux).

Towards an Arbitrary-Lagrangian-Eulerian MOR framework for advection dominated problems: calibration, optimization and regression

Davide Torlo[1] and Monica Nonino[2]

[1]SISSA MathLab, SISSA, Trieste, 34136, Italy
[2]Fakultät für Mathematik, Universität Wien, 1090 Wien, Austria
davide.torlo@sissa.it; monica.nonino@univie.ac.at

Abstract

Classical model order reduction (MOR) techniques have always struggled to compress information for problems advecting steep features. Their linear nature does not allow to accelerate the slow decay of the Kolmogorov N-width of these problems. In recent years, many new nonlinear algorithms and frameworks have been presented to overcome this issue. In [1], a MOR technique was proposed for unsteady parametric advection-dominated scalar 1D hyperbolic problems, giving a complete offline and online description and showing time savings in the online phase. The key of the work consists of an arbitrary Lagrangian–Eulerian approach that modifies both the offline and online phases of the MOR process. The technique makes use of various algorithms such as Greedy, EIM, POD and multilayer perceptron. This allows for calibrating the advected features on the same position, strongly compressing the reduced spaces, and outperforming classical methods on many equations with nonlinear fluxes and with different boundary conditions.

We want to extend this framework to systems of equations with multiple traveling features. In particular, we have in mind a classical test in compressible flow: the Sod shock tube problem, where a shock, a contact and a rarefaction wave develop from the initial conditions. The geometrical transformations used in [1] need now to align more than just one feature. This raises various questions on the techniques to use to minimize the Kolmogorov N-width decay, on the regularity of the calibration map, and on the regression techniques to use for the calibration in the online phase. We try to study various methods, including some optimization strategies, POD-NN, multilayer perceptron, and similar, to answer such questions. The whole process tries not to be too problem-specific, but some bottlenecks quickly arise. We will show some very encouraging tests on a parametric Sod tube test problem.

Keywords: Model order reduction, POD-NN, advection dominated, Sod shock tube

References

[1] D. Torlo (2020). *Model reduction for advection dominated hyperbolic problems in an ALE framework: Offline and online phases.* arXiv preprint arXiv:2003.13735.

SUPG-stabilised Dynamical Low Rank Methods for Advection-Dominated Problems

Thomas Trigo Trindade [1] and Fabio Nobile [1]

[1]CSQI, EPFL
{thomas.trigotrindade, fabio.nobile}@epfl.ch

Abstract

The Streamline Upwind Petrov-Galerkin (SUPG) is a popular method to control the spurious oscillations that often arise in the numerical solution to advection-dominated problems when using the finite element method. The Dynamical Low Rank (DLR) approach consists in approximating the solution to a time-dependent random PDE by $u(t,x,\omega) \approx \sum_{i=1}^{R} U_i(t,x)Y_i(t,\omega)$, where both the physical basis $\{U_i(t,x)\}_{i=1}^{R}$ and the stochastic basis $\{Y_i(t,\omega)\}_{i=1}^{R}$ are dynamically evolved in time. As such, the standard DLR framework can be very well-suited to efficiently simulate the evolution of coherent features in transport problems, however it remains subject to spurious oscillations. In this work, we derive SUPG-stabilised Dynamical Low-Rank equations for advection-dominated problems. We investigate a class of time-marching schemes that allows to recover a variational formulation on a "skewed" testing space. This tool is used to derive norm-stability estimates of the numerical solution that are comparable to those of the full order model. We propose extensions of this method such as mean-stabilisation in the case of a transport term with small stochasticity. Numerical examples illustrate the effectiveness of the method.

Keywords: Dynamical Low-Rank Approximations, Petrov-Galerkin, Stabilisation of Advection-Dominated Problems

References

[1] Y. Kazashi, F. Nobile, and E. Vidličková (2021). *Stability properties of a projector-splitting scheme for dynamical low rank approximation of random parabolic equations*. Numerische Mathematik, 149, 973–1024.

MS12 - Structure-Preserving and Efficient Neural Networks for Scientific Machine Learning

Dynamic Neural Networks

Chinmay Datar[1, 2], Felix Dietrich[2], and Wil Schilders[1, 3]

[1]Institute of Advanced Study, Technical University of Munich, Germany
[2]Department of Computer Science, Technical University of Munich, Germany
[3]Department of Mathematics and Computer Science, Eindhoven University of Technology, Netherlands
{chinmay.datar, felix.dietrich}@tum.de; w.h.a.schilders@tue.nl

Abstract

Black-box machine learning models are often not interpretable. This limits their applicability in problems involving high-stake decisions [1], including problems in science and engineering. Moreover, in most deep learning applications, neural architecture search involves iterating over many different architectures, often resulting in substantial computational cost. In this work, we show how to construct interpretable Dynamic Neural Networks (DyNN) to simulate Linear-Time-Invariant (LTI) systems.

A dynamic neural network is a system of coupled Ordinary Differential Equations (ODEs) [2], [3]. The state of each neuron is a solution of a first or second order ODE. We show that DyNNs are interpretable, and describe how to construct their topology using properties of the underlying LTI system.

Firstly, to construct computationally efficient DyNNs with sparser connections, we propose a sequence of similarity transformations for LTI systems. In particular, we block-diagonalize the state matrix of the LTI system. We show how this block diagonal structure unravels a special structure in the topology of the corresponding DyNN. Secondly, we derive a mapping from the LTI system matrices to weights of the DyNN. One can compute the trainable parameters of the DyNN directly using this mapping, in a training-free manner. Moreover, one can precisely determine the number of neurons, number of layers and the connections between the neruons required to simulate the underlying LTI system using a DyNN.

As an example, we simulate an LTI system using a DyNN. An open and vital research direction is designing dynamic neural network architectures for non-linear dynamical systems. We demonstrate how to design DyNN architectures on some toy examples of non-linear systems.

Keywords: dynamic neural networks, linear-time-invariant systems, ordinary differential equations, interpretable artificial intelligence

References

[1] C. Rudin, (2019). *Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead.* Nature machine intelligence, 1(5), 206-215.

[2] P.B.L. Meijer, (1996). *Neural network applications in device and subcircuit modelling for circuit simulation.* Philips Electronics.

[3] W.H.A. Schilders, (2009). *Predicting the topology of dynamic neural networks for the simulation of electronic circuits.* Neurocomputing, 73(1-3), 127-132.

Learning a Mesh Motion Technique with Application to Fluid-Structure Interaction and Shape Optimization

Ottar Hellan*[1], Johannes Haubner[2], and Miroslav Kuchta†[1]

[1]Simula Research Laboratory, Oslo, Norway
[2]Institute of Mathematics and Scientific Computing, University of Graz, Austria
{hellanottar, miroslav}@simula.no; johannes.haubner@uni-graz.at

Abstract

Mesh degeneration is a bottleneck for fluid-structure interaction (FSI) simulations and for shape optimization via the method of mappings. In both cases, an appropriate mesh motion technique is required. The choice is typically based on heuristics, e.g., the solution operators of partial differential equations (PDE), such as the Laplace or biharmonic equation. Especially the latter, which shows good numerical performance for large displacements, is expensive. Moreover, from a continuous perspective, choosing the mesh motion technique is to a certain extent arbitrary and has no influence on the physically relevant quantities. Therefore, we consider approaches inspired by machine learning. We present a hybrid PDE-NN approach, where the neural network (NN) serves as parameterization of a coefficient in a second order nonlinear PDE. We ensure existence of solutions for the nonlinear PDE by the choice of the neural network architecture. In addition, we present an approach where a neural network is used as an additive correction to a Laplace equation extension. We assess the quality of the learned mesh motion techniques by applying them to a FSI benchmark problem.

Keywords: Fluid-structure interaction, shape optimization, neural networks, partial differential equations, hybrid PDE-NN, mesh moving techniques, data-driven approaches

References

[1] J. Haubner, M. Kuchta (2022). *Learning a Mesh Motion Technique with Application to Fluid-Structure Interaction and Shape Optimization.* arXiv:2206.02217.

*Ottar Hellan acknowledges support from the Research Council of Norway, grant 303362.
†Miroslav Kuchta acknowledges support from the Research Council of Norway, grant 303362.

Structure-preserving neural networks for coupled dissipative systems

Quercus Hernández[1], Alberto Badías[2], Francisco Chinesta[3], and Elías Cueto[1]

[1]Aragon Institute of Engineering Research (I3A), University of Zaragoza
[2]Higher Technical School of Industrial Engineering, Polytechnic University of Madrid
[3]ESI Chair at the PIMM Lab, Arts et Metiers Institute of Technology
{quercus, ecueto}@unizar.es; alberto.badias@upm.es; francisco.chinesta@ensam.eu

Abstract

The use of AI in engineering simulations has attracted important research activity as an intersection between physics, computer science, engineering and mathematics. Since the first machine learning-based models showed great performance in real world engineering simulations, the field has gained increased popularity and more complex architectures have emerged which overcome the limitations of black-box approaches. The use of inductive biases such as invariances and equivariances in the learning procedure has been proven not only to improve the global performance of the predictions but also to better extrapolate to data outside of the training samples. This is the case of the so-called structure-preserving deep learning, in which the predictions are forced to satisfy certain known basic physical laws acting as a strong topological inductive bias.

Common structure-preserving algorithms are the ones targeted for conservative phenomena in which the Hamiltonian potential function plays a central role. A variation of those algorithms recently proposed an extension to dissipative phenomena [1], which is based on including an extra metric term to the dynamics together with its respective potential function (entropy). This is called the GENERIC or metriplectic structure of the system, and forces the predictions to fulfil the laws of thermodynamics. However, these algorithms require the full description of the state variables of the dynamical system, which is not convenient if the computational resources are limited or only partial information is required or available.

To overcome those limitations, we propose a deep learning algorithm based on structure-preserving neural networks to learn open dissipative systems. Thus, the complete system is divided into different subdomains which are coupled via energy and entropy ports at each boundary. The resulting port-metriplectic neural network [2] is an extension of the port-Hamiltonian counterpart in conservative systems. The algorithm is presented in two different variations, depending on the application and known information of the complete system.

Keywords: Artificial Intelligence, Machine Learning, Port-metriplectic, Thermodynamics, GENERIC

References

[1] Q. Hernández, A. Badías, F. Chinesta, E. Cueto (2021). *Structure-preserving neural networks.* Journal of Computational Physics, 426, 109950.

[2] Q. Hernández, A. Badías, F. Chinesta, E. Cueto (2023). *Port-metriplectic neural networks: thermodynamics-informed machine learning of complex physical systems.* Computational Mechanics, 1-9.

A Generalized Framework of Neural Networks for Hamiltonian Systems

Philipp Horn[1], Veronica Saz Ulibarrena[2], Barry Koren[1], and Simon Portegies Zwart[2]

[1]Centre for Analysis, Scientific Computing and Applications (CASA),
Eindhoven University of Technology, The Netherlands
[2]Leiden Observatory, Leiden University, The Netherlands
{p.horn, b.koren}@tue.nl; {ulibarrena, spz}@strw.leidenuniv.nl

Abstract

When solving Hamiltonian systems using numerical integrators, preserving the symplectic structure is crucial [1]. At the same time, solving chaotic problems requires integrators to approximate the trajectories with extreme precision. This can be very computationally expensive. However, for example in [2] it was shown that a neural network can be a viable alternative to numerical integrators. Offering high accuracy solutions for the chaotic N-body problem many orders of magnitudes faster.

To understand when it is useful to add physics constraints into neural networks, we analyze three well-known neural network topologies that include a symplectic structure inside the NN architecture [3, 4]. Between these neural network topologies many similarities can be found [5]. This allows us to formulate a generalized framework for these topologies. With the new framework, we can find novel topologies by transitioning between the established ones.

We compare these new Generalized Hamiltonian Neural Networks (GHNN) against the already established SympNets and HénonNets and physics-unaware multilayer perceptrons. This comparison is performed with data from a pendulum, a double pendulum and a gravitational three-body problem. A special focus lies on the capability of the neural networks to generalize outside the training data. We found that the GHNN outperforms all other neural network architectures.

Keywords: Hamiltonian Systems, Scientific Machine Learning, Structure-Preserving Computing

References

[1] E. Hairer, C. Lubich and G. Wanner (2006). Geometric Numerical Integration, Springer.

[2] P.G. Breen, C.N. Foley, T. Boekholt, S. Portegies Zwart (2020). *Newton versus the machine: solving the chaotic three-body problem using deep neural networks.* Monthly Notices of the Royal Astronomical Society, Vol. 494, 2465–2470.

[3] Z. Chen, J. Zhang, M. Arjovsky and L. Bottou (2020). *Symplectic recurrent neural networks.* In *8th International Conference on Learning Representations*, ICLR.

[4] P. Jin, Z. Zhang, A. Zhu, Y. Tang and G.E. Karniadakis (2020). *SympNets: Intrinsic structure-preserving symplectic networks for identifying Hamiltonian systems.* Neural Networks, Vol. 132, 166–179.

[5] P. Horn, V. Saz Ulibarrena, B. Koren and S. Portegies Zwart (2022). *Structure-Preserving Neural Networks for the N-body Problem. ECCOMAS.*

Preserving physical-invariances in the closure of Reynolds-averaged Navier-Stokes equations with neural-networks

Davide Oberto[1], Maria Strazzullo[1], and Stefano Berrone[1]

[1]Department of Mathematical Sciences, Politecnico di Torino
{davide.oberto, maria.strazzullo, stefano.berrone}@polito.it

Abstract

Reynolds-averaged Navier-Stokes (RANS) equations are obtained by averaging procedure from the classic Navier-Stokes equations for incompressible flows to reduce the computational effort. RANS equations read

$$\begin{cases} \nabla \cdot \mathbf{u} = 0 \\ \dfrac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} = -\nabla p - \nabla \cdot \boldsymbol{\tau}, \end{cases}$$

where $\mathbf{u}$ and p are the averaged velocity and pressure fields respectively, ν is the kinematic viscosity and τ is the Reynolds stress tensor (RST). The latter is a symmetric tensor that needs to be modeled to close the RANS equations. Classically, this is performed by deducing additional partial differential equations obtained heuristically through physical arguments. While these models have decades of history and are well-established, they can be highly inaccurate for some types of flow.

Recently, several studies took advantage of machine learning techniques to learn the mapping between the averaged fields and the RST to increase the accuracy of RANS models by using high-fidelity data (i.e. data coming directly from the Navier-Stokes equations). In this framework, data-driven models should satisfy the same invariances properties of the physical system they are describing.

In this talk, we present a data-driven model that predicts the divergence of the RST and guarantees both Galilean and frame-reference rotation invariances by construction. Analogously to [1], a constitutive assumption of the divergence of the RST from mean fields is derived. This hypothesis is fundamental to obtain the inputs of the data-driven model and the structural vector basis used to expand the divergence of the RST. The obtained neural network predicts the coefficients of the linear combination and it is called vector basis neural network (VBNN). We also tackle the problem of bad-conditioning of the data-driven RANS equations by defining a neural network that predicts a turbulent viscosity that can be treated implicitly in the RANS system.

Numerical experiments are presented to show the improvements of our approach compared to standard RANS models.

Keywords: Reynolds-averaged Navier-Stokes equations, data-driven turbulence modelling

References

[1] J. Ling, A. Kurzawski, J. Templeton (2016). *Reynolds averaged turbulence modelling using deep neural networks with embedded invariance*, Journal of Fluid Mechanics, vol. 807, pp. 155-166.

[2] S. Berrone, D. Oberto (2022). *An invariances-preserving vector basis neural network for the closure of Reynolds-averaged Navier–Stokes equations by the divergence of the Reynolds stress tensor*. Physics of Fluids, 34 (9): 095136.

Learning a Lattice Boltzmann Collisional operator using Physics Constrained Neural Networks

Giulio Ortali[1], Alessandro Corbetta[1], Nicola Demo[2], Alessandro Gabbana[1], Gianluigi Rozza[2], and Federico Toschi[1]

[1]Eindhoven University of Technology, Eindhoven, The Netherlands
[2]Scuola Internazionale di Studi Superiori Avanzati (SISSA), Trieste, Italy
{g.ortali, a.corbetta, a.gabbana, f.toschi}@tue.nl; {grozza, ndemo}@sissa.it

25 Apr 2023

Abstract

In this work we explore the possibility of using Artificial Neural Networks for the task of learning novel collisional operators for the Lattice Boltzmann Method (LBM)[1].

The LBM is a broad class of computational methods, originating from the kinetic theory of gases, able to accurately model the dynamics of fluid flows at the mesoscopic level.

The fluid flow is described by the dynamics of a set of discrete particle distribution functions (populations) following the stream and collide paradigm, in which at each time step populations hop from lattice-site to lattice-site and then incoming populations collide among one another.

We take into consideration the problem of learning the single relaxation time BGK collision operator using data from 3D turbulent flows. We show that in order to achieve accuracy and stability it is crucial to supply the Neural Network with hard constraints on the conservation of mass and momentum, and to carefully design the training set.

We also present early results in the direction of learning a correction to the BGK collision operator that accounts for subgrid effects in under-resolved Turbulent flows.

Keywords: Machine Learning, Fluid Dynamics, Lattice Boltzmann Method, Turbulence

References

[1] S. Succi. *The Lattice Boltzmann Equation*. Oxford University Press

[2] A. Corbetta, A. Gabbana, V. Gyrya, D. Livescu, J. Prins, F. Toschi (2023). *Toward learning Lattice Boltzmann collision operators*. Eur. Phys. J. E 46: 10.

Hybrid integration of the gravitational N-body problem with Artificial Neural Networks

Veronica Saz Ulibarrena[1], Philipp Horn[2], Simon Portegies Zwart[1], Elena Sellentin[1], Barry Koren[2], and Maxwell X. Cai[1]

[1]Leiden Observatory, Leiden University, the Netherlands
[2]Eindhoven University of Technology, the Netherlands
{ulibarrena, spz, sellentin}@leidenuniv.nl; {p.horn, b.koren}@tue.nl;
maxwell.cai@intel.com

Abstract

The complexity of the gravitational N-body problem scales with N^2 according to Newton's equation of gravitation [1]. This leads to the need of larger computational resources as the number of bodies increases. In order to alleviate this problem, we use Artificial Neural Networks (ANNs) to substitute expensive parts of the integration of a planetary system. We use the integrator proposed by Wisdom and Holman [2], where the keplerian part of the integration, which can be solved analytically, is separated from the N^2 part, which we solve using neural networks.

We compare the performance of a Hamiltonian Neural Network [3] which includes physics constraints into its architecture with a conventional Deep Neural Network. We study the advantages and limitations of the two topologies and compare their performance with the baseline Wisdom-Holman integrator.

When using neural networks to substitute parts of the integrator, the problem of accumulation of errors becomes crucial; if the neural network is not able to provide a solution within a certain accuracy, error propagation leads to unphysical solutions. To mitigate this problem, we develop a hybrid integrator that chooses between the network's prediction and the numerical computation if the first is not accurate enough. With this hybrid approach, we show that for a number of minor bodies ≥ 60, using ANNs improves the computational cost of the simulation while allowing for an accurate reproduction of the trajectory of the bodies.

Keywords: Machine Learning, Gravitational N-body problem, Numerical integrator, Planetary systems, Physics-aware Neural Networks, Hybrid method

References

[1] I. Newton (1999). *The Principia: mathematical principles of natural philosophy.* Univ of California Press.

[2] J. Wisdom, M. Holman (1991). *Symplectic maps for the n-body problem.* The Astronomical Journal, Vol. 102, 1528–1538.

[3] S. Greydanus, M. Dzamba, J. Yosinski (2019). *Hamiltonian neural networks.* Advances in neural information processing systems, Vol. 32.

[4] M. X. Cai, S. Portegies Zwart, D. Podareanu (2021). *Neural symplectic integrator with hamiltonian inductive bias for the gravitational n-body problem.* arXiv preprint arXiv:2111.15631.

On the influence of hyperparameters on the convergence of adaptive gradient methods

Lu Xia[1], Stefano Massei[2], and Michiel E. Hochstenbach[1]

[1]Department of Mathematics and Computer Science, Eindhoven University of Technology, Eindhoven, The Netherlands
[2]Department of Mathematics, Università di Pisa, Pisa, Italy
{l.xia1, m.e.hochstenbach}@tue.nl; stefano.massei@unipi.it

Abstract

First-order optimization methods such as stochastic gradient descent (SGD) are widely applied in the training of neural networks due to their efficiency. However, the constant learning stepsize along each gradient coordinate often restricts the convergence speed of SGD. Therefore, numerous adaptive gradient methods have been proposed to achieve faster convergence. Among them, Adam [1] is the most popular one due to its robustness in choosing hyperparameters. However, the nonuniform scaling of the gradient may cause worse performances on the unseen data, a phenomenon is often called *poor generalization*. Many methods have emerged to bridge this generation gap between adaptive and non-adaptive gradient methods; see, e.g., SWATS [2], AdaBound [3], and AdaBelief [4]. These optimizers update the exponential moving average of the gradient using different second raw moment estimates (uncentred variances).

In many studies [1, 4, 5], the major objective is to assess the convergence of the algorithm, either by ensuring that the algorithm regret is of the order $\mathcal{O}(\sqrt{K})$, or by showing that $\lim_{K\to\infty} E\,[\,\|\nabla f(\mathbf{x}^{(K)})\|\,] = 0$. There is still room for improvement in understanding how the hyperparameters of the optimizers affect the convergence. In this study, we theoretically investigate the influence of hyperparameters on the convergence of adaptive gradient methods. We prove that the Adam-type optimizers have linear convergence as the vanilla gradient descent method under the Polyak–Łojasiewicz (PL) inequality. We compare both theoretically and numerically the speed of convergence when changing the hyperparameters, β_2 and the learning rate, for Adam and its variants.

Keywords: adaptive gradient methods, convergence analysis

References

[1] D. P. Kingma, J. Ba (2015). *A Method for Stochastic Optimization.* In *Proc. ICLR 2015.*

[2] N. S. Keskar, R. Socher (2017). *Improving generalization performance by switching from Adam to SGD.* ArXiv preprint: 1712.07628.

[3] L. Luo, Y. Xiong, Y. Liu, X. Sun (2019). *Adaptive Gradient Methods with Dynamic Bound of Learning Rate.* In *Proc. ICLR 2019.*

[4] J. Zhang, T. Tang, Y. Ding, S. C. Tatikonda, N. Dvornek, X. Papademetris, J. Dunca (2020). *Adabelief optimizer: Adapting stepsizes by the belief in observed gradients.* In *Proc. NeurIPS 2020.*

[5] M. Zaheer, S. Reddi, D. Sachan, S. Kale, S. Kumar (2018). *Adaptive Methods for Nonconvex Optimization.* In *Proc. NeurIPS 2018.*

MS13 - Nonlinear problems in fluid mechanics and related problems

Convergence Analysis for Pseudomonotone Parabolic Problems

Michael Růžička[1] and Alex Kaltenbach[2]

[1]Department of Applied Mathematics, University of Freiburg
[2]Institute of Mathematics, Technical University of Berlin
rose@mathematik.uni-freiburg.de; kaltenbach@math.tu-berlin.de

Abstract

In this talk, we present an abstract framework, which provides convergence of fully discrete approximations, using a nonconforming spatial approximation, to weak solutions of abstract pseudomonotone problems. The method is illustrated on a Local Discontinuous Galerkin (LDG) approximation both of the steady and unsteady p-Navier–Stokes system.

Keywords: Convergence of fully discrete approximations, Local Discontinuous Galerkin, p-Navier–Stokes system.

References

[1] A. Kaltenbach and M. Růžička (2023). *A Local Discontinuous Galerkin approximation for the p-Navier-Stokes system, Part I: Convergence analysis*, SIAM J. Num. Anal., **61**:1613–1640.

[2] A. Kaltenbach and M. Růžička (2023). *Analysis of a fully-discrete, non-conforming approximation of evolution equations and applications*, Math. Models Methods Appl. Sci., **33**:1147–1192.

Relaxed Kacanov scheme for the p-Laplacian

Anna Balci*[1], Lars Diening[1], and Johannes Storn[1]

[1]Department of Mathematics, Bielefeld University
{akhripun, jstorn}@math.uni-bielefeld.de; lars.diening@uni-bielefeld.de

Abstract

We introduce a globally convergent relaxed Kacanov scheme for the computation of the discrete minimizer to the p-Laplace problem with large p. The iterative scheme is easy to implement since each iterate results only from the solve of a weighted, linear Poisson problem. It neither requires an additional line search nor involves unknown constants for the step length. The rate of convergence is independent of the underlying mesh. Using duality approach we are able to obtain the results for large p. This complements the previous result for $p < 2$ obtained in [2]. The talk is based on the results with Diening and Storn, see [1].

Keywords: p-laplace, relaxed Kacanov scheme

References

[1] A. Balci, L. Diening, J. Storn (2022). *Relaxed Kacanov scheme for the p-Laplacian with large p.*

[2] L. Diening, M. Fornasier, R. Tomasi, M. Wank (2020). *A relaxed Kačanov iteration for the p-Poisson problem.* Numer. Math, 145, 1–34, https://doi.org/10.1007/s00211-020-01107-1.

*Anna Balci thans DFG for the support

Structure preserving finite element schemes for a non-Newtonian flow

Gabriel R. Barrenechea*[1], Tristan Pryer[2], and Emmanuil Georgoulis[3]

[1]University of Strathclyde, Glasgow, UK
[2]University of Bath, Bath, UK
[3]Heriot-Watt University, Edinburgh, UK, and NTUA Athens, Greece
gabriel.barrenechea@strath.ac.uk

Abstract

We propose a finite element discretisation of a three-dimensional non-Newtonian flow whose dynamics are described by an Upper Convected Maxwell model. The scheme preserves structure in the sense that the velocity is divergence-free and the overall discretisation is energy consistent with the underlying problem. We investigate the problem's complexity and devise relevant timestepping strategies for effcient solution realisation. We showcase the method with several numerical experiments, confirm the theory and demonstrate the efficiency of the scheme.

Keywords: non-Newtonian flow, upper convected Maxwell, Capillarity

*This work has been partially funded by the Leverhulme Trust through the Research Project Grant No. RPG-2021-238.

Boundary regularity for nonlinear systems depending on the symmetric gradient

Linus Behn[1] and Lars Diening[1]

[1]Faculty of Mathematics, Bielefeld University
linus.behn@math.uni-bielefeld.de; lars.diening@uni-bielefeld.de

Abstract

We study the global regularity of solutions u of nonlinear systems depending on the symmetric gradient $\varepsilon u := \frac{1}{2}(\nabla u + \nabla^T u)$. For example, this includes the symmetric p-Laplace system $\operatorname{div}(|\varepsilon u|^{p-2}\varepsilon u) = 0$ for all $1 < p < \infty$. Our result extends the prior results of Seregin and Shilkin [3] and Berselli and Růžička [1, 2] by considering more general Orlicz-growth conditions.

Keywords: symmetric gradient, boundary regularity, Orlicz growth, p-Laplace system, non-linear elasticity

References

[1] L. C. Berselli, M. Růžička (2022). *Natural second-order regularity for parabolic systems with operators having (p, δ)-structure and depending only on the symmetric gradient.* Calc. Var. PDE 61.

[2] L. C. Berselli, M. Růžička (2020). *Global regularity for systems with p-structure depending on the symmetric gradient.* Adv. Nonlinear Anal. 9.

[3] G. A. Seregin, T. N. Shilkin (1997). *Regularity of minimizers of some variational problems in plasticity theory.* Zap. Nauchn. Sem. S.-Peterburg. Otdel. Mat. Inst. Steklov. (POMI) 243.

Quasioptimal nonconforming discretisations of the p-Laplace equation

Jan Blechta[1], Alexei Gazca[2], Alex Kaltenbach[2], and Michael Růžička[2]

[1]Faculty of Mathematics and Physics, Charles University
[2]Mathematical Institute, University of Freiburg
{alexei.gazca, rose, alex.kaltenbach}@mathematik.uni-freiburg.de;
blechta@karlin.mff.cuni.cz

Abstract

The classical arguments for obtaining error estimates for Finite Element discretisations of elliptic problems lead to more restrictive assumptions on the regularity of the exact solution when applied to nonconforming methods. The work of Gudi [1] first got around this obstacle by employing tools from a posteriori error analysis; however, the estimates obtained in [1] are not truly minimal in its regularity assumptions, since a data oscillation term still appears in the error estimate. In a series of works [2, 3, 4], Veeser and Zanotti were able to characterise genuinely quasioptimal discretisations of linear symmetric elliptic problems, i.e. those in which the discretisation error is equivalent to the best approximation error; in particular, they showed that a necessary condition is that the method be well-defined for forcing terms in the dual space $H^{-1}(\Omega)$, and they achieve this by constructing an appropriate smoothing operator E_h that maps test functions into a conforming subspace. In the same spirit (but working with the equation directly, since the Hilbert structure is not available), we derive for the first time error estimates for nonlinear problems with a p-structure that only assume the natural $W^{1,p}$-regularity of the exact solution, and which do not contain any data oscillation terms.

Keywords: Discontinuous Galerkin, minimal regularity, p-Laplace, quasioptimality

References

[1] T. Gudi (2010). *A new error analysis for discontinuous finite element methods for linear elliptic problems.* Math. Comp., 79:2169-2189.

[2] A. Veeser, P. Zanotti (2018). *Quasi-optimal nonconforming methods for symmetric elliptic problems. I–Abstract theory.* SIAM J. Numer. Anal., 56(3):1621-1642.

[3] A. Veeser, P. Zanotti (2019). *Quasi-optimal nonconforming methods for symmetric elliptic problems. II–Overconsistency and classical nonconforming elements.* SIAM J. Numer. Anal., 57(1):266-292.

[4] A. Veeser, P. Zanotti (2018). *Quasi-optimal nonconforming methods for symmetric elliptic problems. III–Discontinuous Galerkin and other interior penalty methods.* SIAM J. Numer. Anal., 56(5):2871-2894.

A modified Kačanov iteration scheme for the numerical solution of quasilinear elliptic diffusion equations

Pascal Heid[1] and Thomas P. Wihler[2]

[1]Department of Mathematics, Technical University of Munich
[1]Munich Center for Machine Learning
[2]Mathematics Institute, University of Bern
pascal.heid@ma.tum.de; thomas.wihler@unibe.ch

Abstract

Kačanov's method is an efficient iterative nonlinear solver for a class of quasilinear elliptic diffusion equations. However, to guarantee the convergence to a solution of the given problem, the classical theorem requires the diffusion coefficient to be monotonically decreasing. In particular, in the context of fluid flows, convergence is only assured for shear-thinnig fluids. In this talk, we introduce a modified Kačanov method, which allows for adaptive damping, and, thereby, to derive a new convergence analysis, which no longer requires the standard monotonicity assumption. We further present two different adaptive strategies for the practical selection of the damping parameter. Finally, the performance of the modified scheme is demonstrated with some numerical experiments in the context of finite element discretisations.

Keywords: Quasilinear elliptic PDEs, Kačanov's method, adaptive damping

References

[1] P. Heid, T. P. Wihler (2022). *A modified Kačanov iteration scheme with application to quasilinear diffusion models.* ESAIM: M2AN, 56, 433-450.

Convergence rate for a space-time discretization for incompressible generalized Newtonian fluids: the Dirichlet problem for $p > 2$

Mirjam Hoferichter[1] and Michael Růžička[2]

[1]Institute of Applied Mathematics, University of Freiburg, Germany
mirjam.hoferichter@mathematik.uni-freiburg.de
[2]Institute of Applied Mathematics, University of Freiburg, Germany
rose@mathematik.uni-freiburg.de

Abstract

We present convergence rates for solutions of the equations describing the unsteady motion of incompressible shear-thickening fluids with homogeneous Dirichlet boundary conditions. A full space-time semi-implicit scheme based on a backward Euler scheme in time and a Finite Element discretization in space is considered. Berselli and Růžička were the first to obtain error estimates without the introduction of intermediate semi-discrete problems in [1] which strongly inspired the presented proof.
The main novelty is the consideration of the shear-thickening case $p > 2$ for which convergence rates have, up until now, only been proven for the generalized Stokes equation using intermediate semi-discrete problems (see [2]).

Keywords: Space-time descretization, Generalized Newtonian fluids, Error analysis, shear-thickening

References

[1] L. Berselli, M. Růžička (2021). *Optimal error estimate for a space-time discretization for incompressible generalized Newtonian fluids: the Dirichlet problem.* Partial Differ. Equ. Appl., 2.4, 1–23.

[2] S. Eckstein, M. Růžička (2018). *On the full space-time discretization of the generalized Stokes equations: The Dirichlet case.* SIAM J. Numer. Anal., 56.4, 2234–2261.

Numerical investigation of blood flows with general boundary conditions

Jaroslav Hron*[1] and Jana Brunátová[1]

[1]Faculty of Mathematics nad Physics, Charles University, Prague
jaroslav.hron@mff.cuni.cz

Abstract

Most studies of patient-specific blood flow models prescribe a no-slip boundary condition at the walls. Although its implementation is straightforward, its validity at the blood-vessel wall interface is questionable. It has been suggested in Nubar1971 that a slip boundary condition can be considered for blood flow in certain situations. In [**nolte2019**], the slip boundary condition is used to compensate for geometry inaccuracies in patient-specific blood flow simulations.

We will discuss the combination of a non-Newtonian blood viscosity model with a Navier-type slip boundary condition, which assumes a linear proportionality between the tangential part of the wall velocity and the shear stress using an additional parameter. We incorporate the slip condition into a weak formulation using Nitsche method, [**Chabiniok2021**, **Chabiniok2022**]. We then discuss some implementation issues associated with its discretization using the finite element method and the efficient numerical solution of the resulting nonlinear system.

Keywords: Navier-Stokes equations, slip boundary condition, blood flow

*The work was supported by the Ministry of Health of the Czech Republic, grant nr. NU22-08-00124

Error analysis for a local discontinuous Galerkin approximation for systems of p-Navier–Stokes type

Alex Kaltenbach[1] and Michael Růžička[2]

[1]Institute of Mathematics, Technical University of Berlin
[2]Department of Applied Mathematics, University of Freiburg
kaltenbach@math.tu-berlin.de; rose@mathematik.uni-freiburg.de

Abstract

In this talk, we propose a Local Discontinuous Galerkin (LDG) approximation for systems of p-Navier–Stokes type involving a new numerical flux in the stabilization term and a new discretization of the convective term. A priori error estimates are derived for the velocity, which are optimal for all $p > 2$ and $\delta \geq 0$. A new criterion is presented that yields a priori error estimates for the pressure, which are optimal for all $p > 2$ and $\delta \geq 0$.

Keywords: Local Discontinuous Galerkin, p-Navier–Stokes system, a priori error analysis

References

[1] A. Kaltenbach, M. Růžička (2023). *A Local Discontinuous Galerkin approximation for the p-Navier-Stokes system, Part I: Convergence analysis*, SIAM J. Num. Anal., accepted.

[2] A. Kaltenbach, M. Růžička (2023). *A Local Discontinuous Galerkin approximation for the p-Navier-Stokes system, Part II: Convergence rates for the velocity*, SIAM J. Num. Anal., accepted.

[3] A. Kaltenbach, M. Růžička (2023). *A Local Discontinuous Galerkin approximation for the p-Navier-Stokes system, Part III: Convergence rates for the pressure*, SIAM J. Num. Anal., accepted.

Pressure robust discretisations of the nonlinear Stokes equations

Christian Kreuzer[1], Lars Diening[2], Adrian Hirn[3], and Pietro Zanotti[4]

[1]Fakultät für Mathematik, TU Dortmund University
[2]Fakultät für Mathematik, Universität Bielefeld
[3]Faculty Mechanical and Systems Engineering, Esslingen University
[4]Dipartimanto di Matematica, Universita di Pavia
christian.kreuzer@tu-dortmund.de; lars.diening@uni-bielefeld.de;
Adrian.Hirn@hs-esslingen.de; pietro.zanotti@unipv.it

Abstract

In standard finite element discretisations of power law Stokes problems

$$-\operatorname{div}|\nabla u|^{r-2}\nabla u + \nabla p = f, \qquad -\operatorname{div} u = 0,$$

for certain ranges of the exponent r, suboptimal convergence rates are observed; see [1, 2]. For example, using the mini element for powers $r > 2$, convergence rates $r'/2$ with the dual exponent $r' = r/(r-1)$ are proved, which are suboptimal due to $r'/2 < 1$ in this case. Numerical results confirm the theoretical rates and thus show that the suboptimality is not just a technical artefact [1]. This can be explained as follows: The nonlinear constitutive law acts on a subspace subject to the linear divergence constraint with corresponding Lagrange multiplier, the fluid pressure. Consequently, the natural error measures for the velocity and pressure are the quasi-norm energy distance and the $L^{r'}$ norm, respectively. The suboptimal rates result now from the interaction of the velocity and the pressure error together with some missmatch of their respective error measures.

In a series of papers, we have recently developed together with Pietro Zanotti and Rüdiger Verfürth, pressure robust and quasi optimal variants of some standard Stokes discretisations; see e.g. [3] Here one main feature is that the velocity error is fully decoupled from the pressure. We shall demonstrate for the Crouzeix-Raviart first order velocities with piecewise constant pressure, that the developed pressure robust techniques can be used to remedy the suboptimal approximation results for nonlinear Stokes problems. In particular, we prove first order convergence of the velocity error in the quasi-norm independently of the exponent r.

If time permits, we conclude the talk by extending the ideas to construct quasi-optimal and pressure robust quadratic velocity approximations in 2 dimensions.

Keywords: Nonlinear Stokes equations, Pressure robust methods, Quasi-optimality

References

[1] L. Belenki, L. Berselli, L. Diening, M. Růžička (2012). *Isogeometric analysis: approximation, stability and error estimates for h-refined meshes.* SIAM J. Numer. Anal., 50(2), 373–397.

[2] A. Hirn (2013). *Approximation of the p-Stokes Equations with Equal-Order Finite Elements*, Journal of Mathematical Fluid Mechanics, 15(1), 65-88.

[3] C. Kreuzer, R. Verfürth, P. Zanotti (2021). *Quasi-Optimal and Pressure Robust Discretizations of the Stokes Equations by Moment- and Divergence-Preserving Operators*, Comput. Methods Appl. Math., 21(2), 423–443.

Finite element approximation for fluids with non-standard boundary conditions

Alexei Gazca Orozco[1], Erika Maringová [2], and Tabea Tscherpel[3]

[1]Mathematical Institute, Albert Ludwigs University of Freiburg, Germany
[2]Institute of Science and Technology Austria (ISTA), Austria
[3]Department of Mathematics, TU Darmstadt, Germany
alexei.gazca@mathematik.uni-freiburg.de; erika.maringova@ist.ac.at;
tscherpel@mathematik.tu-darmstadt.de

Abstract

The flow of incompressible non-Newtonian fluids is determined by non-linear constitutive relation between the stress tensor and the strain rate. Besides this, many non-Newtonian fluids also exhibit complex behaviour at the boundary. Phenomena such as slip, stick-slip and dynamical boundary conditions are typical examples.

Existence of weak solutions for the incompressible fluid flow subject to such boundary conditions is proved in [1]. For the numerical approximation with finite elements one has to circumvent the so-called Babuška paradox [2]. This refers to the fact, that when imposing inhomogeneous boundary conditions strongly, the approximate solutions may converge to a function that does not satisfy the boundary conditions. For this reason we employ the Nitsche penalisation approach, cf. [3]. By this means, for polytopal domains and certain mixed finite element spaces we investigate convergence properties of the approximate solutions.

Keywords: non-Newtonian fluids, boundary conditions, Nitsche method

References

[1] A. Abbatiello, M. Bulíček, Maringová (2021). *On the dynamic slip boundary condition for Navier-Stokes-like problems*. Math. Models Methods Appl. Sci. 31, no. 11, 2165–2212.

[2] R. Verfürth (1985). *Finite element approximation of steady Navier-Stokes equations with mixed boundary conditions*. RAIRO Modél. Math. Anal. Numér. 19, no. 3, 461–475.

[3] I. G. Gjerde, L. R. Scott (2022). *Nitsche's method for Navier-Stokes equations with slip boundary conditions*. Math. Comp. 91, no. 334, 597–622.

Temporal regularity of power-law fluids under stochastic perturbations

Jörn Wichmann*[1]

[1]School of Mathematics, Monash University
Joern.Wichmann@monash.edu

Abstract

Humans have always been interested in fluids. However, many interesting aspects have not been understood yet. In this talk we focus on regularity results for power-law fluids in the regime of laminar flow. These are modelled by the p-Stokes system.

Already in the absence of turbulence, additional difficulties arise through the non-linear structure of the system as well as the low regularity of the stochastic perturbation. We will elaborate on the difficulties and try to build up an intuition on what regularity is natural. Finally, we present the temporal regularity results and give an application of the natural regularity within the development of numerical algorithms.

Keywords: Power-law fluids, SPDEs, Strong solutions, Regularity

*Author 1 thanks someone.

MS14 - Goal-oriented Error Estimation and Adaptivity

Goal-oriented multirate techniques for coupled flow and transport and their challenges

Marius P. Bruchhäuser[1], Markus Bause[1], and Mathias Anselmann[1]

[1]Faculty of Mechanical and Civil Engineering, Helmut Schmidt University Hamburg
{bruchhaeuser, bause, anselmann}@hsu-hamburg.de

Abstract

The efficient numerical approximation of multi-physics and multi-scale problems is associated with an ever-increasing complexity. This increases even further if one of the subproblems is additionally assumed to be convection-dominated. Challenges include, inter alia, different characteristic time scales, different characteristic spatial scales by means of layers and sharp moving fronts, and thus an efficient handling of the underlying discretization parameters in space and time likewise. In order to increase numerical efficiency, we present a cost-efficient space-time adaptive algorithm based on the Dual Weighted Residual (DWR) method applied to a coupled model problem of flow and convection-dominated transport. Here, the transport problem is modeled by a convection-diffusion equation, whereas the flow problem is modeled by a viscous time-dependent Stokes flow problem. Consistent with an underlying goal functional, local error indicators manage the adaptive mesh refinement process automatically by marking the respective cells in space and time. The algorithm includes a multirate approach using different time step sizes adapted to the dynamics and characteristic scales of the respective subproblems. Moreover, the interaction of goal-oriented error control and stabilization techniques is analyzed. In numerical examples, we show robustness and efficiency of the underlying algorithm and demonstrate the importance of stabilization in a strongly convection-dominated case. Finally, the efficient solution of the algebraic systems with block structure of growing complexity for higher order polynomial degrees in time is briefly addressed. The potential of a flexible geometric multigrid preconditioner is illustrated.

Keywords: Coupled Problems, Space-Time Adaptivity, Goal-Oriented A Posteriori Error Control, Dual Weighted Residual Method, SUPG Stabilization, Multirate, Cost-Efficiency, Geometric Multigrid Method

References

[1] M. P. Bruchhäuser, M. Bause (2022). *A cost-efficient space-time adaptive algorithm for coupled flow and transport*. Comput. Methods Appl. Math., accepted, 1–29.

[2] M. Anselmann, M. Bause (2023). *A geometric multigrid method for space-time finite element discretizations of the Navier–Stokes equations and its application to 3d flow simulation*. ACM Trans. Math. Softw., 49(1), 1–25.

[3] M. P. Bruchhäuser, U. Köcher, M. Bause (2022). *On the implementation of an adaptive multirate framework for coupled transport and flow*. J. Sci. Comput., 93(59).

[4] M. P. Bruchhäuser (2022). *Goal-oriented space-time adaptivity for a multirate approach to coupled flow and transport*. Ph.D. thesis, Helmut-Schmidt-University/University of the Federal Armed Forces Hamburg. DOI: 10.24405/14380

[5] U. Köcher, M. P. Bruchhäuser, M. Bause (2019). *Efficient and scalable data structures and algorithms for goal-oriented adaptivity of space–time FEM codes*. Software X, 10:100239.

Rate-optimal goal-oriented adaptive FEM for semilinear elliptic PDEs

Roland Becker[1], Maximilian Brunner[2], Michael Innerberger[2], Jens Markus Melenk[2], and Dirk Praetorius[2]

[1]Université de Pau et des Pays de l'Adour, IPRA-LMAP, France
[2]TU Wien, Institute of Analysis and Scientific Computing, Austria
maximilian.brunner@asc.tuwien.ac.at

Abstract

The talk presents some results of our recent works [1, 2]: For a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ and given $f, g \in \mathrm{L}^2(\Omega)$, we aim to approximate the linear goal quantity

$$G(u^\star) := \int_\Omega g\, u^\star \,\mathrm{d}x$$

where $u^\star \in \mathrm{H}^1_0(\Omega)$ is the weak solution of the semilinear elliptic PDE

$$-\mathrm{div}(\boldsymbol{A}\nabla u^\star) + b(u^\star) = f \quad \text{in } \Omega \quad \text{subject to} \quad u^\star = 0 \quad \text{on } \partial\Omega. \tag{1}$$

Here, the diffusion matrix $\boldsymbol{A} \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$ is uniformly positive definite, and the smooth nonlinearity $b(\,\cdot\,)$ is monotone and satisfies certain growth conditions. For a conforming FEM subspace $\mathcal{X}_H \subset \mathrm{H}^1_0(\Omega)$, the discrete formulation of the *primal problem* (1) reads: Find $u^\star_H \in \mathcal{X}_H$ such that

$$\langle \boldsymbol{A}\nabla u^\star_H, \nabla v_H\rangle + \langle b(u^\star_H), v_H\rangle = \langle f, v_H\rangle \quad \text{for all } v_H \in \mathcal{X}_H, \tag{2}$$

where $\langle v, w\rangle := \int_\Omega v\, w \,\mathrm{d}x$ denotes the $\mathrm{L}^2(\Omega)$-scalar product.

We approximate $G(u^\star)$ by means of the computable quantity $G(u^\star_H)$. The optimal error control of the goal error $G(u^\star) - G(u^\star_H)$ involves the *(practical) dual problem*: Find $z^\star[u^\star_H] \in \mathrm{H}^1_0(\Omega)$ such that

$$\langle \boldsymbol{A}\nabla z^\star[u^\star_H], \nabla v\rangle + \langle b'(u^\star_H) z^\star[u^\star_H], v\rangle = G(v) \quad \text{for all } v \in \mathrm{H}^1_0(\Omega),$$

while the FEM implementation will deal with its Galerkin approximation $z^\star_H[u^\star_H] \in \mathcal{X}_H$. We prove the goal error estimate

$$C^{-1}|G(u^\star) - G(u^\star_H)| \,\le\, \|u^\star - u^\star_H\|_{\mathrm{H}^1_0(\Omega)}\, \|z^\star[u^\star_H] - z^\star_H[u^\star_H]\|_{\mathrm{H}^1_0(\Omega)} + \|u^\star - u^\star_H\|^2_{\mathrm{H}^1_0(\Omega)}.$$

Based on residual error estimators, we formulate a goal-oriented adaptive algorithm (GOAFEM), which guarantees convergence and, as the main contribution, optimal algebraic convergence rates [1]. As an extension, we briefly discuss a cost-optimal `solve`-module that steers the interplay of discretization and linearization for semilinear problems [2].

Keywords: goal-oriented adaptive algorithm, optimal convergence rates, semilinear PDEs, quantity of interest, *a posteriori* error estimation

References

[1] R. Becker, M. Brunner, M. Innerberger, J.M. Melenk, D. Praetorius (2022). *Rate-optimal goal-oriented adaptive finite element method for semilinear elliptic PDEs.* Comput. Math. Appl., 118:18–35.

[2] R. Becker, M. Brunner, M. Innerberger, J.M. Melenk, D. Praetorius (2023). *Cost-optimal adaptive iterative linearized FEM for semilinear elliptic PDEs.* Accepted for publication in ESAIM: M2AN.

Goal-oriented error estimates for nonlinear PDEs including linearization and algebraic errors

Vít Dolejší[1] and Scott Congreve[1]

[1]Charles University, Faculty of Mathematics and Physics, Prague
{dolejsi, congreve}@karlin.mff.cuni.cz

Abstract

When solving numerically partial differential equations (PDEs), we are often not interested in the approximate solution itself but in a quantity of interest given by a (possibly nonlinear) target functional. In order to estimate the error of the quantity of interest, an adjoint problem has to be formulated and solved, cf. [1, 5]. For nonlinear PDEs, the adjoint problem has to be set on a linearization (usually differentiation) of the primal one. The error arising from the linearization of the primal problem and the target functional are usually neglected, an exception is the numerical analysis in [4].

In this talk, we present a novel approach where the errors arising from the linearization of the PDE and the target functional are not neglected but appear as additional terms in the final error estimate, cf. [2]. For practical computations, these terms are approximated by a local higher-order reconstruction operator. The presented approach is not restricted to the linearization by a differentiation but additional covers other types of linearizations; for example, the Kačanov method or Zarantonello iterations.

Finally, we present an adaptive algorithm which equilibrates the discretization, linearization and algebraic errors. Several numerical examples demonstrate the efficiency of this algorithm in connection with a standard mesh adaptive technique and the anisotropic *hp*-mesh adaptation [3].

Keywords: goal-oriented error estimates, linearization errors, mesh adaptation

References

[1] R. Becker and R. Rannacher (2021). *An optimal control approach to a-posteriori error estimation in finite element methods.* Acta Numerica, 10, 1–102

[2] V. Dolejší and S. Congreve (2023). *Goal-oriented error analysis of iterative Galerkin discretizations for nonlinear problems including linearization and algebraic errors*, J. Comput. Appl. Math., 427, 115134

[3] V. Dolejší and G. May (2022). *Anisotropic hp-Mesh Adaptation Methods.* Birkhäuser.

[4] Endtmayer, B., Langer, U., Wick, T.(2020) *Two-side a posteriori error estimates for the dual-weighted residual method.* SIAM J. Sci. Comput. 1, A371–A394.

[5] M. Giles and E. Süli (2002). *Adjoint methods for PDEs: a posteriori error analysis and postprocessing by duality.* Acta Numerica, 11, 145–236.

Efficiency and Reliability for Adjoint Based Error Estimates using Interpolations

Sven Beuchler[1,2], Bernhard Endtmayer[1,2], Ulrich Langer[3], and Thomas Wick[1,2]

[1]Leibniz Universität Hannover, Institut für Angewandte Mathematik
[2]Cluster of Excellence PhoenixD, Leibniz Universität Hannover
[3]Institute of Numerical Mathematics, Johannes Kepler Universtiy Linz
{beuchler, endtmayer, thomas.wick}@ifam.uni-hannover.de;
ulanger@numa.uni-linz.ac.at

Abstract

In this talk, we derive efficiency and reliability for goal oriented error estimation using higher-order interpolations and enriched solutions. In [2], efficiency and reliability was already shown for enriched approximations. However, the computation of enriched solutions requires a lot of resources. In literature, this problem can be solved by using some higher-order interpolation. Here, we derive a similar result for arbitrary interpolations. Similar as in [2], we require a saturation assumption for the goal functional evaluated the interpolation. The results of our results can be used to create a new family of algorithms. The talk will be concluded with some numerical test.

Keywords: Regularized parabolic p-Laplacian, goal-oriented adaptivity, efficiency, reliability

References

[1] B. Endtmayer, U. Langer, T. Wick (2020). *Two-side a posteriori error estimates for the dual-weighted residual method*. SIAM J. Sci. Comput., 42(1):A371–A394.

[2] B. Endtmayer, U. Langer, T. Wick (2021). *Reliability and efficiency of DWR-type a posteriori error estimates with smart sensitivity weight recovering*. Computational Methods in Applied Mathematics, 21(2):351–371.

MORe DWR: Space-time goal-oriented error control for incremental POD-based ROM

Hendrik Fischer[1,2], Julian Roth[1,2], Thomas Wick[1,2],
Ludovic Chamoin[2], and Amelie Fau[2]

[1]Leibniz Universität Hannover, Institute of Applied Mathematics
[2]Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay LMPS - Laboratoire de Mecanique Paris-Saclay

Abstract

In this presentation, the dual-weighted residual (DWR) method [1, 2] is applied to obtain a certified incremental proper orthogonal decomposition (POD) based reduced order model [3]. A novel approach called MORe DWR (Model Order Reduction with Dual-Weighted Residual error estimates) [4] is being introduced. It marries tensor-product space-time reduced-order modeling with time slabbing [5] and an incremental POD basis generation [6] with goal-oriented error control based on dual-weighted residual estimates. The error in the goal functional is being estimated during the simulation and the POD basis is being updated if the estimate exceeds a given threshold. This allows an adaptive enrichment of the POD basis in case of unforeseen changes in the solution behavior which is of high interest in many real-world applications. Consequently, the offline phase can be skipped, the reduced-order model is being solved directly with the POD basis extracted from the solution on the first time slab and –if necessary– the POD basis is being enriched on-the-fly during the simulation with high-fidelity finite element solutions. Therefore, the full-order model solves can be reduced to a minimum, which is demonstrated on numerical tests for the heat equation and elastodynamics. We conclude the talk with recent developments and preliminary extensions of our presented framework.

Keywords: Tensor-Product Space-Time Reduced-Order Modeling, Dual-Weighted Residual method, goal-oriented error control, incremental Proper Orthogonal Decomposition

References

[1] R. Becker, R. Rannacher (1996). *A feed-back approach to error control in finite element methods: basic analysis and examples*. East-West J. Numer. Math., 4, 237–264

[2] R. Becker, R. Rannacher (2001). *An optimal control approach to a posteriori error estimation in finite element methods*. Acta Numer., 10, 1–102

[3] H. Fischer, T. Wick, A. Fau (2022). *Reduced-order modeling for parametrized time-dependent Navier-Stokes equations*. PAMM.

[4] H. Fischer, J. Roth, T. Wick, L. Chamoin, A. Fau (2023). *MORe DWR: Space-time goal-oriented error control for incremental POD-based ROM*. https://doi.org/10.48550/ARXIV.2304.01140.

[5] J. Roth, J.P. Thiele, U. Köcher, T. Wick (2022). *Tensor-product space-time goal-oriented error control and adaptivity with partition-of-unity dual-weighted residuals for nonstationary flow problems*. https://doi.org/10.48550/ARXIV.2210.02965.

[6] N. Kühl, H. Fischer, M. Hinze, T. Rung (2023). *An Incremental Singular Value Decomposition Approach for Large-Scale Spatially Parallel & Distributed but Temporally Serial Data–Applied to Technical Flows*. https://doi.org/10.48550/ARXIV.2302.09149.

Using Neural Networks to Estimate Errors Generated by Uncertain Data in the Poisson Equation

Vilho Halonen[1], Ilkka Pölönen[1], and Monika Wolfmayr[2]

[1]Faculty of Information Technology, University of Jyväskylä
[2]Institute of Information Technology, JAMK University of Applied Sciences
{vihebeha, ilkka.polonen}@jyu.fi; monika.wolfmayr@jamk.fi

Abstract

Uncertainty errors have been dealt with in the past using propabilistic methods [3] and analytical methods such as the worst case scenario method [2]. More recently analytical bounds for the radius of the solution set have been derived using a posteriori error estimates of the functional type [1]. Propabilistic methods which usually involve Monte-Carlo sampling are computationally very expensive and analytical methods for complex PDE's tend to be either unknown or unsatisfactorily coarse. We suggest using neural networks to approximate the radius of the solution set for an uncertain problem. A dataset was made for training such a network in the case of the Poisson equation with an uncertain source term. One training example has as input two source term functions of the poisson equation and as output the distance between the two different solutions generated by the source terms. The neural network performs in a comparable way to analytical bounds (which come from functional a posteriori estimates) and a raw monte-carlo sampling computation. This will be attempted for nonlinear PDE's in later research.

Keywords: Uncertainty quantification, Neural Networks

References

[1] Repin, Sergey (2010). *A Posteriori Error Estimates for Partial Differential Equations*. Radon. Ser. on Comput. and Appl. Mathematics 4. Berlin: De Gruyter. 4. 10.1515/9783110203042.

[2] I. Hlavacek, J. Chleboun, I. Babuska (2004). *Uncertain Input Data Problems and the Worset Scenario Method*. Elsevier, Amsterdam.

[3] G.I. Schuëller (1997). *A state-of-the-art report on computational stochastic mechanics*. Probabilistic Engineering Mechanics, Vol.12, 4, 197–321, ISSN 0266-8920.

Space-time goal-oriented error control for incremental POD-ROM using MORe DWR and temporal multirate FEM applied to porous media

Julian Roth[1,2], Hendrik Fischer[1,2], Martyna Soszyńska[3], Thomas Wick[1,2], Ludovic Chamoin[2], Amélie Fau[2], and Thomas Richter[3]

[1]Leibniz Universität Hannover, Institut für Angewandte Mathematik, AG Wissenschaftliches Rechnen, Welfengarten 1, 30167 Hannover, Germany
[2]Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS, LMPS - Laboratoire de Mécanique Paris-Saclay, 91190 Gif-sur-Yvette, France
[3]Otto-von-Guericke Universität Magdeburg, Institute of Analysis and Numerics, Universitätsplatz 2, 39106 Magdeburg, Germany
{roth, fischer, wick}@ifam.uni-hannover.de;
{ludovic.chamoin, amelie.fau}@ens-paris-saclay.fr;
{martyna.soszynska, thomas.richter}@ovgu.de

Abstract

In this talk, we present two adaptive methodologies for the efficient simulation of porous media.

In the first part of this talk, we apply the MORe DWR (Model Order Reduction with Dual-Weighted Residual error estimates) algorithm [1] to a benchmark problem from poroelasticity. The MORe DWR method introduces a goal-oriented adaptive incremental proper othogonal decomposition (POD) based reduced order model (ROM). Therein, the error in the reduced goal functional is being estimated during the simulation and the POD basis is being enriched on-the-fly if the estimate exceeds a given threshold, which reduces the total number of full-order model solves for the simulation of the porous medium.

In the second part of this talk, we propose and computationally investigate a monolithic space-time multirate scheme for the displacement equation coupled to Darcy flow in a poro-elastic medium. The novelty lies in the monolithic formulation of the multirate approach as this requires a careful design of the functional framework, corresponding discretization, and implementation. Our method of choice is a tensor-product Galerkin space-time discretization. The methodology is applied to the well-known Mandel's benchmark [3].

Keywords: Reduced-Order Modeling, Space-Time FEM, Dual-Weighted Residual method, Goal-oriented error control, incremental Proper Orthogonal Decomposition, multirate, temporal discretization, Mandel benchmark

References

[1] H. Fischer, J. Roth, T. Wick, L. Chamoin, A. Fau (2023). *MORe DWR: Space-time goal-oriented error control for incremental POD-based ROM.* https://doi.org/10.48550/ARXIV.2304.01140.

[2] J. Roth, M. Soszyńska, T. Richter, T. Wick (2023). *A monolithic space-time temporal multirate finite element framework for interface and volume coupled problems.* https://doi.org/10.48550/ARXIV.2307.12455.

[3] J. Mandel (1953). *Consolidation des sols (Étude mathématique).* Géotechnique. https://doi.org/10.1680/geot.1953.3.7.287.

Goal-Oriented Adaptive Space-Time Finite Element Methods for Regularized Parabolic p-Laplace Problems

Bernhard Endtmayer[1,2], Ulrich Langer[3], and Andreas Schafelner[3]

[1]Leibniz Universität Hannover, Institut für Angewandte Mathematik, AG Numerische Mathematik
[2]Cluster of Excellence PhoenixD, Leibniz Universität Hannover
[3]Institute of Numerical Mathematics, Johannes Kepler Universtiy Linz
endtmayer@ifam.uni-hannover.de; ulanger@numa.uni-linz.ac.at;
andreas.schafelner@jku.at

Abstract

We consider goal-oriented adaptive space-time finite-element discretizations of the regularized parabolic p-Laplace problem on completely unstructured simplicial space-time meshes. The adaptivity is driven by the dual-weighted residual (DWR) method since we are interested in an accurate computation of some possibly nonlinear functionals at the solution. Such functionals represent goals in which engineers are often more interested than the solution itself. The DWR method requires the numerical solution of a linear adjoint problem that provides the sensitivities for the mesh refinement. This can be done by means of the same full space-time finite element discretization as used for the primal non-linear problems. The numerical experiments presented demonstrate that this goal-oriented, full space-time finite element solver efficiently provides accurate numerical results for different functionals.

Keywords: Regularized parabolic p-Laplacian, space-time finite element discretization, goal-oriented adaptivity

Goal-oriented error control for the finite cell method

Andreas Schröder[1], Paolo Di Stolfo[1], and Andreas Rademacher[2]

[1]Department of Mathematics, University of Salzburg
[2]Center for Industrial Mathematics, University of Bremen
andreas.schroeder@plus.ac.at; arademac@uni-bremen.de

Abstract

The finite cell method is a combination of a fictitious domain method with a finite element method. It is based on the replacement of the possibly complicated physical domain by an embedding domain of a geometrically simple shape which can easily be meshed. The variational formulation of the problem and its finite element discretization is defined on the embedding domain. An indicator function is used to incorporate the geometry of the physical domain. Mainly two computational error sources occur in the finite cell method: the discretization error and the quadrature error.

The talk presents some concepts of the finite cell method and discusses a posteriori error control for this method. The focus is on the application of the dual weighted residual approach (DWR) which enables the control of the error with respect to a user-defined quantity of interest. Based on the DWR approach, an adaptive strategy is proposed which tries to balance the error contributions resulting from discretization and quadrature. The strategy consists in either refining the finite cell mesh or its associated quadrature mesh. Several numerical experiments demonstrate the applicability of the error control and the adaptive scheme for linear and nonlinear problems.

Keywords: finite cell method, error control, dual weighted residual approach

References

[1] P. Di Stolfo, A. Rademacher, A. Schröder (2019). *Dual weighted residual error estimation for the finite cell method.*, J. Numer. Math., 27(2), 101–122.

[2] P. Di Stolfo, A. Düster, S. Kollmannsberger, E. Rank, A. Schröder (2019). *A posteriori error control for the finite cell method.* PAMM, 19(1).

[3] P. Di Stolfo, A. Schröder (2022). *Error control and adaptivity for the finite cell method.* In *Non-standard discretisation methods in solid mechanics*, eds.: J. Schröder et al., Cham: Springer. Lect. Notes Appl. Comput. Mech., 98, 377–403.

Cost-optimal goal-oriented AFEM for linear elliptic PDEs

Maximilian Brunner[1], Dirk Praetorius[1], and Julian Streitberger[1]

[1]TU Wien, Institute of Analysis and Scientific Computing, Austria
julian.streitberger@asc.tuwien.ac.at

Abstract

For a given bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ and given right-hand side $f \in L^2(\Omega)$, we consider the nonsymmetric second-order linear elliptic PDE

$$-\operatorname{div}(\boldsymbol{A}\nabla u^\star) + \boldsymbol{b}\cdot\nabla u^\star + c\,u^\star = f \quad \text{in } \Omega \quad \text{subject to} \quad u^\star = 0 \quad \text{on } \partial\Omega, \tag{1}$$

with diffusion matrix $\boldsymbol{A} \in [L^\infty(\Omega)]^{d\times d}_{\rm sym}$, convection term $\boldsymbol{b} \in [L^\infty(\Omega)]^d$, and reaction term $c \in L^\infty(\Omega)$. With the principal part $a(u,v) := \langle \boldsymbol{A}\nabla u, \nabla v\rangle_{L^2(\Omega)}$, the weak form of (1) seeks $u^\star \in H^1_0(\Omega)$ with

$$b(u^\star, v) := a(u^\star, v) + \langle \boldsymbol{b}\cdot\nabla u^\star + c\,u^\star, v\rangle_{L^2(\Omega)} = \langle f, v\rangle_{L^2(\Omega)} + \langle \boldsymbol{f}, \nabla v\rangle_{L^2(\Omega)} =: F(v) \quad \text{for all } v \in H^1_0(\Omega). \tag{2}$$

We suppose that $b(\cdot\,,\cdot)$ satisfies the assumptions of the Lax–Milgram lemma on $H^1_0(\Omega)$ so that (2) admits a unique solution $u^\star \in H^1_0(\Omega)$. In contrast to standard adaptive FEM that aims to approximate $u^\star \in H^1_0(\Omega)$, goal-oriented adaptive FEM aims at computing a linear *quantity of interest*, e.g., $G(u^\star)$, e.g., $G(u^\star) := \langle g, u^\star\rangle_{L^2(\Omega)}$ for given $g \in L^2(\Omega)$. The so-called dual problem seeks $z^\star \in H^1_0(\Omega)$ such that

$$b(v, z^\star) = G(v) \quad \text{for all } v \in H^1_0(\Omega). \tag{3}$$

By defining the discrete goal $G_H(u_H, z_H) := G(u_H) + \big[F(z_H) - b(u_H, z_H)\big]$ for finite element approximations $u_H \approx u^\star$ and $z_H \approx z^\star$, we can exploit continuity of $b(\cdot\,,\cdot)$ to control the goal error by

$$|G(u^\star) - G_H(u_H, z_H)| = |b(u^\star - u_H, z^\star - z_H)| \le C\,\|u^\star - u_H\|_{H^1_0(\Omega)}\,\|z^\star - z_H\|_{H^1_0(\Omega)}. \tag{4}$$

We formulate and analyze a goal-oriented adaptive finite element algorithm that steers the adaptive mesh refinement, and the inexact iterative solutions of the arising linear systems in the spirit of [1]. While the analysis in [3] for symmetric PDEs (with $\boldsymbol{b} = 0$) is considerably less challenging, the iterative solver for the nonsymmetric problem employs, as an outer loop, the so-called Zarantonello iteration to symmetrize (2)–(3) and, as an inner loop, an optimal geometric multigrid algorithm [2]. We prove that the proposed goal-oriented adaptive iteratively symmetrized finite element method (GAISFEM) leads to full linear convergence and, as our main contribution, to optimal convergence rates with respect to the overall computational cost, i.e., the total computational time.

Keywords: nonsymmetric PDEs, goal-oriented adaptive finite element method, optimal convergence rates, cost-optimality

References

[1] M. Brunner, P. Heid, M. Innerberger, A. Miraçi, D. Praetorius, J. Streitberger (2022). *Adaptive FEM with quasi-optimal overall cost for nonsymmetric linear elliptic PDEs*. arXiv:2212.00353.

[2] M. Innerberger, A. Miraçi, D. Praetorius, J. Streitberger (2022). *hp-robust multigrid solver on locally refined meshes for FEM discretizations of symmetric elliptic PDEs*. arXiv:2210.10415.

[3] R. Becker, G. Gantner, M. Innerberger, D. Praetorius (2023). *Goal-oriented adaptive finite element methods with optimal computational complexity*, Numer. Math., 153, 111–140.

Adaptive Mixed Finite Elements Methods based on Goal Oriented A Posteriori Error Estimates

Dominika Thiede[1], Andreas Rademacher[1], and Lothar Banz[2]

[1]Center for Industrial Mathematics, University of Bremen
[2]Department of Mathematics, University of Salzburg
{dothiede, arademac}@uni-bremen.de; lothar.banz@plus.ac.at

Abstract

We consider the following Poisson problem: Let $u : \Omega \to \mathbb{R}$ be the solution of

$$-\Delta u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega, \quad u = g \text{ on } \Gamma_g$$

in the domain $\Omega \subset \mathbb{R}^d, d \in \{2, 3\}$. In this case, f and g are given functions and Γ_g is a lower dimensional closed manifold in the interior of Ω.
Now mixed finite elements are developed and analyzed which realize the condition $u = g$ on Γ_g in the weak sense. On the one hand, relating to the domain triangulation with quadrilaterals and the grid size h, we choose piecewise bilinear functions for the solution space. On the other hand, the Lagrange multiplier is approximated with piecewise constant functions on an exact discretization of Γ_g with grid size H. The approximation of the Lagrange multiplier is independent of the discretization of the domain. We show the inf-sup stability for H/h small enough. Satisfying the above condition increases the numerical complexity due to the non-matching meshes. For this reason, we consider a second approach, using the same solution spaces but also taking into account the domain discretization in the approximation of the Lagrange multiplier. We ensure the inf-sup condition by adding least-squares residual terms to the original bi-linear and linear forms as in [1]. We perform an a priori error analysis for both approaches. In this talk, we discuss especially the a posteriori error estimation using the dual weighted residual (DWR) method for these two solution approaches. The problem we consider is motivated by the handling of Dirichlet boundary conditions in the fictitious domain approach.

Keywords: finite cell methods, mixed finite element methods, elliptical problem

References

[1] L. Banz, H. Gimperlein, A. Issaoui, & E. Stephan (2017). *Stabilized mixed hp-BEM for frictional contact problems in linear elasticity. Numerische Mathematik*, 217–263.

A posteriori error estimates robust with respect to the strength of nonlinearities

André Harnist[1,2], Koondanibha Mitra[3], Ari Rappaport[1,2], and Martin Vohralík[1,2]

[1]Inria Paris, France
[2]CERMICS, Ecole des Ponts, Marne-la-Vallée, France
[3]Faculty of Sciences, Hasselt University, Belgium
koondanibha.mitra@uhasselt.be; {andre.harnist, ari.rappaport, martin.vohralik}@inria.fr

Abstract

A posteriori estimates enable to certify errors committed in numerical approximations of solutions of partial differential equations. For linear model problems, the equilibrated flux reconstruction technique yields an upper bound on the unknown error which is guaranteed and fully computable. It is, importantly, also robust, i.e., the overestimation factor (effectivity index) is uniformly bounded in all situations: for any domain size and shape, problem data, regular or singular exact solution, as well as for all combinations of the two basic discretization parameters – the number of mesh elements (mesh size h) and the polynomial degree p. Moreover, the flux, obtained by a local postprocessing, is of independent interest since it is always locally conservative.

This talk addresses nonlinear problems, where standard approaches do not give estimates robust with respect to the strength of the nonlinearities (the overestimation factor increases when the problem is more and more nonlinear). We consider nonlinear strongly monotone and Lipschitz-continuous elliptic problems and derive estimates that include, and build on, common iterative linearization schemes such as Zarantonello, Picard, Newton, or M- and L-ones. We derive two approaches that give robustness: we either estimate the energy difference that we augment by the discretization error of the current linearization step, or we design iteration-dependent norms that feature weights given by the current linearization iterate. The second setting allows for error localization and an orthogonal decomposition into discretization and linearization components. Numerical experiments illustrate the theoretical findings, with the overestimation factors close to the optimal value of one for any strength of the nonlinearities. Details are given in [1,2].

Keywords: nonlinear elliptic problem, finite element method, iterative linearization, energy difference, residual, dual norm, a posteriori error estimate, robustness, equilibrated flux reconstruction

References

[1] A. Harnist, K. Mitra, A. Rappaport, M. Vohralík (2023). *Robust energy a posteriori estimates for nonlinear elliptic problems.* HAL Preprint 04033438.

[2] K. Mitra, M. Vohralík, (2023). *Guaranteed, locally efficient, and robust a posteriori estimates for nonlinear elliptic problems in iteration-dependent norms. An orthogonal decomposition result based on iterative linearization.* In preparation.

MS15 - Mathematical and computational models of cells, cell-populations, and applications thereof

Numerical simulation of active cell surfaces - from pattern formation to cell division

Sebastian Aland[1,2]

[1]Institute of Numerical Mathematics and Optimization, TU Freiberg, Germany
[2]Faculty of Informatics/Mathematics, HTW Dresden, Germany
sebastian.aland@math.tu-freiberg.de

Abstract

Shape changes of single cells are governed by the actomyosin cortex, a thin layer of active material underneath the cell surface. Besides the imposed rigidity, the cortical surface exerts an active contractile tension, the strength of which being controlled by the concentration of force-generating molecules. The complex interplay of molecule transport and surface hydrodynamics gives rise to pattern formation and self-organized shape dynamics. Despite the biological importance of these phenomena, the system is far from being understood. To improve this understanding, we present a numerical model of such an active surface immersed in viscous fluids [4]. The cortex is modelled as a viscoelastic surface material, described by a freely evolving Finite-Element grid [2]. The dynamics is coupled to a surface concentration equation of force-generating molecules (e.g. actomyosin). We analyze the emerging mechanochemical patterns and shape changes and show that the activity of the surface can lead to cell division or cell migration [1, 3].

Keywords: Free boundary problems, Cell biology, Two-phase flow

References

[1] M. Bonati, L.D. Wittwer, S. Aland, E.F. Fischer-Friedrich (2022). *On the role of mechanosensitive binding dynamics in the pattern formation of active surfaces*. New Journal of Physics, 24(7):073044.

[2] E. De Kinkelder, L. Sagis, S. Aland (2021). *A numerical method for the simulation of viscoelastic fluid surfaces*. Journal of computational physics, 440:110413.

[3] E. De Kinkelder, E. Fischer-Friedrich, S. Aland (2022). *Chiral flows can induce neck formation in viscoelastic surfaces*. ArXiv preprint arXiv:2211.07183.

[4] L.D. Wittwer, S. Aland (2022). *A computational model of self-organized shape dynamics of active surfaces in fluids*. ArXiv preprint arXiv:2203.00099.

Blocked Gibbs Particle Smoothing Algorithm for Jump-Diffusion Approximations of Biochemical Reaction Networks

Derya Altıntan[1], Bastian Alt[2], and Heinz Koeppl [2]

[1]Department of Mathematics, Hacettepe University
[2] Department of Electrical Engineering and Information Technology, Technische Universität Darmstadt
deryaaltintan@hacettepe.edu.tr; {bastian.alt, heinz.koeppl}@tu-darmstadt.de

Abstract

Biochemical reaction networks (BRNs) consist of species that collaborate and adjust the dynamics of each other via reaction channels. These networks generally have a multi-scale nature concerning the reaction rates and species abundances. In [1], the authors proposed jump-diffusion approximation to exploit this multi-scale nature. The strategy of this hybrid model is to separate the BRN into fast and slow reaction sets and model the fast set by using Langevin approximation while a Markov jump process is maintained for the slow set. Generally, it is a difficult task to estimate the unknown states/parameters of BRNs, therefore, statistical methods that can be utilized to infer these hidden quantities are needed.

In this talk, we develop a Gibbs sampling strategy, namely the blocked Gibbs particle smoothing algorithm, which combines a Sequential Monte Carlo (SMC) algorithm involving forward-filtering and backward-smoothing steps and a Monte Carlo Markov chain (MCMC) based method to estimate the hidden states/parameters of BRNs modeled with the jump-diffusion approximation. The algorithm is a two-layered algorithm including state and parameter inference steps. In the state inference step, we sample hidden states from the conditional posterior distribution of the states given the reaction rates and the observation data by utilizing a forward-filtering backward-smoothing algorithm based on the bootstrap filter [2]. In the parameter inference step, we sample from the conditional posterior distribution of the reaction rates given the states obtained in the state inference step and the observation data using a MCMC method [3]. Finally, we present numerical results for a multi-scale birth-death process to validate the algorithm's efficiency.

Keywords: Jump-diffussion approximation, Markov chain Monte Carlo, sequential Monte Carlo, Gibbs sampling, bootstrap filtering

References

[1] A. Ganguly, D. Altıntan, H. Koeppl (2015). *Jump-Diffusion Approximation of Stochastic Reaction Dynamics: Error Bounds and Algorithms*. Multiscale Model. Simul., 13, 1390–1419.

[2] N. Gordon, J. Neil, D. J. Salmond, A. F. Smith (1993). *Novel approach to nonlinear/non-Gaussian Bayesian state estimation*. In *IEE proceedings F (radar and signal processing)*, 140, 107–113.

[3] S. Brooks, A. Gelman, G. Jones, X. L. Meng (2011). *Handbook of Markov Chain Monte Carlo*. CRC press.

Morphological stability for *in silico* models of avascular tumors

Erik Blom[1] and Stefan Engblom[2]

[1]Division of Scientific Computing, Department of Information Technology, Uppsala University
{erik.blom, stefane}@it.uu.se

Abstract

Stochastic models of cell populations are capable of capturing features that arise from the inherent variability of biological processes. The probabilistic nature of these models are also particularly useful when we seek to infer, e.g., Bayesian posterior distributions from biological data. However, stochastic models are notoriously difficult to analyse and thus achieving a good model understanding is more computationally demanding than for models that are amenable to analysis.

In this minisymposium talk, we present the morphological stability analysis of a stochastic cell population model of avascular tumor growth using the model's mean-field counterpart. We investigate the emergent morphological properties of the deterministic mean-field model using linear stability analysis and show how the morphological instabilities of the stochastic model can be partially understood as perturbations in the deterministic model. As an example, we find that morphological instabilities are amplified during nutrient starvation and that the Saffman-Taylor instability plays a central part in the morphological development of our model.

In short, we talk about how the morphological properties of a stochastic model of avascular tumor growth can be analysed from the perspective of its mean-field counterpart.

Keywords: Avascular tumor modeling, Cell population modeling, Morphological stability

References

[1] E. Blom, S. Engblom (2023). *Morphological stability for in silico models of avascular tumors.* Manuscript.

[2] S. Engblom, D. B. Wilson, R. E. Baker (2018). *Scalable population-level modelling of biological cells incor- porating mechanics and kinetics in continuous time.* Roy. Soc. Open Sci. 5(8):180379.

Modelling the transport of radiative particles: The impact of tumour heterogeneous properties

Victor Ogesa Juma[1], Diego Sainz-De Mena[1], María Teresa Sánchez[2], and José Manuel García-Aznar*[1]

[1]Multiscale in Mechanical and Biological Engineering, Aragon Institute of Engineering Research (I3A), University of Zaragoza, 50018 Zaragoza, Spain
[2]Centro Universitario de la Defensa Zaragoza, Zaragoza, Spain
{vjuma,dsainz, tererua, jmgaraz}@unizar.es

Abstract

Radiotherapy is a widely used method in cancer therapy, and it uses high doses of radiation to kill cancer cells and shrink tumours by exposing them to high-energy rays. The accurate calculation of radiation dosage is a critical component of radiotherapy treatment planning, relying heavily on mathematical models that incorporate the heterogeneous properties of tumours. Recently, deterministic models have gained attention due to their ability to simplify the calculations while maintaining accuracy.

In this talk, I will explore the application of the Boltzmann transport equation (BTE) in radiotherapy treatment planning, showcasing its effectiveness in modelling the behaviour of tumours. I will also demonstrate how dose deposition models and tumour growth models can be integrated to provide a comprehensive understanding of the dynamics of tumours following radiotherapy treatment. Additionally, I will discuss the use of the finite element method (FEM) to simulate real-world clinical cases, allowing for more accurate predictions of patient outcomes.

Finally, I will highlight the significance of magnetic resonance imaging (MRI) data in extracting tumour properties and its role in enhancing dose calculation models.

Keywords: Finite element method, Radiative particle transport, Boltzmann transport equation, Numerical methods, DIPG, Mathematical modelling, Photon transport

References

[1] L. Martí-Bonmatí, Á. Alberich-Bayarri, R. Ladenstein, I. Blanquer, J.D. Segrelles, L. Cerdá-Alberich, E. Neri (2020). *PRIMAGE project: predictive in silico multiscale analytics to support childhood cancer personalised evaluation empowered by imaging biomarkers.* European radiology experimental, 4(1), 1–11.

[2] D. Sainz-DeMena, J.M. García-Aznar, M.Á. Pérez, C. Borau, (2022). *Im2mesh: A Python Library to Reconstruct 3D Meshes from Scattered Data and 2D Segmentations, Application to Patient-Specific Neuroblastoma Tumour Image Sequences.* Applied Sciences, 12(22), 11557.

[3] J.L. Bedford (2019). *Calculation of absorbed dose in radiotherapy by solution of the linear Boltzmann transport equations.* Physics in Medicine & Biology, 64(2), 02TR01.

*This work has received funding from the European Union's Horizon 2020 research and innovation program under PRedictive In-silico Multiscale Analytics to support cancer personalized diaGnosis and prognosis, empowered by imaging biomarkers (PRIMAGE) grant agreement No. 826494.

Bridging the gap between individual-based and continuum models of growing cell populations

Fiona R. Macfarlane[1]

[1]School of Mathematics and Statistics, University of St Andrews

Abstract

Stochastic individual-based modelling approaches allow for the description of single cells in a biological system. These models generally include rules that each cell follows independently of other cells in the population and allow for heterogeneity of population to be considered. However, these models cannot be analysed mathematically. Therefore, it can be beneficial to derive the corresponding deterministic model from the underlying random walk of the stochastic model. The resulting deterministic models, usually partial differential equations (PDEs), can then be analysed to provide further information about the biological systems studied. We have developed a range of simple IB models that describe biological systems with various properties of interest, such as chemotaxis and pressure-dependent growth and proliferation. Ultimately, the results illustrate how the simple rules governing the dynamics of single cells in our individual-based model can lead to the emergence of complex spatial patterns of population growth observed in continuum models. These models can be applied to a variety of biological situations such as bacterial population growth and tumour invasion processes.

Model selection identifies proliferative heterogeneity in mouse microglia development

W. Duncan Martinson[1], Carles Falco[1], Marta Pereira[2], Amanda Sierra[2], and José Carrillo[1]

[1]University of Oxford Mathematical Institute, Oxford, UK
[2]Achucarro Basque Center for Neuroscience, Bilbao, Spain
william.martinson@maths.ox.ac.uk

Abstract

Microglia, the resident immune cells of the brain, have recently been found to play key roles in neuronal development and synapse formation. By contrast, the mechanisms that drive microglia to acquire their mature functions remain poorly understood. We address this knowledge gap by developing a data-inspired mathematical model for mouse microglia development following birth. We apply Bayesian inference and model selection techniques to fit and evaluate several different mathematical frameworks that aim to describe *in vivo* observations of how the density of microglia change over time in the cerebellum and hippocampus. We find that a model in which microglia form a heterogeneous population best explains the available data. The fitted parameter values suggest that the basis of this heterogeneity lies in the ability of cells to proliferate. Individual model simulations imply that microglia transition from a highly proliferative to a more quiescent phenotype in the weeks following birth, with this change largely driven by interactions with other brain cells such as neurons or radial glial cells. Our model predictions motivate new biological experiments confirming the existence of such proliferative heterogeneity and demonstrate the synergistic benefits of collaboration between theoretical and experimental biologists.

Keywords: Bayesian inference, data-driven modeling, model selection, microglia, developmental biology, population dynamics

Towards a full digital liver twin of drug-induced damage, regeneration and disease progression

Jieling Zhao[1,2], Seddik Hammad[3], Ahmed Ghallab[2], Steven Dooley[3], Jan G. Hengstler[2], and Dirk Drasdo[1,2]

[1]Inria de Saclay, Palaiseau, France
[2]IfADo, Dortmund, Germany
[3]Molecular Hepatology Section, Department of Medicine II, Medical Faculty Mannheim Heidelberg University, Mannheim, Germany

Abstract

Digital twin is the projection of the real world object to the digital world. It has been widely used to study the biological and medical phenomena such as to understand the biomechanical growth control mechanisms of liver regeneration [1] and to explore the extrapolation strategies for drug-induced liver injury [2]. In this talk, we present a digital twin of the liver and its application to drug-induced liver damage, liver regeneration and fibrosis formation as a prominent example of a disease process. This digital twin is based on a biophysics-based computational model which can accurately capture the deformation of cells, capillaries, and extracellular matrix according to their biomechanical properties. As drug-induced damage overdosing paracetamol (acetaminophen) is studied in a multilevel model integrating drug detoxification in each individual hepatocytes according to the processes in the respective liver zones (zonatation). The regeneration process triggered by the drug is based on a complex cross-talk between cells exchanging extracellular signals. This intercellular signaling network is integrated into the digital twin to allow the communication between various cell types through corresponding signals. We show that for the application of liver regeneration, the digital twin could help identify a set of successful alternative mechanisms controversly discussed in the biological and medical community for a perfect liver recovery and predict the effect of depletion certain cell types[3]. Repetitive damage has been shown to cause fibrosis characterized by deposition of extracellular matrix but the mechanism leading to the characteristic spatial pattern of fibrosis are not understood. The digital twin proposes a mechanism of how the fibrotic pattern is formed. In summary, here we show the potential of the digital twin for studying complex biological/medical problems at subcellular level and its role as a pillar complementary to real-world experiments in future.

Keywords: Digital twin, Cell mechanics, Intercellular signal network, Liver regeneration & fibrosis

References

[1] S. Hoehme, S. Hammad, J. Boettger, B. Begher-Tibbe, P. Bucur, E. Vibert, R. Gebhardt, J. G. Hengstler, D. Drasdo (2023). *Digital twin (...) after partial hepatectomy.* iScience 26, 105714.

[2] J. Dichamp, G. Celliere, A. Ghallab, R. Hassan, N. Boissier, U. Hofmann, J. Reinders, S. Sezgin, S. Zuhlke, J. G. Hengstler, D. Drasdo (2023). *In vitro to in vivo (...) liver twin.* Frontiers in Bioengineering and Biotechnology 11, 1049564.

[3] J. Zhao, A. Ghallab, R. Hassan, S. Dooley, J. G. Hengstler, D. Drasdo. *A liver digital twin for in silico testing of cellular and intercellular mechanisms in regeneration after drug-induced damage.* Accepted in iScience.

MS16 - Theoretical and numerical developments for high-dimensional parametric PDEs

An adaptive finite element stochastic Galerkin method based on multilevel expansions

Henrik Eisenmann[1], Markus Bachmayr[1], Martin Eigel[2], and Igor Voulis[3]

[1]RWTH Aachen
[2]WIAS Berlin
[3]Uniservität Göttingen
[1]eisenmann@igpm.rwth-aachen.de

Abstract

The subject of this work is a stochastic Galerkin method for second-order elliptic partial differential equations with random diffusion coefficients. It combines operator compression in the stochastic variables with adaptive finite-element approximation in the spatial variables. We provide a convergence analysis for the method. Numerical experiments illustrate optimal or close to optimal complexity.

Keywords: parameter-dependent elliptic partial differential equations, stochastic Galerkin method

High-dimensional and adaptive approximation of micromagnetics

Michael Feischl[1] and Andrea Scaglioni[2]

[1,2]Institute for Analysis and Scientific Computing, TU Wien
michael.feischl@tuwien.ac.at

Abstract

We consider the stochastic Landau-Lifschitz-Gilbert equation, an SPDE model for dynamic micromagnetism. We first convert the problem to a (highly nonlinear) PDE with parametric coefficients using the Doss-Sussmann transform and the Lévy-Ciesielsky parametrization of the Brownian motion. We prove analytic regularity of the parameter-to-solution map and estimate its derivatives. These estimates are used to to prove convergence rates for piecewise-polynomial sparse grid methods. Moreover, we propose novel time-stepping methods to solve the underlying deterministic equations.

Keywords: Landau-Lifshitz-Gilbert equation, sparse grids, approximation

Dimension truncation error analysis for high-dimensional numerical integration: lognormal setting and beyond

Philipp A. Guth[1] and Vesa Kaarnioja[2]

[1]Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences, philipp.guth@ricam.oeaw.ac.at
[2]Department of Mathematics and Computer Science, Free University of Berlin, vesa.kaarnioja@fu-berlin.de

Abstract

Partial differential equations (PDEs) with uncertain or random inputs have been considered in many studies of uncertainty quantification. In forward uncertainty quantification, one is interested in analyzing the stochastic response of the PDE subject to input uncertainty, which usually involves solving high-dimensional integrals of the PDE output over a sequence of stochastic variables. In practical computations, one typically needs to discretize the problem in several ways: approximating an infinite-dimensional input random field with a finite-dimensional random field, spatial discretization of the PDE using, e.g., finite elements, and approximating high-dimensional integrals using cubatures such as quasi-Monte Carlo methods. In this presentation, we focus on the error resulting from dimension truncation of an input random field. Using a Taylor series approach we obtain theoretical dimension truncation rates for a wide class of problems and we provide a simple checklist of conditions that a parametric mathematical model needs to satisfy in order for our dimension truncation error bound to hold. Some of the novel features of our approach include that our results are applicable to non-affine parametric operator equations, dimensionally-truncated conforming finite element discretized solutions of parametric PDEs, and even compositions of PDE solutions with smooth nonlinear quantities of interest. As a specific application of our method, we derive an improved dimension truncation error bound for elliptic PDEs with lognormally parameterized diffusion coefficients. Numerical examples support our theoretical findings.

Keywords: Numerical integration, uncertainty quantification, parametric partial differential equation, lognormal random field

References

[1] P. A. Guth, V. Kaarnioja (2022). *Generalized dimension truncation error analysis for high-dimensional numerical integration: lognormal setting and beyond.* Preprint arXiv:2209.06176 [math.NA].

Isogeometric analysis of rough random acoustic scattering

Jürgen Dölz[1], Wei Huang[2], and Michael Multerer[2]

[1]Institute for Numerical Simulation, University of Bonn
[2]Euler Institute, Università della Svizzera italiana
doelz@ins.uni-bonn.de; {wei.huang, michael.multerer}@usi.ch

Abstract

We study the numerical solution of forward time-harmonic acoustic scattering problems by rough randomly deformed obstacles in three-dimensional space using a fast isogeometric boundary element method. As in [1], realizations of the random scatterer can efficiently be computed by simply updating the NURBS mappings which represent the scatterer. However, unlike [1], we consider a rough random deformation field on the boundary determined by an identity expectation and a covariance operator with slowly decaying eigenvalues. Employing samplets, cp. [2], for the compression of the covariance operator, we use the Cholesky decomposition with nested dissection reordering to obtain a representation of the deformation field. Due to the slow decay of the covariance operator's eigenvalues, higher order quadrature methods for the computation of quantities of interest, such as the scattered wave's expectation and correlation in free space via an artificial, fixed interface enclosing the random obstacle, are not indicated. Therefore, we resort to the multilevel Monte Carlo method. Numerical results for the forward problem validate the proposed approach.

Keywords: Uncertainty Quantification; Helmholtz scattering; Isogeometric Analysis; Boundary Integral Methods; Samplets; Multilevel Monte Carlo

References

[1] J. Dölz, H. Harbrecht, C. Jerez-Hanckes, M. Multerer (2022). *Isogeometric multilevel quadrature for forward and inverse random acoustic scattering*. Computer Methods in Applied Mechanics and Engineering, 388, 114242.

[2] H. Harbrecht, M. Multerer (2022). *Samplets: Construction and scattered data compression*. Journal of Computational Physics, 471, 111616.

Density estimation in RKHS with application to Korobov spaces in high dimensions

Yoshihito Kazashi[1] and Fabio Nobile[2]

[1]Department of Mathematics and Statistics, University of Strathclyde, United Kingdom
[2]Institute of Mathematics, École Polytechnique Fédérale de Lausanne, Switzerland
y.kazashi@strath.ac.uk; fabio.nobile@epfl.ch

Abstract

I will be talking about a kernel-based method for estimating a probability density function (pdf) from an i.i.d. sample. Our estimator is a linear combination of kernel functions, the coefficients of which are determined by a linear equation. I will present an error analysis for the mean integrated squared error in a general reproducing kernel Hilbert space setting. This theory is then applied to estimate pdfs belonging to weighted Korobov spaces, for which a dimension independent convergence rate is established. Under a suitable smoothness assumption, our method attains a rate arbitrarily close to the optimal rate.

This talk will be based on [1].

Keywords: Density estimation in high dimensions, Kernel approximation in high dimensions, Quasi-Monte Carlo methods

References

[1] Y. Kazashi, F. Nobile (2023). *Density estimation in RKHS with application to Korobov spaces in high dimensions*. SIAM J. Numer. Anal., 62(2), 1080–1102. https://doi.org/10.1137/22M147476X.

Bifurcation diagrams of PDEs with parametric uncertainty

Christian Kuehn[1], Chiara Piazzola[1], and Elisabeth Ullmann[1]

[1]Department of Mathematics, Technical University of Munich, Germany
{ckuehn, elisabeth.ullmann}@ma.tum.de; chiara.piazzola@tum.de

Abstract

Complex physical phenomena can often be described by PDEs with random coefficients, possibly involving a large number of uncertain parameters. Crucially, the presence of such uncertainty might render into very different behavior of the modeled phenomenon, e.g. due to the randomness of the stability region of an equilibrium.

In this talk, we consider model equations such as the Allen-Cahn equation with polynomial nonlinearity. We take a look at bifurcation diagrams and regard them as random objects, meaning that e.g. equilibria and bifurcation points are random quantities. As such, they call for uncertainty quantification methods. In particular, we investigate the forward uncertainty quantification problem, i.e. the propagation of the uncertainty of the model coefficients to such quantities by means of sparse grids and the polynomial chaos method.

Keywords: PDEs with pametric uncertainty, linear stability, bifurcation points

A dimension-adaptive sparse grid method for random elliptic PDEs using adaptive finite elements

Uta Seidler[1] and Michael Griebel[1,2]

[1]Institute of Numerical Simulation, University of Bonn
[2]Fraunhofer Institute for Algorithms and Scientific Computing SCAI
{seidler, griebel}@ins.uni-bonn.de

Abstract

We present an adaptive algorithm for the computation of quantities of interest of random elliptic partial differential equations. We consider PDE problems where the source of randomness is given by the diffusion coefficient which is parametrized by means of a Kahunen-Loève expansion. One common approach is to approximate the equivalent parametric problem by a restriction of the countably infinite dimensional parameter space to a finite-dimensional parameter set and subsequently apply a spatial discretization and an approximation in the parametric variables.

In our method, we use a dimension-adaptive sparse grid approach to balance a stochastic collocation method with the spatial discretization. In contrast to established methods with uniform finite element meshes, we apply an adaptive finite element method as spatial discretizaton.

Our adaptive algorithm uses the benefit-cost ratio to steer the adaptive process in the dimension-adaptive combination technique and to balance the quadrature levels with different spatial discretizations. In order to define a hierarchy of spatial discretization, we consider a decreasing sequence of error tolerances and construct non-uniform meshes using suitable adaptive finite element error estimators.

Applying an adaptive spatial refinement, allows us to adjust to the spatial regularity of the problem and our method performs well even if spatial singularities are present.

Keywords: uncertainty quantification, high-dimensional approximation, adaptive sparse grids, combination technique, adaptive finite elements

Multilevel quadrature rules for optimal control problems constrained by random PDEs

Fabio Nobile[1] and Tommaso Vanzan[2]

[1]École Polytechinique Fédérale de Lausanne, fabio.nobile@epfl.ch
[2]École Polytechinique Fédérale de Lausanne, tommaso.vanzan@epfl.ch

Abstract

In this talk, we consider the minimization of the expected value of a functional constrained by a random elliptic partial differential equation. One common approach to solve such problems is to discretize a-priori the probability space by replacing the continuous expectation with a Monte Carlo or Quasi Monte Carlo approximation. Since the computational cost grows with the number of quadrature nodes, several techniques have been proposed in the last years to ease the computational burden, including sparse grids and multilevel Monte Carlo methods. However, the methods proposed have the drawback of involving negative quadrature weights which may lead to the loss of the convexity of the continuous optimization problem. In this work, we propose a novel and different approach to use general multilevel quadrature formulae to solve optimal control problems under uncertainty, while preserving the properties of the continuous optimization problem. We conclude by showing the efficacy through numerical experiments on nonlinear problems.

Keywords: optimization under uncertainty, combination technique, parametric regularity, sparse grids, MLMC

MS17 - Analysis and Numerics for Systems of Nonlinear PDEs in Mathematical Biology

Asymptotic study of a neuroscience PDE model with singular boundary condition

Elena Ambrogi [*1] and Delphine Salort[2]

[1]Laboratoire Jacques-Louis Lions, Sorbonne Université - Inria Paris, France
[2]Laboratoire de Biologie Computationnelle et Quantitative, Sorbonne Université, France
elena.ambrogi@sorbonne-université.fr; delphine.salort@sorbonne-université.fr

Abstract

The Integrate and Fire model is a class of mean-field evolutionary equations which describes the activity of a population of neurons via their membrane potential. The structure of this equation is shared by many models of neural network, and the investigation of its qualitative properties is still an open and challenging question. We study the asymptotic behaviour of the linear I&F model, which presents a singular boundary condition. We prove, via a Doeblin-Harris theorem [1], that the solutions converge exponentially fast to the unique stationary state in a L^1-weighted norm [3]. We additionally illustrate some numerical simulations [2] for the model and (depending on time) for some generalizations of it.

Keywords: mathematical neuroscience, Doeblin-Harris theorem, asymptotic behaviour

References

[1] José A. Cañizo and Stéphane Mischler (2023). *Harris-type results on geometric and subgeometric convergence to equilibrium for stochastic semigroups.* Journal of Functional Analysis, 284(7):109830.

[2] Jingwei Hu, Jian-Guo Liu, Yantong Xie, and Zhennan Zhou (2021). *A structure preserving numerical scheme for Fokker-Planck equations of neuron networks: numerical analysis and exploration.* J. Comput. Phys., 433:Paper No. 110195, 23.

[3] Delphine Salort, Didier Smets (2022). *Convergence towards equilibrium for a model with partial diffusion.* ⟨hal-03845918⟩

[*]thanks M.J. Cacéres, J.A. Cañizo and B. Perthame

Fast numerical solvers for pattern formation problems in mathematical biology

Karolína Benková*[1], John Pearson[2], and Mariya Ptashnyk[3]

[1]MAC-MIGS, The Maxwell Institute for Mathematical Sciences, Heriot-Watt University & University of Edinburgh, Scotland, UK
[2]School of Mathematics, University of Edinburgh, Scotland, UK
[3]Department of Mathematics, Heriot-Watt University, Scotland, UK
{k.benkova, j.pearson}@ed.ac.uk; m.ptashnyk@hw.ac.uk

Abstract

Many of the mechanisms governing pattern formation in embryonic development have been identified and described by systems of PDEs. As some of the parameters or functions in these PDEs may be impossible to measure in laboratory conditions, we can use optimal control theory, in particular PDE-constrained optimization, to identify them. Given experimental data as the desired states, we can pose a minimisation problem so that the equations in the constraints evolve the state as close as possible to the desired state while also minimising the amount of control (or external biological mechanism) applied. In this talk, we will present a numerical solver for a problem with reaction-diffusion PDEs as constraints, by making use of a preconditioner for the large-scale saddle-point problems that arise. Moreover, we will discuss how to solve the numerical problems that arise when the PDEs are chemotaxis equations, present the flux-corrected transport technique, and outline how this could be applied within the optimization setting.

Keywords: Optimal control, PDE-constrained optimisation, Pattern formation, Chemotaxis equations, Flux-corrected transport

References

[1] R. Strehl, A. Sokolov, D. Kuzmin, S. Turek (2010). *A Flux-Corrected Finite Element Method for Chemotaxis Problems*. Computational Methods in Applied Mathematics, 10: 219–232.

[2] T. Apel, T.G. Flaig (2012). *Crank-Nicolson Schemes for Optimal Control Problems with Evolution Equations*. SIAM Journal on Numerical Analysis, 50: 1484–1512.

[3] S. Leveque, J.W. Pearson (2022). *Parameter-Robust Preconditioning for Oseen Iteration Applied to Stationary and Instationary Navier–Stokes Control*. SIAM Journal on Scientific Computing, 44: 694–722.

[4] S. Leveque, J.W. Pearson (2021). *Fast Iterative Solver for the Optimal Control of Time-dependent PDEs with Crank–Nicolson Discretization in Time*. Numerical Linear Algebra Appl., 129:1–23.

*EPSRC Centre for Doctoral Training in Mathematical Modelling, Analysis and Computation (MAC-MIGS) funded by the UK Engineering and Physical Sciences Research Council (grant EP/S023291/1), Heriot-Watt University & University of Edinburgh

Toward Bayesian models of growing tumors

Stefan Engblom[1] and Erik Blom[1]

[1]Department of Information Technology, Division of Scientific Computing, Uppsala University, Sweden
{stefane, erik.blom}@it.uu.se

Abstract

The study of growing tumors has been a long-standing challenge in cancer research. For this reason it has also been a recurrent modeling theme *in silico*, e.g., relying on PDEs or agent-based simulation frameworks. Inspired by experimental progress and improved *in vitro* data streams we aim to develop a Bayesian model of avascular tumors. This requires the development of a well-understood and highly parsimonious computational model, preferably from first principles. The model should also be equipped with a rigorous mathematical analysis, which enables the formation of sound Bayesian priors. The challenge is then to intersect the available data with the computational model in a Bayesian sense.

In the talk, we will present a stability analysis of a certain mean-field PDE model, which serves as the basis of our computational model. We will explain how a suitable likelihood can be deduced from a stochastic interpretation of the model. We will also present preliminary results from a synthetic setting.

In summary, we take the first steps toward a Bayesian approach to analyzing experimental data from *in vitro* tumors. We anticipate that our work opens up for an improved analytic understanding of avascular tumor growth.

Keywords: Computational cell biology, Saffman-Taylor instability, Kalman filter, Avascular tumor model.

References

[1] E. Blom, S. Engblom (2023). *Morphological stability for in silico models of avascular tumors.* Manuscript.

[2] S. Engblom, D. B. Wilson, R. E. Baker (2018). *Scalable population-level modelling of biological cells incorporating mechanics and kinetics in continuous time.* Roy. Soc. Open Sci., 5(8):180379.

Bridging modelling and numerical simulations

Christian Engwer[1] and Mariya Ptashyk[2]

[1]Applied Mathematics, University of Münster, Germany
[2]Department of Mathematics, Heriot-Watt University, The Maxwell Institute for Mathematical Sciences, Scotland, UK
christian.engwer@uni-muenster.de; m.ptashnyk@hw.ac.uk

Abstract

The advance in the experimental possibilities and availability of data allow us to develop complex models for a better understanding of many different biological processes. In this talk we will set the stage for the following talks, introducing the fundamental challenges and questions.

We discuss challenges to link mathematical models back to biological or medical data, how numerical methods can contribute and how this leads to new mathematical research questions in modelling and numerics. We will showcase the necessity for sophisticated modelling, as well as the development of modern numerical schemes, taking examples from real clinical and biological applications.

Keywords: Multi-scale Modelling, Elliptic Partial Differential Equations, Parabolic Differential Equations, Medical Imaging, Stationary Approximation

Curvotaxis - How does curvature influence cellular motion?

Lea Happel[1] and Axel Voigt[1,2]

[1]Institute of Scientific Computing, TU Dresden, Germany
[2]Center for Systems Biology Dresden & Cluster of Excellence, Physics of Life, TU Dresden, Germany
Lea.Happel@tu-dresden.de

Abstract

Cells sense and respond to local curvature [2], essentially by aligning the filaments with the principal curvature directions. Such an alignment can be explained by extrinsic curvature effects, as established in the theory of surface liquid crystals. In the context of cell alignment these implications are not explored. We attempt to close this gap here with including terms to account for extrinsic curvature effects in our energy.

Curvature influences not only the shape of a single cells, it also plays an important role regarding cellular motion. Recently first experimental results point to a strong connection between (extrinsic) curvature and collective cell rotation. This is mainly investigated for cylindrical epithelial tissues of MDCK cells. Mathematically this has been modelled by a coarse-grained continuous active polar gel model [5] with ad hoc added linear curvature terms, similar to [1]. These models neglect cellular properties and cell interactions. We therefore propose a multiphase field model similar to [4] to take these properties into account and add terms that account for extrinsic curvature contributions. We consider cylindrical shapes and compare our results with the experimental data of MDCK cells [3]. Additionally we give a short outlook on surfaces with non-constant Gaussian curvature.

Keywords: Collective Motion, Active Matter, Extrinsic Curvature Effects, Phase Field Model, Surface Cahn Hilliard, Surface Finite Elements, Mathematical Biology

References

[1] S. Bell, S.-Z. Lin, J.-F. Rupprecht, J. Prost (2022). *Active Nematic Flows over Curved Surfaces.* Physical Review Letter, 129:118001.

[2] S.J.P. Callens, R.J.C. Uyttendaele, L.E. Fratila-Apachitei, A.A. Zadpoor (2020). *Substrate curvature as a cue to guide spatiotemporal cell and tissue organization.* Biomaterials, 232:119739.

[3] A. Glentis, C. Blanch-Mercader et al. (2022). *The emergence of spontaneous coordinated epithelial rotation on cylindrical curved surfaces.* Science Advances, 8:eabn5406.

[4] L. Happel, D. Wenzel, A. Voigt (2022). *Effects of curvature on epithelial tissue - Coordinated rotational movement and other spatiotemporal arrangements.* Europhysics Letter, 138(6):67002.

[5] I. Nitschke, M. Nestler, S. Praetorius, H. Löwen, A. Voigt (2018). *Nematic liquid crystals on curved surfaces: a thin film limit.* Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 474:20170686.

Active contraction of axons: Mathematical modelling, numerical implementation and comparison with experiments

Giulio Lucci*[1], Dario Andrini[2], Valentina Balbi[3], Giulia Bevilacqua[4], Giulia Pozzi[1], and Davide Riccobelli[2]

[1]Department of Mathematical Sciences, Politecnico di Torino, Italy
[2]MOX - Department of Mathematics, Politecnico di Milano, Italy
[3]School of Mathematical and Statistical Sciences, NUI Galway, Ireland
[4]Department of Mathematics, University of Pisa, Italy

Abstract

Recent experimental evidence suggests that axons, i.e. the slender protrusions of neurons that carry electro-chemical signals to neighbouring cells, possess a very mechanosensitive cytoskeleton. In particular, the axonal cortex that surrounds the cytoplasm is capable of developing an active contractility both in the axial and in the hoop directions [2] when the axon undergoes mechanical deformations or alterations due to drugs. However, the mechanisms that guide the synergistic interplay between the axial and circumferential active contractions are not yet fully elucidated.

Motivated by these observations, we present a mathematical model for axon mechanics based on the active strain theory [1, 3]. The axon is considered as a continuum elastic body composed of an inner passive part, representing the cytoplasm, and an outer coating able to actively contract in two directions. Then, the evolution equations for the active strains are derived in a thermodynamically consistent way by using the Coleman-Noll procedure. Such an approach allows to shed light on the coupling between the axial and circumferential contractions, which naturally emerges through the Mandel stress tensor [1]. Under the simplifying assumption of incompressibility, we propose a qualitative analysis of the system and prove the existence of a stable equilibrium solution for the active strains, which we study as a function of the applied stretch. Finally, we discuss the numerical implementation of the model and show the results of numerical simulations, compared with experimental data [2]. The results about variations in the axonal diameter following drug treatments or uniaxial stretch are in very good agreement with experimental findings. In particular, our model outcomes support the hypothesis of a coupled mechanism between the axial and hoop active stretches.

Keywords: Axons, Active contractility, Nonlinear elasticity, Finite element simulations

References

[1] D. Andrini, V. Balbi, G. Bevilacqua, G. Lucci, G. Pozzi, D. Riccobelli (2022). *Mathematical modelling of axonal cortex contractility.* Brain Multiphysics 3:100060.

[2] A. Fan, A. Tofangchi, M. Kandel, G. Popescu, and T. Saif (2017). *Coupled circumferential and axial tension driven by actin and myosin influences in vivo axon diameter.* Sci. Rep. 7:14188.

[3] D. Riccobelli (2021). *Active elasticity drives the formation of periodic beading in damaged axons.* Phys. Rev. E 104:024417.

*giulio.lucci@polito.it

Stokes-flow models of tissue growth

Chandrasekhar Venkataraman[1] and John King[2]

[1]School of Mathematical and Physical Sciences, University of Sussex, UK
[2]School of Mathematical Sciences, University of Nottingham, UK
c.venkataraman@sussex.ac.uk; john.king@nottingham.ac.uk

Abstract

We formulate, analyse and numerically simulate what are arguably the simplest Stokes-flow free boundary problems relevant to tissue growth, extending the classical Stokes free boundary problem by incorporating (i) a volumetric source (the nutrient-rich case) and (ii) a volumetric sink, a surface source and surface compression (the nutrient-poor case). Both two- and three-dimensional cases are considered. A number of phenomena are identified and characterised thereby, most notably a buckling-associated instability in case (ii).

Keywords: Stokes flow, Free boundary problems, Finite elements, Tissue growth

References

[1] J.R. King, C. Venkataraman (2021). *Free boundary problems for Stokes flow, with applications to the growth of biological tissues.* Interfaces and Free Boundaries, 23, 433–458.

Simulation of Post Burned Skin using Principles from Morphoelasticity

Fred Vermolen[1] and Ginger Egberts*[2]

[1]Department of Mathematics and Statistics, University of Hasselt, Belgium
[2]Delft Institute of Applied Mathematics, Delft University of Technology, The Netherlands
Fred.Vermolen@uhasselt.be; egberts.ginger@gmail.com

April 21, 2023

Abstract

Burn injuries can leave hypertrophic scars and/or contractures in skin. Hypertrophic scars impair the patient's appearance, and contractures negatively impact the patient's mobility. Some burn injuries develop both or one of the earlier-mentioned complications, whereas sometimes a burn with the same characteristics does not at all lead to any problems. Our research is devoted to mathematically simulate the evolution of post-burnt skin. The model is based on principles from morphoelasticity, where microstructural changes of the tissue are combined with stresses and displacement that result from cellular traction forces. The mechanical model is nonlinearly coupled to a biochemical model for the balance of several cell types (fibroblasts and myofibroblasts), chemokines and collagen. During the talk, some mathematical issues will be addressed, such as monotonicity of the numerical solution, stability of the (exact) solution [1], as well as stability of the numerical solution. Furthermore, we will show some of the implications and uncertainty quantification [2] of the model as well as a clinical application of the model [3, 4].

Keywords: Morphoelasticity, Stability, Uncertainty Quantification

References

[1] G. Egberts, F.J. Vermolen, P.P.M. van Zuijlen (2023). *Stability of a two–dimensional biomorphoelastic model for post–burn contraction.* J. Math.Biol. 86 (4): 59.

[2] G. Egberts, F.J. Vermolen, P.P.M. van Zuijlen (2023). *Sensitivity of a two–dimensional biomorphoelastic model for post–burn contraction.* Biomech. Modell. Mechanobiol. 22: 105–121.

[3] G. Egberts, M. Schaaphok, F.J. Vermolen, P.P.M. van Zuijlen (2022). *A Bayesian finite-element trained machine learning approach for predicting post–burn contraction.* Neur. Comput. Appl. 34 (11): 8635–8642.

[4] G. Egberts, F.J. Vermolen, P.P.M. van Zuijlen (2023). *High speed predictions of post–burn contraction using a neural network trained on 2D–finite element simulations.* Front. Appl. Math. Stat. 9: 1098242.

*The Dutch Burns Foundation is thanked for financial support in Project 17.105.

MS18 - Efficient numerical methods for direct or inverse wave propagation problems

Using spectral information for the robust solution of positive Maxwell problems via domain decomposition

Niall Bootland[1], Victorita Dolean[2,3], Frédéric Nataf[4], and Pierre-Henri Tournier[4]

[1]STFC Rutherford Appleton Laboratory, UK
[2]Department of Mathematics and Statistics, University of Strathclyde, UK
[3]Laboratoire J.A. Dieudonné, CNRS, University Côte d'Azur, France
[4]Laboratoire J.-L. Lions, Sorbonne University, France
niall.bootland@stfc.ac.uk; {nataf, tournier}@ljll.math.upmc.fr;
work@victoritadolean.com

Abstract

We consider the solution of linear systems arising from finite element discretisations of positive Maxwell problems using domain decomposition. In order to provide a robust solver, we design adaptive coarse spaces that complement a near-kernel space made locally from the gradient of scalar functions. The new class of preconditioner is inspired by the idea of subspace decomposition, but is based on spectral coarse spaces, and are specially designed for curl-conforming discretisations of Maxwell's equations in heterogeneous media. This extends results for the nodal auxiliary space preconditioner of Hiptmair and Xu [1] to an approach that is further robust in the variable coefficient case and for non-convex domains at the expense of a larger coarse space. Numerical results will demonstrate the effectiveness of our approach even with the presence of many holes penetrating the domain, where the nodal auxiliary space preconditioner fails.

Keywords: Maxwell's equations, domain decomposition, preconditioning

References

[1] R. Hiptmair, J. Xu (2007). *Nodal auxiliary space preconditioning in* **H**(**curl**) *and* **H**(div) *spaces.* SIAM J. Numer. Anal. 45(6), 2483–2509.

Time-dependent electromagnetic scattering from dispersive material laws

Jörg Nick[1], Selina Burkhard*[2], and Christian Lubich[1]

[2]Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, Germany
[2]selina.burkhard@kit.edu
[1]Mathematisches Institut, Universität Tübingen, Germany

Abstract

Electromagnetic scattering problems in the context of time-varying material laws are a natural topic of interest, both in the physical and the mathematical literature.

In the present talk, we study the numerical treatment of a scattering problem

$$\begin{aligned} \varepsilon^{\pm}(\partial_t)\,\partial_t \mathbf{E}^{\pm} - \operatorname{curl} \mathbf{H}^{\pm} &= 0, \\ \mu^{\pm}(\partial_t)\,\partial_t \mathbf{H}^{\pm} + \operatorname{curl} \mathbf{E}^{\pm} &= 0, \end{aligned} \quad \text{in } \Omega^{\pm},$$

where $\varepsilon(\partial_t)$ denotes a temporal convolution with a kernel function determined by the physical properties of the medium. Inside of the scatterer Ω^-, a general class of retarded material laws determines the wave-material interaction. The above Maxwell equations are equipped with transmission conditions on the boundary $\Gamma = \partial\Omega^{\pm}$,

$$\begin{aligned} \gamma_T \mathbf{E}^- &= \gamma_T \mathbf{E}^+ + \gamma_T \mathbf{E}^+_{\mathrm{inc}}, \\ \gamma_T \mathbf{H}^- &= \gamma_T \mathbf{H}^+ + \gamma_T \mathbf{H}^+_{\mathrm{inc}}, \end{aligned} \quad \text{on } \Gamma,$$

enforcing continuity of the electromagnetic fields. The resulting problem formulation is nonlocal in time (in the interior of the scatterer) and posed on an unbounded domain Ω^+, thus creating a challenging problem for practical computations.

In order to overcome these difficulties, a formulation based on time-dependent boundary integral equations is proposed and analyzed, which is fully formulated on the surface of the scatterer. Discretizing the boundary integral equation by convolution quadrature in time and boundary elements in space yields a provably stable and convergent method, that is fully parallel in time and space. Under regularity assumptions on the exact solution we derive error bounds with explicit convergence rates in time and space.

Keywords: error analysis, full discretization, electromagnetic scattering problems, retarded material laws, convolution quadrature, boundary elements

*Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173.

Strong norm error bounds for quasilinear wave equations under weak CFL-type conditions

Benjamin Dörich*[1], Jan Leibold[1], and Bernhard Maier[1]

[1]Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, Germany
[1]benjamin.doerich@kit.edu

Abstract

In this talk, we consider a class of quasilinear wave equations

$$\lambda(u(t))\partial_t^2 u(t) = \Delta u(t) + f(t, u(t), \partial_t u(t)),$$

on a smooth, bounded domain. We discretize it in space with isoparametric finite elements, and apply a semi-implicit Euler and midpoint rule as well as the exponential Euler method to obtain three fully discrete schemes. We first derive error bounds in norms which are stronger than the classical $H^1 \times L^2$ energy norm, and then show how this allows us to obtain only weak CFL-type conditions and to include linear elements. We will first discuss the spatially discretized case in order to transfer the techniques to the fully discrete case.

Keywords: error analysis, full discretization, quasilinear wave equation, nonconforming space discretization, isoparametric finite elements, a-priori error bounds

References

[1] B. Dörich, J. Leibold, B. Maier (2021). *Maximum norm error bounds for the full discretization of non-autonomous wave equations*. CRC 1173 Preprint 2021/47, Karlsruhe Institute of Technology.

[2] B. Dörich (2022). *Strong norm error bounds for quasilinear wave equations under weak CFL-type conditions*. CRC 1173 Preprint 2022/52, Karlsruhe Institute of Technology.

*Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173.

Symplectic FEM–QTT solution of the acoustic wave equation

Sara Fraschini[1], Vladimir Kazeev[1], and Ilaria Perugia[1]

[1]Fakultät für Mathematik, Universität Wien
{sara.fraschini, vladimir.kazeev, ilaria.perugia}@univie.ac.at

Abstract

Dealing with wave propagation problems presents challenges such as high-frequency oscillations and singularities [2]. As a result, accurate finite element approximations may require high mesh resolution, leading to large computational complexities. In this setting, suitable compression techniques, like the Quantized Tensor Train (QTT) decomposition [4, 5], are necessary to make computations affordable. The QTT decomposition is a multilevel construction that successively separates the levels of the data. The reason why this tensor-structured approach is appealing is that it results in compressed and adaptive approximations that rely on simple discretizations [1, 3]. In this talk, we devise a symplectic Hamiltonian finite element method for the acoustic wave equation, motivated by the enhanced accuracy of energy-preserving numerical methods. By employing a BPX preconditioner, the energy-conservative scheme that we provide is uniformly well-conditioned with respect to the discretization parameter. We then investigate the multilevel low-rank tensor structure of the proposed numerical scheme by exploiting the self-similarity of data across different refinement levels, resulting in QTT complexity reduction.

Keywords: Acoustic wave equation, Quantized tensor train decomposition, Finite element method, Symplecticity, BPX preconditioner

References

[1] M. Bachmayr, V. Kazeev (2020). *Stability of low-rank tensor representations and structured multilevel preconditioning for elliptic PDEs.* Found. Comput. Math., 20(5), 1175–1236.

[2] P. Bansal, A. Moiola, I. Perugia, Ch. Schwab (2021). *Space–time discontinuous Galerkin approximation of acoustic waves with point singularities.* IMA J. Numer. Anal., 41(3), 2056–2109.

[3] V. Kazeev, Ch. Schwab (2018). *Quantized tensor-structured finite elements for second-order elliptic PDEs in two dimensions.* Numer. Math., 138, 133–190.

[4] I. V. Oseledets (2010). *Approximation of $2^d \times 2^d$ matrices using tensor decomposition.* SIAM J. Matrix Anal. Appl., 31(4), 2130–2145.

[5] I. V. Oseledets (2011). *Tensor-train decomposition.* SIAM J. Sci. Comput., 33(5), 2295–2317.

Adaptive Spectral Decompositions For Inverse Medium Problems

Daniel H. Baffet[1], Yannik G. Gleichmann[1], and Marcus J. Grote[1]

[1]Department of Mathematics and Computer Science, University of Basel, Switzerland
{Daniel.Baffet, Yannik.Gleichmann, Marcus.Grote}@unibas.ch

April 29, 2023

Abstract

A nonlinear optimization method is proposed for the solution of inverse medium problems with spatially varying properties. The inverse medium problem is formulated as a PDE-constrained optimization problem and solved by a standard gradient based method. Instead of a grid-based discrete representation, however, the medium is projected to a finite-dimensional subspace [1, 2], which is iteratively adapted during the optimization. Each subspace is spanned by the first few eigenfunctions of a linearized regularization penalty functional chosen a priori. The eigenfunctions are selected according to both their approximation properties and the cost functional's sensitivities [3]. By repeatedly adapting both the dimension and the basis of the search space, regularization is inherently incorporated at each iteration without the need for extra Tikhonov penalization. Convergence is proved under an angle condition, which is included into the resulting *Adaptive Spectral Inversion* (ASI) algorithm. The ASI approach compares favorably to standard grid-based inversion using L^2-Tikhonov regularization when applied to an elliptic inverse problem. The improved accuracy resulting from the new angle condition is further demonstrated via numerical experiments from time-dependent inverse scattering problems.

Keywords: Inverse medium problem, wave scattering, full waveform inversion

References

[1] D.H. Baffet, M.J. Grote, J.H. Tang (2021). *Adaptive spectral decompositions for inverse medium problems*, Inverse Problems, 37, 025006.

[2] D.H. Baffet, Y.G. Gleichmann, M.J. Grote (2022). *Error estimates for adaptive spectral decompositions*. J. Sc. Comp., 93:68.

[3] M.J. Grote, and Y.G. Gleichmann (2023). *Adaptive spectral inversion for inverse medium problems*, preprint, arXiv:2303.05229v1.

Fast solution of time domain electromagnetic wave problems with spline differential forms

Bernard Kapidani[1] and Rafael Vázquez Hernández[1]

[1]Institute of Mathematics, École Polytechnique Fédérale de Lausanne
{bernard.kapidani, rafael.vazquez}@epfl.ch

Abstract

We present a new structure-preserving numerical method which exhibits high order convergence and, contrarily to other high order geometric methods, does not rely on the geometric realization of any dual mesh. We use B-spline based de Rham complexes to construct two exact sequences of discrete differential forms: the primal sequence starts from the space of tensor-product splines which are of degree p in each Cartesian direction and are at least continuously differentiable. Similarly, the dual sequence starts from the space of tensor-product splines of degree $p-1$, which in the parametric domain coincides with the last space of the primal sequence. The differential operators (gradient, curl and divergence) are synthesised into the exterior derivative operator, and due to the high continuity of splines they are well defined both for the primal and the dual sequence. The method is completed with two sets of discrete Hodge-star operators, which relate the spaces of the two sequences, mapping the space of primal k-forms into the space of dual $(n-k)$-forms, and vice versa. These discrete Hodge star operators encapsulate all the metric-dependent properties, and discretise constitutive equations [1].

We introduce a particular choice of the discrete Hodge-star operators inspired by [1] and how to compute them through the fast inversion of Kronecker product matrices. Their stability is ultimately based on the stable pairing between univariate spline spaces of degree p and $p-2$ [2, 3]. We apply the method to the solution of the initial boundary value problem for Maxwell's equations, where we show it to exhibit high order convergence and energy conservation in the usual semi-discrete in space sense, with computational times much lower than for standard Galerkin discretizations [4]. We will also present preliminary results about the extension of the approach to multi-patch geometries, exploiting discontinuous approximation spaces.

Keywords: Splines, Differential Forms, Maxwell, Discontinuous Galerkin

References

[1] R. Hiptmair (2001). *Discrete Hodge operators.* Numer. Math., 90, 265–289. https://doi.org/10.1007/s002110100295.

[2] E. Brivadis, A. Buffa, B. Wohlmuth, L. Wunderlich (2015). *Isogeometric mortar methods.* Comput. Methods Appl. Mech. Eng., Isogeometric Analysis Special Issue, 284, 292–319. https://doi.org/10.1016/j.cma.2014.09.012.

[3] B. Kapidani, R. Vázquez Hernández (2022). *High order geometric methods with splines: an analysis of discrete Hodge-star operators.* SIAM J. Sci. Comput., 44, A3673–A3699. https://epubs.siam.org/doi/10.1137/22M1481762.

[4] B. Kapidani and R. Vázquez Hernández (2023). *High order geometric methods with splines: fast solution with explicit time-stepping for Maxwell equations.* Submitted. http://arxiv.org/abs/2302.04979, arXiv:2302/04979.

Automated approach for source location in shallow waters

Angèle Niclas[1] and Josselin Garnier[1]

[1]CMAP, CNRS, École polytechnique, Institut Polytechnique de Paris, France
{angele.niclas, josselin.garnier}@polytechnique.edu

Abstract

This talk aims to present a fully automated method for recovering the location of a source and medium parameters in shallow waters. Specifically, we consider a scenario where an unknown source emits low-frequency sound waves (typically less than 500 Hz) in a coastal environment. A single hydrophone records the signal at a distance of more than 1 km from the source.

To model the shallow water environment, we use a semi-infinite Pekeris waveguide with a finite layer of water and an infinite layer of sediments. One of the most commonly used and robust techniques to solve the inverse problem in this scenario is Time-of-Arrival estimation (see, for instance, [1]). This method involves measuring the modal travel times $t_n(\omega)$ at the hydrophone and using this information to estimate the distance to the source. Most existing experimental methods take advantage of the modal dispersion curves in the time-frequency domain and consist in warping the signal to extract each modal component, recovering the dispersion curves $\omega \mapsto t_n(\omega)$ associated with each mode using time/frequency analysis, and matching estimated dispersion curves with simulated replicas.

We aim here to present a completely automated method based on these techniques to recover source location in shallow waters using different theoretical arguments:

- Theoretical tools are introduced to understand the robustness of the warping method, and an automated way to separate modal components in the signal is provided.
- Using the spectrogram of each modal component, we investigate the best way to recover modal travel times and provide stability estimates.
- A penalized minimization algorithm is presented to recover estimates of the source location and some medium parameters.

The proposed method is tested on experimental data of right whale gunshot [3] and combustive sound sources [2], demonstrating its effectiveness in real-world scenarios.

Keywords: Underwater acoustics, Source localization, Time-of-Arrival estimation, Shallow water environment

References

[1] J. Bonnel, A. Thode, D. Wright, R. Chapman (2020). *Nonlinear time-warping made simple: A step-by-step tutorial on underwater acoustic modal separation with a single hydrophone.* The Journal of the Acoustical Society of America, 147(3):1897–1926.

[2] J. Bonnel, Y.-T. Lin, D. Eleftherakis, J. A. Goff, S. Dosso, R. Chapman, J. H. Miller, G. R. Potty, (2018). *Geoacoustic inversion on the new england mud patch using warping and dispersion curves of high-order modes.* The Journal of the Acoustical Society of America, 143(5):405–411.

[3] A. Thode, J. Bonnel, M. Thieury, A. Fagan, C. Verlinden, D. Wright, C. Berchok, J. Crance (2017). *Using nonlinear time warping to estimate north pacific right whale calling depths in the bering sea.* The Journal of the Acoustical Society of America, 141(5):3059–3069.

A paraxial approach for the inverse problem of vibroacoustic imaging in frequency domain

Teresa Rauscher*[1]

[1]Department of Mathematics, University of Klagenfurt
teresa.rauscher@aau.at

Abstract

Vibroacoustography by means of ultrasound is an imaging method that was developed to achieve higher resolutions while avoiding the drawbacks of scattering and stronger attenuation. High frequency waves are sent into the medium, they interact nonlinearly and therefore excite a wave field that basically propagates at the difference frequency. Since these high frequency waves show a strongly preferred direction of propagation, we make use of a paraxial approach to arrive at a system of PDEs that involve space dependent parameters. Their reconstruction then yields a spatial image of the region of interest. In this talk, we will deal with the paraxial modeling of vibroacoustic imaging, present a numerical method and derive the adjoint system for solving the inverse problem with Landweber iteration.

Keywords: Vibroacoustic imaging, Paraxial approximation, Parameter identification in PDEs

References

[1] M. Fatemi, J.F. Greenleaf (1998). *Ultrasound-stimulated vibro-acoustic spectography.* Science, 280:82-85.

[2] B. Kaltenbacher (2022). *On the inverse problem of vibro-acoustography.* Meccanica. See also arXiv:2109.01907 [math.AP].

[3] B. Kaltenbacher, T. Rauscher (2023). *Simultaneous reconstruction of sound speed and nonlinearity parameter in a paraxial model of vibro-acoustography in frequency domain.* In submission. See also arXiv:2303.17236 [math.NA].

[4] A.E. Malcolm, F. Reitich, J. Yang, J.F. Greenleaf, M. Fatemi (2008). *A combined parabolic-integral equation approach to the acoustic simulation of vibro-acoustic imaging.* Ultrasonics, 48:553-558.

[5] T. Rauscher. *A paraxial approach for the inverse problem of vibroacoustic imaging in frequency domain.* In preparation.

*supported by the Austrian Science Fund (FWF): DOC 78

A p-version of convolution quadrature in wave propagation

Alexander Rieder[1]

[1]Institute for Analysis and Scientific Computing, TU Wien

Abstract

In this talk, we present a novel approach towards boundary element methods for wave propagation. It is based on the convolution quadrature idea by Lubich [1], but, instead of relying on reducing the timestep size in order to achieve higher accuracy, we use the p-refinement paradigm of increasing the order of the method while keeping the timestep size fixed. To get an easily computable and analyzable scheme, we rely on the ideas of discontinuous Galerkin timestepping [2]. This allows us to design a scheme which is root-exponentially convergent for certain very smooth initial conditions. We talk about possibilities to analyze this new scheme, as well its practical implementation and challenges.

Keywords: Convolution quadrature, boundary element method, discontinuous Galerkin

References

[1] C. Lubich (1988). *Convolution quadrature and discretized operational calculus. I.* Numer. Math., 52(2):129–145.

[2] D. Schötzau and C. Schwab (2000). *An hp a priori error analysis of the DG time-stepping method for initial value problems.* Calcolo, 37(4):207–232.

Convergence analysis of semi-implicit multi-step one-shot methods for regularized linear inverse problems

Marcella Bonazzoli[1], Houssem Haddar[1], and Tuan-Anh Vu[1]

[1]Inria, UMA, ENSTA Paris, Institut Polytechnique de Paris, France
{marcella.bonazzoli, houssem.haddar, tuan-anh.vu}@inria.fr

Abstract

When an inverse problem is solved by a gradient-based optimization algorithm, the corresponding forward and adjoint problems, which are employed to compute the gradient, can be also solved iteratively. The idea of iterating at the same time on the inverse problem unknown and on the forward and adjoint problem solutions yields to the concept of one-shot inversion methods. This was first introduced in [3]. We are especially interested in the case where the inner iterations for the direct and adjoint problems are incomplete, that is, stopped before achieving a high accuracy on their solutions. Here, we begin with the simplest framework: we focus on general linear inverse problems and generic fixed-point iterations for the associated forward problem. In [1, 2], we analyze variants of the so-called multi-step one-shot methods, in particular semi-implicit schemes with a regularization parameter. By studying the eigenvalues of the block matrix of the coupled iterations, we establish sufficient conditions on the descent step for convergence. Several numerical experiments are provided to illustrate the convergence of these methods in comparison with the classical gradient descent, where the forward and adjoint problems are solved exactly by a direct solver instead. We observe that very few inner iterations are enough to guarantee good convergence of the inversion algorithm, even in the presence of noisy data.

Keywords: inverse problems, one-shot methods, convergence analysis, parameter identification

References

[1] M. Bonazzoli, H. Haddar, T.A. Vu (2022). *Convergence analysis of multi-step one-shot methods for linear inverse problems*, Research Report RR-9477, Inria Saclay, ENSTA ParisTech.

[2] M. Bonazzoli, H. Haddar, T.A. Vu (2023, preprint). *On the convergence analysis of one-shot inversion methods.*

[3] S. Ta'asan. *"One Shot" Methods for Optimal Control of Distributed Parameter Systems I: Finite Dimensional Control*, Technical Report 91-2, ICASE, Hampton, 1991.

Wave propagation in time-varying media

Barbara Verfürth[1]

[1]Institute for Numerical Simulation, University of Bonn
verfuerth@ins.uni-bonn.de

Abstract

In the last years, there has been an increasing interest in time-modulated materials to obtain enhanced properties. As mathematical model, we study the classical wave equation with time-dependent coefficient, which may also include spatial multiscale features.

In the main part, we present a numerical multiscale method for spatially multiscale, (slowly) time-evolving coefficients [1]. The method is inspired by the Localized Orthogonal Decomposition (LOD) and entails time-dependent multiscale spaces. We provide a rigorous a priori error analysis for the considered setting. Numerical examples illustrate the theoretical findings and investigate an adaptive approach for the computation of the time-dependent basis functions. This part of the talk is based on joint work with Bernhard Maier.

Finally, we give a brief outlook on the case when the coefficients are multiscale with respect to time. As temporal and spatial scales may couple in many ways, we focus on spatially homogeneous, temporal multiscale coefficients as first step.

Keywords: waves, multiscale method, numerical homogenization, time-varying media

References

[1] B. Maier, B. Verfürth (2022). *Numerical upscaling for wave equations with time-dependent multiscale coefficients*. Multiscale Model. Simul., 20(4), 1169–1190.

Simultaneous interface identification and soundspeed reconstruction of layered media using acoustic wave

Otmar Scherzer[1,2,3] and Huidong Yang[1,3]

[1]Faculty of Mathematics, University of Vienna
[2]Johann Radon Institute for Computational and Applied Mathematics (RICAM)
[3]Christian Doppler Laboratory for Mathematical Modeling and Simulation of Next Generations of Ultrasound Devices (MaMSi)
{otmar.scherzer, huidong.yang}@univie.ac.at

Abstract

We present a full waveform inversion (FWI) method of simultaneous interface identification and soundspeed reconstruction in layered media using an acoustic pressure wave equation. The method is based on the numerical solution of the underlying acoustic wave equation in a layered medium of piecewise constant soundspeed. We have employed a conventional space-time finite difference discretization scheme for the simulations of both the forward and backward wave propagation arising in the inversion procedure. In particular, a certain number of sources are placed on the top of the layered medium. We iteratively identify the interface and reconstruct the soundspeed from the measured pressure at the receivers. For this, we formulate the least-square misfit between synthetic and observed data, as a functional with respect to both the interface and soundspeed parameter, which aims to simultaneously recover both the interface and soundspeed. The inverse is recast into a PDE constrained optimization problem subject to the wave equation. A gradient descent algorithm is used to solve such an optimization problem. For this, the descent direction is computed via the shape derivative with respect to the interface, and via the adjoint state method using Lagrange multipliers with respect to the soundspeed.

Keywords: FWI, inversion, gradient descent, shape derivative, acoustic wave equation, interface identification, adjoint state method, Lagrange multipliers, soundspeed reconstruction, ultrasound imaging

MS19 - Addressing Industrial Challenges in The Numerical Modeling of Flow and Geomechanics in Porous Media

Disorder: An Innovative numerical algorithm for randomness estimation in seismic exploration

Saleh Al-Dossary[1] and Qiang Fu[1]

[1]Saudi Aramco
{Saleh.dossary.6, qiang.fu.2}@aramco.com

Abstract

Seismic exploration, which is both the kernel of current hydrocarbon exploration in energy industry, and an important application of applied geophysics, relies on the development of numerical algorithms. Reliable characterization and accurate identification of geological features, such as fault and channel, from seismic data is one of the top priority prerequisites for seismic exploration. Although seismic data are usually stratified, coherent and continuous, there are areas in seismic data that look chaotic i.e. high randomness zones. Thus, the industry requires an innovative numerical algorithm for randomness estimation in seismic exploration. The randomness of seismic data is mainly due to three reasons: 1) random reflection/refraction energy from certain subsurface geological structures, e.g. fraction zone, gas chimney, karst collapse, and terminated unconformity; 2) suboptimum acquisition and consequential low data quality, e.g. all kinds of noise; 3) imperfect data processing/imaging procedure, e.g. inaccurate migration velocity, imaging artifacts, and operator aliasing. A reliable method to estimate the spatial distribution of the randomness level in seismic data is essential and indispensable for geological feature (e.g. fracture, fault, channel, gas chimney) characterization. Estimation of randomness spatial distribution with high resolution will assist geological feature characterization in multiple ways: 1) identify certain geological features such as fracture zones, gas chimneys, karst collapse, terminated unconformity or other random reflection/refraction related features; 2) indicate seismic data quality and random noise level, e.g. recognizing boundary problem between merged surveys; 3) provide covariance matrix for seismic inversion or uncertainty index for interpretation and reservoir simulation. There have been numerous early attempts at estimating the randomness level in seismic data, among them are cross-correlation based algorithms, structure tensor-based algorithms, grey level co-occurrence matrix-based algorithms, etc. In this article, an innovative numerical algorithm: disorder seismic attribute, is proposed to address this problem, which differs from its forerunners. This method is based on convolutional filtering method and uses a second order differential operator designed by optimization approach, which is sensitive to chaotic and noisy area but not organized area.

Keywords: Seismic noise, Chaos, Convolutional filtering

References

[1] J. Immerkaer (1996). *Fast noise variance estimation.* Computer Vision and Image Understanding, 64, 300–302.

[2] B. Dash, K.A. Obaidullah (1970). *Determination of signal and noise statistics using correlation theory.* Geophysics, 35, 24–32.

A Priori Error Estimates for a Discretized Multirate Fixed-Stress Split Poro-Elastic System

Tameem Almani[1] and Kundan Kumar[2]

[1]Saudi Aramco, Dhahran, Saudi Arabia
[2]Department of Mathematics, University of Bergen, Norway
tameem.almani@aramco.com; kundan.kumar@math.uib.no

Abstract

Recently, the coupling between reservoir flow and geomechanics received more importance and attention, as more unconventional resources are being extracted and utilized worldwide. To solve the underlying coupled problem, several sequential coupling schemes were proposed and analyzed. In such schemes, the flow and mechanics problems are solved separately (decoupled), and a coupling iteration is imposed between the two to ensure convergence for a particular time step. Due to the different time-scales of the two sequentially coupled problems, the flow problem can assume a finer time step compared to the mechanics problem resulting in what is known as the multirate scheme [1]. In this work, we derive a priori error estimates for the multirate fixed stress split iterative coupling scheme. This scheme is a generalization of the well-known fixed-stress split scheme [2] in which the flow problem takes multiple fine time steps within one coarse mechanics time step. To the best of our knowledge, this is the first time in literature a priori error estimates are derived for the multirate fixed stress split iterative coupling scheme in poro-elastic media.

Keywords: Multirate scheme, Fixed stress split, Coupled flow and geomecahnics problem, A priori error estimates

References

[1] T. Almani, K. Kumar, A. Dogru, G. Singh, M. F. Wheeler (2016). *Convergence analysis of multirate fixed-stress split iterative schemes for coupling flow with geomechanics.* Computer Methods in Applied Mechanics and Engineering 311, 180-207.

[2] V. Girault, M. F. Wheeler, T. Almani, S. Dana (2019). *A priori error estimates for a discretized poro-elastic–elastic system solved by a fixed-stress algorithm.* Oil & Gas Science and Technology–Revue d'IFP Energies nouvelles 74, 24.

Comparison of the different CFD coupled DEM models for polymer flooding

Yerlan Amanbek[1], Daniyar Kazidenov[1], and Sagyn Omirbekov[1]

[1]Department of Mathematics, Nazarbayev University, Astana, Kazakhstan
{yerlan.amanbek, daniyar.kazidenov, sagyn.omirbekov}@nu.edu.kz

Abstract

Polymer Flooding is one of the techniques used in the development of reservoirs to increase oil recovery. In addition, Sand Production has the damaging impact on the production of wells. In this talk, we compare different CFD-DEM numerical models for Sand Production using different mathematical formulations in CFD, such as the Polymer Flooding, and the modified cohesive contact model in DEM. Several CFD-DEM model implementations are considered with mathematically similar formulations [1, 2]. The Polymer Flooding problem in CFD is treated as a non-Newtonian flow using the power law model. We present numerical results of Sand Production rates in weakly consolidated sandstone for the different considered models.

Keywords: CFD-DEM model, Navier-Stokes equations, Polymer flooding

References

[1] F. Chen, E.C. Drumm, G. Guiochon (2011). *Coupled discrete element and finite volume solution of two classical soil mechanics problems.* Computers and Geotechnics, 38(5), 638-647P.

[2] L. Guo, K. Morita, Y. Tobita (2014). *Numerical simulation of gas–solid fluidized beds by coupling a fluid-dynamics model with the discrete element method.* Annals of Nuclear Energy, 72, 31-38.

Solving Groundwater Flow Equation using Physics-Informed Neural Networks

Salvatore CUOMO*[1]

[1]Department of Mathematics and Applications, University of Naples Federico II
salvatore.cuomo@unina.it

Abstract

In recent years, Scientific Machine Learning (SciML) methods for solving partial differential equations (PDEs) have gained wide popularity. Within such a paradigm, Physics-Informed Neural Networks (PINNs) are novel deep learning frameworks for solving forward and inverse problems with non-linear PDEs. Recently, PINNs have shown promising results in different application domains. In this paper, we approach the groundwater flow equations numerically by searching for the unknown hydraulic head. Since singular terms in differential equations are very challenging from a numerical point of view, we approximate the Dirac distribution by different regularization terms. Furthermore, from a computational point of view, this study investigate how a PINN can solve higher-dimensional flow equations. In particular, we analyze the approximation error for one and two-dimensional cases in a statistical learning framework. The numerical experiments discussed include one and two-dimensional cases of a single or multiple pumping well in an infinite aquifer, demonstrating the effectiveness of this approach in the hydrology application domain.

Keywords: Physics-Informed Neural Networks, Hydraulic Head, Scientific Machine Learning.

References

[1] S. Cuomo, V.S.D. Cola, F. Giampaolo, G. Rozza, M. Raissi, F. Piccialli (2022). *F. Scientific Machine Learning through Physics-Informed Neural Networks: Where we are and What's next.* Journal of Scientifc Computing.

[2] S. Cuomo, F. Giampaolo, S. Izzo, C. Nitsch, F. Piccialli, C. Trombetti (2022). *A physics-informed learning approach to Bernoulli-type free boundary problems.* Computers & Mathematics with Applications, 128, 34-43.

*joint work with M.O.D.A.L. Laboratory - Naples, `http://www.labdma.unina.it`, Università degli Studi di Napoli Federico II

Mixed discretization for coupled flow and mechanics in a fractured porous medium

Kundan Kumar[1], Omar Duran[1], Maarten de Hoop[2], and Solveig Stefansdottir[1]

[1]Vista CSD, Department of Mathematics, University of Bergen, Norway
[2]Simons Chair, CAM and Earth Science, Rice University, USA
{kundan.kumar, omar.duran, solveig.stefansdottir}@uib.no; mvd2@rice.edu

Abstract

We present a mixed dimensional model for a fractured poro-elasic medium. The fracture is a lower dimensional surface embedded in a bulk poro-elastic matrix. The flow equation on the fracture is a Darcy type model that follows the cubic law for permeability. The bulk poro-elasticity is governed by fully dynamic Biot equations. The resulting model is a mixed dimensional type where the fracture flow on a surface is coupled to a bulk flow and geomechanics model. We consider a fully mixed discretization for the model equations. We consider a fully mixed Biot formulation based on a weakly symmetric stress-displacement-rotation elasticity system and Darcy velocity-pressure flow formulation. For the fracture flow, we consider again a Darcy velocity-pressure formulation but now on the fracture surface. Existence and uniqueness of a solution are established for the continuous weak formulation. Stability and error estimates are derived for both the semi-discrete, continuous-in-time, and fully discrete mixed finite element approximation. Numerical experiments are presented to verify the theoretical results. We further discuss the extensions including considering a fully dynamic Biot equation, that is, including an inertia term and iterative methods for the coupled model.

Keywords: Fractured porous medium, Darcy flow, Mixed discretizations, Biot model

References

[1] V. Girault, M. F. Wheeler, K. Kumar, G. Singh (2019). *Mixed formulation of a linearized lubrication fracture model in a poro-elastic medium.* Contributions to Partial Differential Equations and Applications, Springer, 171–219.

[2] V. Girault, M. F. Wheeler, B. Ganis, and M. E. Mear (2015). *A lubrication fracture model in a poro-elastic medium. mathematical models and methods in applied sciences.* Mathematical Models and Methods in Applied Sciences, 25, 587–645.

[3] I. Ambartsumyan, E. Khattatov, J. M. Nordbotten, I. Yotov (2020).*A multipoint stress mixed finite element method for elasticity on simplicial grids.* SIAM Journal on Numerical Analysis 58, 1, 630-656.

Parallel multiscale methods on High-Performace-Computing (HPC) Architectures: Design aspects and performance analysis

Abdulrahman Manea[1]

[1]Saudi Aramco
abdulrahman.manea@aramco.com

Abstract

Multiscale methods are popular multi-level methods that allow the efficient solution of coupled flow and transport problems using two (or more) resolution scales. In their general form, multiscale methods map the problem into an auxiliary reduced-size space to solve it efficiently there and then map it back to the original (i.e. reference) space. They can be applied as a single-pass method to obtain an approximate solution, or used in an iterative setting to converge to the exact solution (within machine-precision). In the latter settings, multiscale-based solvers are of particular interest for large-scale scalable computing as they inherently have a large degree of parallelism, offering huge potential to effectively exploit contemporary massively parallel high-performance-computing (HPC) architectures. However, a multiscale-based solver involves multiple kernels with varying control and data-flow patterns requiring special design for achieving good scalability. This is demonstrated by two widely-adopted multiscale methods, namely the Multiscale Finite Volume (MSFV) method (Jenny et al. 2003) and the Multiscale Restriction-Smoothed Basis (MsRSB) (Møyner and Lie 2016) method, where both methods are used within the algebraic multiscale solver (AMS) framework (Wang et al. 2014). The parallel design of both methods is discussed on two common HPC architectures, namely, the multi-core architecture and the GPU architecture. This includes analyzing design choices for key kernels in both solvers, such as basis function computation, coarse-scale solver, prolongation, restriction and local smoothing. The parallel scalability of the two parallel multiscale-based solvers is demonstrated using problems derived from the highly heterogeneous SPE10 Comparative Solution Benchmark (Christie and Blunt 2001), with problem sizes ranging from millions to tens of millions of unknowns. The multi-core implementation is benchmarked on Intel's Cascade Lake Xeon® Gold 6246 CPU, while the GPU implementation is benchmarked on Nvidia Volta V100 GPUs.

Keywords: Multiscale Methods, Parallel Linear Solvers, High-Performance Computing, Multi-core Parallelization, GPU Parallelization

References

[1] M. Christie, M. Blunt (2001). *Tenth SPE comparative solution project: A comparison of upscaling techniques*. SPE Reservoir Evaluation & Engineering, 4(04):308–317.

[2] O. Møyner, K.A. Lie.(2016). *A multiscale restriction-smoothed basis method for compressible black-oil models*. SPE Journal 21.

[3] P. Jenny, S.H. Lee, H.A. Tchelepi (2003). *Multi-scale Finite-volume Method for Elliptic Problems in Subsurface Flow Simulation*. J. Comput. Phys., 187(1):47–67, May 2003. ISSN 0021-9991. doi: 10.1016/S0021-9991(03)00075-5.

A linear iterative scheme for nonlinear, degenerate parabolic equations modelling unsaturated flow in porous media

Ayesha Javed[1], Koondanibha Mitra[1], and Iuliu Sorin Pop[1]

[1]Data Science Institute, Computational Mathematics Group, Hasselt University
{ayesha.javed, koondanibha.mitra, sorin.pop}@uhasselt.be

Abstract

Porous media flow models are nonlinear evolution equations that may degenerate into elliptic, or hyperbolic ones, depending on the value of the unknown in the model. A prominent example is the Richards equation, which can be casted in the general form

$$\partial_t b(u) - \Delta B(u) = f, \text{ in } [0,T) \times \Omega. \tag{1}$$

Here $T > 0$ is a maximal time and $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ is a Lipschitz domain. f is a given source term (it may depend on u as well), while b and B are given, Lipschitz-continuous functions that may have vanishing derivatives

$$0 \leq b'(u) \leq L_b, \quad \text{and} \quad 0 \leq B'(u) \leq L_B,$$

for all $u \in \mathbb{R}$, for some $Lb, L_B > 0$. Boundary and initial conditions complete the model.

In this talk, we consider the time-discrete elliptic equations, obtained after applying, say, an Euler implicit discretisation. In view of the degenerate character of (1), the Newton scheme is converging under severe restrictions on the time step. Also, a regularisation step is required to guarantee that the iterations are well posed. We present first an iterative scheme that does not require any regularisation. The scheme builds on the ideas in [1, 2]. For this scheme, we prove the linear convergence under a mild restriction (if any) on the time step. This convergence is proved at the level of the elliptic problem, so it is not restricted to any spatial discretisation or mesh. Moreover, each iteration uses the same linear operator (or discretisation matrix), which reduces the total computational complexity. Finally, we present a modified scheme that combines the ideas in [1] and [3], showing an improved the convergence behaviour still with mild restrictions on the time step, at the expense of having an iteration-dependent operator, thus re-calculating the discretisation matrix at every iteration.

Keywords: Degenerate parabolic equations, unsaturated flow in porous media, linear iterative schemes, convergence analysis

References

[1] I.S. Pop, F.A. Radu, P. Knabner (2004). *Mixed finite elements for the Richards' equation: linearization procedure.* J. Comput. Appl. Math., 168, 365–373.

[2] F. List, F.A. Radu (2016). *A study on iterative methods for solving Richards' equation.* Comput. Geosci., 20, 341–353.

[3] K. Mitra, I.S. Pop (2019). *A modified L-Scheme to solve nonlinear diffusion problems.* Comput. Math. Appl., 77, 1722–1738.

MS20 - Modern simulation & data science techniques for computational fluid dynamics problems in the exascale range

Lineal: An Efficient, Hybrid-Parallel Linear Algebra Library

Kurt Böhm[1]

[1]Institute of Mathematics, TU Clausthal
kurt.boehm@tu-clausthal.de

Abstract

Efficiently solving large sparse systems of linear equations arising from the discretization of PDEs is still a challenging problem. To solve large problems on attainable hardware, the new linear algebra library Lineal has been developed.

Lineal uses the preconditioned CG method as its main solver, with an Algebraic Multigrid solver (an optimized version of the AMG from DUNE ISTL) as its main preconditioner. However, Lineal uses a number of techniques to achieve very low memory requirements while providing low runtimes as well as generic and extensible interfaces.

For stencil-based problems, Lineal can compute the matrix elements on the finest grid on the fly and only needs to store the coarse grid hierarchy explicitly. In this case, only a single value (a single byte for some problems) per cell is needed on the finest grid, which drastically reduces memory consumption compared to explicit matrices. Additionally, matrix-vector products are computed using tiling to improve cache utilization. Alternatively, a Compressed Row Storage (CRS) matrix can be used, which supports indices consisting of an arbitrary number of bytes to reduce memory consumption. Furthermore, floating point types can be mixed (almost) arbitrarily to save memory.

Elementary operations are represented as classes that perform element-wise computations, using inlining to combine operations efficiently. Almost all components are fully multithreaded and use explicit SIMD operations to improve performance. Additionally, recent work has added distributed memory parallelization using MPI, allowing for hybrid-parallel computations that utilize a compute cluster while minimizing communication costs.

Lineal has been successfully used to simulate oxygen diffusion in X-ray scans of soil samples, solving instances with more than 10^9 unknowns in 10 to 120 minutes on a single AMD EPYC system with 32 cores and 256 GB of RAM. Tests using this problem show that Lineal performs well compared to existing libraries in terms of runtime and memory consumption.

Keywords: Algebraic Multigrid, Stencil Operators, Multi-threading, MPI, Hybrid Parallelism, SIMD

Towards performance portable algorithms for shallow water equations on unstructured grids

Markus Büttner[1], Vadym Aizinger[1], and Tobias Kenter[2]

[1]Chair of Scientific Computing, University of Bayreuth
[2]Paderborn Center for Parallel Computing
{markus.buettner, vadym.aizinger}@uni-bayreuth.de; kenter@upb.de

Abstract

In this talk, we will discuss our discontinuous Galerkin (DG) finite element implementation for the shallow water equations on unstructured grids. In the focus of our work is the performance portability between CPUs, GPUs and FPGAs – using a common code base. To achieve this goal, we use the SYCL programming model.

The FPGA port [2] of the original CPU implementation [1] was transferred to SYCL. We will show how the SYCL implementation uses the same code for execution on different hardware, and discuss optimizations beneficial for all hardware platforms as well as device-specific optimizations.

Keywords: Shallow water equations, Discontinuous Galerkin, SYCL, Performance Portability

References

[1] V. Aizinger, C. Dawson (2002). *A discontinuous Galerkin method for two-dimensional flow and transport in shallow water*. Advances in Water Resources, 25, 67–84.

[2] T. Kenter, A. Shambhu, S. Faghih-Naini, V. Aizinger (2021). *Algorithm-hardware co-design of a discontinuous Galerkin shallow-water model for a dataflow architecture on FPGA*. In *Association for Computing Machinery: Proceedings of the Platform for Advanced Scientific Computing Conference*, Geneva, 2021, 1–11.

Numerical Analysis of a Time-Simultaneous Multigrid Solver for Stabilized Convection-Dominated Transport Problems

Wiebke Drews[1], Stefan Turek[1], and Christoph Lohmann[1]

[1]Institute of Applied Mathematics, Department of Mathematics,
TU Dortmund University
{wiebke.drews, stefan.turek, christoph.lohmann}@math.tu-dortmund.de

Abstract

The work to be presented in this talk focuses on the one-dimensional convection-diffusion equation, especially in the regime of small diffusion coefficients, which is solved using a time-simultaneous multigrid algorithm closely related to multigrid waveform relaxation [2]. For spatial discretization we use linear finite elements, while the time integrator is given by e.g. the Crank-Nicolson scheme. Blocking all time steps into a global linear system of equations and rearranging the degrees of freedom leads to a space-only problem with vector-valued unknowns for each spatial node. Then, common iterative solution techniques, such as the block Jacobi method or the preconditioned GMRES method, can be used for the numerical solution of the (spatial) problem and allow parallelization in space. We consider a time-simultaneous multigrid algorithm, which exploits space-only coarsening and the solution techniques mentioned above for smoothing purposes. By treating more time steps simultaneously, the dimension of the system of equations increases significantly and, hence, results in a larger number of degrees of freedom per spatial unknown. This can be used to employ parallel processes more efficiently [1]. In numerical studies, the iterative multigrid solution of a problem with up to thousands of blocked time steps is analyzed. For the special case of the heat equation, it is well known that the number of iterations is bounded from above independently of of the number of blocked time steps, the time step size, and the spatial resolution. Unfortunately, stability problems arise for the standard Galerkin method if the diffusion coefficient is small compared to the grid size and the magnitude of the velocity field. Therefore, the influence of VMS-type stabilization techniques [3] is discussed, which remove artificial oscillations in the solution and aim to improve the convergence behavior of the iterative solution algorithm.

Keywords: Convection-diffusion equations, Multigrid waveform relaxation, Variational multiscale methods

References

[1] J. Dünnebacke, S. Turek, C. Lohmann, A. Sokolov, P. Zajac (2021). *Increased space-parallelism via time-simultaneous Newton-multigrid methods for nonstationary nonlinear PDE problems*. The International Journal of High Performance Computing Applications 35.3, pp. 211-225.

[2] J. Janssen, S. Vandewalle (1996). *Multigrid Waveform Relaxation on Spatial Finite Element Meshes: The Continuous-Time Case*. SIAM Journal on Numerical Analysis 33.2, pp. 456–474.

[3] V. John, S. Kaya, W. Layton (2006). *A two-level variational multiscale method for convection-dominated convection-diffusion equations*. Computer Methods in Applied Mechanics and Engineering 195.33, pp. 4594–4603.

Space-time multigrid methods for stabilized convection-diffusion equations arising from flow problems

Jonas Dünnebacke[1] and Stefan Turek[2]

[1]Institute of Applied Mathematics, Department of Mathematics, TU Dortmund University
{jonas.duennebacke, stefan.turek}@math.tu-dortmund.de

Abstract

Usually time dependent evolution equations are solved time step by time step where in each step a system of equations corresponding to the spatial discretization has to be solved. Such methods can only be parallelized in space, but the size of the spatial problem limits the strong scaling behavior. Using multigrid methods that treat multiple time steps in an all-at-once system the parallel scaling can be improved significantly in comparison to geometric multigrid solvers in a time stepping application [2, 4]. Due to the improved communication pattern between the parallel processes, this holds true even if a time-simultaneous multigrid method without temporal parallelization is used [1].

Here, we numerically analyze how such multigrid methods behave for convection-diffusion(-reaction) equations found in flow problems, when the problems are increasingly transport dominated. Then, we show how stabilization techniques, e.g. the variational multiscale method [3], can remedy the emerging problems depending on the discretization of the problem. Furthermore, we show the behavior of such methods for problems with space and time dependent diffusion and convection parameters, that arise in global-in-time solution strategies of the Navier-Stokes equations.

Keywords: parallel-in-time, space-time multigrid, multigrid waveform relaxation, variational multiscale method

References

[1] J. Dünnebacke, S. Turek, C. Lohmann, A. Sokolov, P. Zajac (2021). *Increased space-parallelism via time-simultaneous newton-multigrid methods for nonstationary nonlinear pde problems.* Int. J. High Perform. Comput. Appl., 35(3), 211–225.

[2] M.J. Gander, M. Neumüller (2014). *Analysis of a New Space-Time Parallel Multigrid Algorithm for Parabolic Problems* SIAM J. Sci. Comput., 38(4), A2173 - A2208.

[3] V. John, S. Kaya, W. Layton (2006). *A two-level variational multiscale method for convection-dominated convection-diffusion equations.* Comput. Methods Appl. Mech. Eng., 195(33-36), 4594–4603.

[4] C. Lubich, A. Ostermann (1987). *Multi-grid dynamic iteration for parabolic equations.* BIT, 27(2), 216–234.

Algorithm re-design and code generation for performance improvements of a discontinuous Galerkin shallow water model on CPUs, GPUs, FPGAs and heterogeneous systems

Sara Faghih-Naini[1,2], Vadym Aizinger[1], Sebastian Kuckuk[3,2], Richard Angersbach[2], Christoph Alt[2], Tobias Kenter[4], and Harald Köstler[3]

[1]Chair of Scientific Computing, University of Bayreuth
[2]Chair of Computer Science 10, Friedrich-Alexander Universität Erlangen-Nürnberg
[3]Erlangen National High Performance Computing Center (NHR@FAU), Friedrich-Alexander Universität Erlangen-Nürnberg
[4]Paderborn Center for Parallel Computing (PC2), Paderborn University
{sara.faghih-naini, vadym.aizinger}@uni-bayreuth.de; {sebastian.kuckuk, richard.angersbach, christoph.alt, harald.koeslter}@fau.de; kenter@upb.de

Abstract

Heterogeneous architectures and accelerator hardware have become a clear trend in current high-performance computing environments.

In this talk, we present new numerical, algorithmic, and computational technologies with the potential to be incorporated into future ocean and atmospheric models after successful evaluation. First, we propose a numerical and algorithmic re-design of a p-adaptive quadrature-free discontinuous Galerkin method for the shallow water equations [1]. Our new approach separates the computations of lower-order degrees of freedom from the rest of the discretization, which lets us overlap computations of the lower-order and the higher-order DG solution components. We use automatic code generation [2] to optimize the kernel distribution between the CPU and GPU, achieving significant performance improvements.

Furthermore, we present a new approach to port shallow water simulations to FPGAs based on the same code generation framework in combination with a template-based stencil processing library that provides FPGA-specific optimizations for a streaming execution model [3].

Keywords: Quadrature-free discontinuous Galerkin discretization, Code generation, Shallow water equations, p-adaptivity, Heterogeneous GPU-CPU system, FPGA

References

[1] S. Faghih-Naini, V. Aizinger, S. Kuckuk, R. Angersbach, H. Köstler (2023). *p-adaptive discontinuous Galerkin method for the shallow water equations on heterogeneous computing architectures.* Submitted to Transactions on Mathematical Software.

[2] S. Faghih-Naini, S. Kuckuk, V. Aizinger, D. Zint, R. Grosso, H. Köstler (2020). *Quadrature-free discontinuous Galerkin method with code generation features for shallow water equations on automatically generated block-structured meshes.* Advances in Water Resources, 138, 103552.

[3] C. Alt, T. Kenter, S. Faghih-Naini, J. Faj, J.-O. Opdenhövel, C. Plessl, V. Aizinger, J. Hönig, H. Köstler (2023). *Shallow Water DG Simulations on FPGAs: Design and Comparison of a Novel Code Generation Pipeline.* Accepted at ISC High Performance.

Nonlinear FETI-DP domain decomposition methods combined with deep learning

Axel Klawonn[1], Martin Lanser[1], and Janine Weber[1]

[1]Department of Mathematics and Computer Science, University of Cologne, Germany
{axel.klawonn,martin.lanser,janine.weber}@uni-koeln.de

Abstract

In nonlinear-FETI-DP domain decomposition methods the choice of the nonlinear elimination set and of the coarse space have a huge impact on the nonlinear and linear convergence behavior. In this talk, we will show new results combining recently developed approaches for the adaptive choice of the nonlinear elimination set with adaptive coarse spaces. Additionally, we will discuss approaches to improve the computational efficiency and nonlinear convergence by enhancing Nonlinear-FETI-DP with techniques from machine learning.

Keywords: Nonlinear Domain Decomposition Methods, Nonlinear FETI-DP, Scientific Machine Learning

References

[1] A. Heinlein, A. Klawonn, M. Lanser (2022). *Adaptive Nonlinear Domain Decomposition Methods with an Application to the p-Laplacian*. SIAM J. Sci. Comput. 0, no. 0, S152-S172

[2] A. Klawonn, M. Lanser, O. Rheinbach, M. Uran (2017). *Nonlinear FETI-DP and BDDC methods: a unified framework and parallel results*. SIAM J. Sci. Comput. 39, no. 6, C417-C451

[3] A. Klawonn, M. Lanser, J. Weber (2022). *Learning Adaptive Coarse Basis Functions of FETI-DP*. Technical Report; https://cds.uni-koeln.de/en/technical-report-series

Robust nonlinear two-level Schwarz domain decomposition methods

Martin Lanser[1], Alexander Heinlein[2], and Axel Klawonn[1]

[1]Department of Mathematics and Computer Science, University of Cologne, Germany
[2]Delft Institute of Applied Mathematics, Delft University of Technology, The Netherlands
{martin.lanser,axel.klawonn}@uni-koeln.de; a.heinlein@tudelft.nl

Abstract

Nonlinear domain decomposition methods (DDMs) are efficient alternatives to classical Newton-Krylov-DDMs. In contrast to the latter ones, in nonlinear DDMs, the nonlinear partial differential equation is decomposed into subdomains before linearization, which often improves the nonlinear convergence behavior. To obtain robustness applying nonlinear DDMs to heterogeneous multi-scale or other sophisticated nonlinear problems, a global and coarse second level should be included. In this talk, several two-level nonlinear Schwarz methods for heterogeneous problems are discussed and compared.

Keywords: Nonlinear Domain Decomposition Methods, Nonlinear Schwarz, ASPIN, RASPEN

References

[1] A. Heinlein, A. Klawonn, M. Lanser (2022). *Adaptive Nonlinear Domain Decomposition Methods with an Application to the p-Laplacian*. SIAM J. Sci. Comput. 0, no. 0, S152-S172

[2] A. Heinlein, M. Lanser (2020). *Additive and hybrid nonlinear two-level Schwarz methods and energy minimizing coarse spaces for unstructured grids*. SIAM J. Sci. Comput. 42, no. 4, A2461-A2488

On the design of global-in-time Navier-Stokes solvers

Christoph Lohmann[1] and Stefan Turek[1]

[1]Department of Mathematics, TU Dortmund University
{christoph.lohmann, stefan.turek}@math.tu-dortmund.de

Abstract

The work to be presented in this talk focuses on the design of a new global-in-time multigrid solution strategy for incompressible flow problems, which highly exploits the Pressure Schur complement (PSC) approach and provides the possibility to use massively parallelizable solution components [1]. For linear problems like the incompressible Stokes equations discretized in space using an inf-sup-stable finite element pair, the fundamental idea is to block the linear systems of equations associated with individual time steps into a single all-at-once saddle point problem for all velocity and pressure unknowns. Then the Pressure Schur complement can be used to eliminate the velocity fields and set up a linear system for all pressure variables only. This algebraic manipulation allows the construction of parallel-in-time preconditioners for the corresponding all-at-once Picard iteration by extending frequently used sequential PSC preconditioners in a straightforward manner (cf. [2]). We show that those preconditioners can be applied very efficiently on modern high performance computing facilities and are asymptotically exact in the limit of vanishing time increments.

To accelerate the convergence of the proposed fixed-point iteration, this iterative solver is embedded as a smoother into a space-time multigrid algorithm, where the computational complexity of the coarse grid problem highly depends on the coarsening strategy in space and/or time. While coarsening in space using commonly used FE intergrid transfer operators significantly reduces the size of the space-time problem, most promising results for convection-dominated problems could be obtained by only coarsening in time using tailor-made prolongation and restriction operators. This procedure even allows the efficient solution of the incompressible Navier-Stokes equations using a nonlinear viscosity model for many time steps by employing Newton's method for linearization.

At the end, the presented multigrid solution strategy only requires the solution of time-dependent linear convection-diffusion-reaction equations and many Poisson problems, which both can be performed efficiently by using algorithms that exploit massive parallelism. The potential of this approach for CFD simulations with large time intervals is illustrated in numerical examples.

Keywords: incompressible Navier-Stokes equations, global-in-time, pressure Schur complement, Newton's method, space-time multigrid

References

[1] Ch. Lohmann, St. Turek. *On the design of global-in-time Newton-Multigrid-Pressure Schur complement solvers for incompressible flow problems.* In progress.

[2] F. Danieli, B. S. Southworth, A. J. Wathen (2022). *Space-Time Block Preconditioning for Incompressible Flow.* SIAM Journal on Scientific Computing, 44.1.

Benchmarking Hybrid Finite Element/Deep Neural Networks and Classical Finite Element Methods in 3D

Nils Margenberg[1], Mathias Anselmann[1], Markus Bause[1], Robert Jendersie[2], Christian Lessig[2], and Thomas Richter[3]

[1] Helmut Schmidt University, Faculty of Mechanical and Civil Engineering, Holstenhofweg 85, 22043 Hamburg, Germany
[2] University of Magdeburg, Institute for Simulation and Graphics, Universitätsplatz 2, 39104 Magdeburg, Germany
[3] University of Magdeburg, Institute for Analysis and Numerics, Universitätsplatz 2, 39104 Magdeburg, Germany

Abstract

Accurate flow simulations remain a challenging task. Combining classical finite element approximation techniques with deep neural neworks adds new aspects to the pure numerics-oriented approach and offers potential for further innovations. In this talk we discuss the use of deep neural networks for augmenting classical finite element simulations in fluid-dynamics.

We first establish new benchmark results for the classical DFG-benchmark in 3D using classical finite element simulations with high accuracy. We extend these settings to higher Reynolds numbers and compare two different FEM libraries: Gascoigne3D and deal.II. We compare the computation of drag and lift forces across the two software platforms and show that they are in good agreement.

At high Reynolds numbers, accurate simulations in 3D settings become increasingly difficult, and the classical methods reach their limits. To address this issue, we discuss approaches to connect the finite element method with neural networks. We propose the Deep Neural Network Multigrid Solver, which combines a geometric multigrid solver with a deep neural network to overcome limitations of classical methods. This approach uses classical simulation techniques where their strengths are eminent, such as the efficient representation of a coarse, large-scale flow field. Neural networks are used when a full resolution of the effects does not seem possible or efficient.

We demonstrate the efficiency, generalizability, and scalability of our proposed approach using 3D simulations. Our focus is particularly on issues of stability, generalizability, and error accuracy, and we establish the error accuracy of our proposed method by comparing it with the newly established benchmark results. Overall, our approach offers potential for further innovations in accurate flow simulations.

Keywords: Navier-Stokes equations, Geometric Multigrid Method, Deep Neural Networks

References

[1] N. Margenberg, D. Hartmann, C. Lessig, T. Richter (2022). *A neural network multigrid solver for the Navier-Stokes equations.* Journal of Computational Physics 460, 110983.

[2] M. Anselmann, M. Bause (2023). *A geometric multigrid method for space-time finite element discretizations of the Navier-Stokes equations and its application to 3d flow simulation.* ACM Trans. Math. Softw.

Fast semi-iterative finite element Poisson solvers for Tensor Core GPUs

Dustin Ruda[1], Stefan Turek[1], Dirk Ribbrock[1], and Peter Zajac[1]

[1]Department of Mathematics, TU Dortmund University
{dustin.ruda, stefan.turek, dirk.ribbrock, peter.zajac}@math.tu-dortmund.de

Abstract

The overarching theme of the work presented is how specialized high performance hardware in the form of Tensor Core GPUs can be extensively exploited for PDE computing. For example, one representative of this hardware, the Nvidia A100, promises a performance of up to 156 TFLOP/s in single precision and 312 TFLOP/s in half precision, but only if dense matrix operations are performed in the mentioned lower precision floating point formats which makes its use in the context of finite element simulations for ill-conditioned Poisson problems challenging.

Novel direct and semi-iterative hardware-oriented finite element Poisson solvers that meet the requirements for exploiting the Tensor Cores are presented. These solvers incorporate explicit preconditioning, referred to as 'prehandling' techniques, to reduce the condition number and thus ensure sufficient accuracy, using hierarchical bases in 2D or generating systems that have this property in the 3D case, respectively. By subsequently applying a Schur complement and exploiting the presence of similar mesh cells, the large, sparse linear system is transformed into multiplications of small, primarily dense matrices.

The direct variant of the method has proven to be highly performant but is limited to special cases in terms of the mesh and finite element space and to the 2D case due to its storage requirements. To extend the possible applications of this idea to higher order spaces, further differential operators and also the 3D case, we consider a semi-iterative variant. It consists of a direct part, complemented by an iterative part given by the conjugate gradient method to solve a smaller part of the unknowns. The largest part of the numerical work of this method, too, is made up of dense matrix operations. This promises high performance when implemented on relevant GPUs.

The main focus is on the new results concerning prehandling in 3D and the algorithmics of the semi-iterative method, including estimates of storage requirements, complexity and performance, as well as studies of its accuracy when using lower precision.

Keywords: Tensor Core GPUs, prehandling, hierarchical finite elements, generating systems, Poisson's equation

References

[1] D. Ruda, S. Turek, P. Zajac, D. Ribbrock (2020). *The Concept of Prehandling as Direct Preconditioning for Poisson-like Problems.* In *Numerical Mathematics and Advanced Applications Enumath 2019. Lecture Notes in Computational Science and Engineering*, eds.: F. J. Vermolen, C. Vuik. Springer, Cham, 1011–1019.

[2] D. Ruda, S. Turek, D. Ribbrock, P. Zajac (2022). *Very fast finite element Poisson solvers on lower precision accelerator hardware: A proof of concept study for Nvidia Tesla V100.* Int. J. High Perform. Comput. Appl., 36(4), 459–474.

Parallel Scalable Domain Decomposition Methods for Incompressible Fluid Flow Problems

L. Saßmannshausen[1], A. Heinlein[2], and A. Klawonn[1,3]

[1]Department of Mathematics and Computer Science, University of Cologne, Weyertal 86-90, 50931 Köln, Germany
[2]Delft Institute of Applied Mathematics, Delft University of Technology, Mekelweg 4, 2628 CD Delft, Netherlands
[3]Center for Data and Simulation Science, University of Cologne, Germany
a.heinlein@tudelft.nl; {axel.klawonn, l.sassmannshausen}@uni-koeln.de

Abstract

Monolithic GDSW (generalized Dryja–Smith–Wildund) preconditioners [1] are two-level Schwarz domain decomposition preconditioners for block systems. They are robust because they account for the coupling terms in the system matrix on both levels, that is, in the local and coarse problems. In comparison, block preconditioners, mostly based on block-diagonal and block-triangular preconditioners, such as the famous SIMPLE (semi-implicit method for pressure linked equations) preconditioner [2], often yield higher iteration counts while having a lower setup cost compared to monolithic approaches.

These highly-scalable parallel GDSW-type preconditioners have been implemented in the solver framework FROSch [3], which is part of the software library Trilinos [4]. These methods have also been extended to suit incompressible fluid flow problems.

In this talk, the parallel performance of these different preconditioning methods for incompressible fluid flow problems is investigated and compared using a finite element implementation based on the FEDDLib [5] finite element software and the Trilinos package FROSch.

Keywords: Domain Decomposition Methods, Navier-Stokes equations, Overlapping Schwarz Preconditioners, Trilinos, Finite Element Method

References

[1] A. Heinlein, C. Hochmuth, A. Klawonn (2019). *Monolithic overlapping Schwarz domain decomposition methods with GDSW coarse spaces for incompressible fluid flow problems.* SIAM Journal on Scientific Computing, 41(4): C291–C316.

[2] S. V. Patankar, D. B. Spalding (1983). *A calculation procedure for heat, mass and momentum transfer in three-dimensional parabolic flows.* Numerical prediction of flow, heat transfer, turbulence and combustion. Elsevier, pages 54–73.

[3] A. Heinlein, A. Klawonn, S. Rajamanickam, O. Rheinbach (2020). *FROSch: A Fast And Robust Overlapping Schwarz Domain Decomposition Preconditioner Based on Xpetra in Trilinos.* Domain Decomposition Methods in Science and Engineering XXV. Springer International Publishing, pages 176–184.

[4] The Trilinos Project Team. *The Trilinos Project Website* `https://trilinos.github.io/`. 2023.

[5] *FEDDLib (Finite Element and Domain Decomposition Library).* GitHub repository `https://github.com/FEDDLib/FEDDLib/`. 2023.

Massively Parallel & Low Precision Accelerator Hardware as Trends in HPC and its Application to CFD

Stefan Turek[1]

[1]Department of Mathematics, TU Dortmund University
stefan.turek@math.tu-dortmund.de

Abstract

The aim of this talk is to present and to discuss how modern, resp., future High Performance Computing (HPC) facilities regarding massively parallel hardware with millions of cores together with very fast, but lower precision accelerator hardware can be exploited in numerical simulations of PDEs so that a very high computational, numerical and hence energy efficiency can be obtained. Here, as prototypical extreme-scale PDE-based applications, we concentrate on nonstationary flow simulations with hundreds of millions or even billions of spatial unknowns in long-time computations with many thousands up to millions of time steps. For the expected huge computational resources in the coming exascale era, such type of spatially discretized problems which typically are treated sequentially, that means one time after the other, are still too small to exploit adequately the huge number of compute nodes, resp., cores so that further parallelism, for instance w.r.t. time, might get necessary.

In this context, we discuss how "parallel-in-space simultaneous-in-time" Newton-Krylov-Multigrid approaches can be designed which allow a much higher degree of parallelism. Moreover, to exploit current accelerator hardware in lower precision (for instance, GPUs or ARM), that means mainly working in single or even half precision, we discuss the concept of "prehandling" (in contrast to "preconditioning") of the corresponding ill-conditioned systems of equations, for instance arising from Poisson-like problems. Here, we assume a transformation into an equivalent linear system with similar sparsity but with much lower condition numbers so that the use of lower precision hardware might get feasible. In our talk, we provide for both aspects numerical results as "proof-of-concept" and discuss the open problems, but also the challenges, particularly for incompressible flow problems.

Keywords: Time-simultaneous Newton-Krylov-Multigrid, prehandling, mixed precision, accelerator hardware, HPC, CFD

References

[1] C. Lohmann, S. Turek (2023). *On the design of global-in-time Newton-Multigrid-Pressure Schur complement solvers for incompressible flow problems*, in progress.

[2] J. Dünnebacke, S. Turek, C. Lohmann, A. Sokolov, P. Zajac (2021). *Increased space-parallelism via time-simultaneous Newton-multigrid methods for nonstationary nonlinear PDE problems*. Int. J. High Perform. Comput. Appl., 35(3), 211–225.

[3] D. Ruda, S. Turek, D. Ribbrock, P. Zajac (2022). *Very fast finite element Poisson solvers on lower precision accelerator hardware: A proof of concept study for Nvidia Tesla V100*. Int. J. High Perform. Comput. Appl., 36(4), 459–474.

MS21 - Surface geometry approximation and vector-valued PDEs

Intrinsic surface VEM for vector Laplacian

Elena Bachini[1], Gianmarco Manzini[2], Annamaria Mazzia[3], and Mario Putti[4]

[1]Department of Mathematics "Tullio Levi-Civita", University of Padua, Italy.
[2]Institute for Applied Mathematics and Information Technologies, CNR, Pavia, Italy.
[3]Department of Civil, Environmental and Architectural Engineering, University of Padua, Italy.
[4]Department of Agronomy, Food, Natural resources, Animals and Environment, University of Padua, Italy.
elena.bachini@unipd.it

Abstract

We present an extension of the geometrically intrinsic formulation of the arbitrary-order Virtual Element Method (VEM) to vector-valued surface Laplacian on polygonal cells. The equation, written in covariant form using an appropriate local reference system, is discretized by the VEM approach. The knowledge of the local parametrization allows us to derive a two-dimensional VEM scheme for the contravariant components of the solution vector. The main advantage of the proposed formulation is that there is no need of additional projections or penalizations as the unknowns of the equation are objects that live intrinsically in the tangent space. We evaluate the method on several surfaces to show experimental convergence rates.

Keywords: vector-valued surface PDEs, geometrically intrinsic operators, virtual element method, polygonal mesh, high-order methods

A mesh-free collocation method for vector surface differential operators

Alejandra Foggia[1,2,3], Abhinav Singh[1,2,3], and Ivo F. Sbalzarini[1,2,3,4]

[1]Technische Universität Dresden, Faculty of Computer Science, Dresden, Germany.
[2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany.
[3]Center for Systems Biology Dresden, Dresden, Germany.
[4]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany.
foggia@mpi-cbg.de

Abstract

Vector-valued partial differential equations (PDEs) on surfaces describe flow processes across science and engineering. These surfaces can have a complex shape, demanding methods that provide accurate solutions beyond approximated and simplified geometries.

We propose a numerical framework that uses a mesh-free collocation method to solve PDEs on curved surfaces. We generalize the Discretization-Corrected Particle Strength Exchange (DC-PSE) [1] method to surface differential operators in a (pseudo) embedding-free way requiring fewer computational resources compared with other embedding and mesh-based methods. Our method can be combined with surface representation methods, such as (meshless) level sets [2], to operate on arbitrary surfaces. Moreover, it is scalable on multi-CPU, enabling simulations of large geometries.

We benchmark the algorithm by computing the Gauss and mean curvature of an ellipsoid and of the Stanford bunny. In addition, we compare the solution of the vector heat equation on a flat surface with a bump obtained with our method and with several Finite Element methods [3]. Finally, we demonstrate the approach in surface-flow problems involving the discretization of vector differential operators on curved manifolds.

Keywords: mesh-free method, collocation method, vector-valued PDE, surface

References

[1] B. Schrader, S. Reboux, I. F. Sbalzarini (2010). *Discretization correction of general integral PSE operators for particle methods.* J. Comp. Phys., 229, 4159–4182.

[2] S. Osher, J. A. Sethian (1988). *Fronts propagating with curvature-dependent speed: Algorithms based on Hamilton-Jacobi formulations.* J. Comp. Phys., 79, 12–49.

[3] E. Bachini, P. Brandner, T. Jankuhn, M. Nestler, S. Praetorius, A. Reusken, A. Voigt (2022). *Diffusion of tangential tensor fields: Numerical issues and influence of geometric properties.* arXiv preprint. arXiv:2205.12581.

Global polynomial level sets for numerical differential geometry of smooth closed surfaces

Michael Hecht[1] and Gentian Zavalani[1]

[1]Center for Advanced Systems Understanding (CASUS), Görlitz, Germany.
m.hecht@hzdr.de

Abstract

We present a computational scheme that derives a global polynomial level set parametrisation for smooth closed surfaces from a regular surface-point set and prove its uniqueness. This enables us to approximate a broad class of smooth surfaces by affine algebraic varieties. From such a global polynomial level set parametrisation, differential-geometric quantities like mean and Gauss curvature can be efficiently and accurately computed. Even 4th -order terms such as the Laplacian of mean curvature are approximated with high precision. The accuracy performance results in a gain of computational efficiency, significantly reducing the number of surface points required compared to classic alternatives that rely on surface meshes or embedding grids. We mathematically derive and empirically demonstrate the strengths and the limitations of the present approach, suggesting it to be applicable to a large number of computational tasks in numerical differential geometry.

Keywords: numerical differential geometry, surface approximation, mean curvature, Gauss curvature, level set, surface diffusion

References

[1] S. K. Thekke Veettil, G. Zavalani, U. Hernandez Acosta, I. F. Sbalzarini, M. Hecht (2023). *Global polynomial level sets for numerical differential geometry of smooth closed surfaces*. To appear in SIAM Journal on Scientific Computing, arXiv preprint. arXiv:2212.11536.

The broken Bramble–Hilbert lemma for differential forms and its applications

Martin W. Licht[1], Snorre H. Christiansen[2], Evan Gawlik[3], and Michael Holst[4]

[1]Department of Mathematics, EPFL, Switzerland.
[2]Department of Mathematics, University of Oslo, Norway.
[3]Department of Mathematics, University of Hawaii at Mānoa, Hawaii.
[4]Department of Mathematics, UC San Diego, USA.
martin.licht@epfl.ch

Abstract

We address the error analysis of finite element methods for vector-valued partial differential equations when the geometry is subject to approximation. The latter condition applies to the numerical analysis over curved domains, surfaces, and manifolds. The broken Bramble–Hilbert lemma is crucial in facilitating error estimates. This talk discusses how the broken Bramble–Hilbert lemma extends to the approximation of differential forms in Sobolev spaces. We generalize the Scott–Zhang and Ern–Guermond interpolants, and we explain how these enable a priori error estimates for finite element approximations of the Hodge-Laplace equation over curved domains. The talk will summarize the key findings of several papers, e.g., [1, 2].

Keywords: finite element method, Scott-Zhang interpolation, Ern-Guermond interpolation, Hodge Laplacian

References

[1] E. Gawlik, M. J. Holst, M. W. Licht (2021). *Local finite element approximation of Sobolev differential forms*. ESAIM: Mathematical Modelling and Numerical Analysis, 55(5), 2075–2099.

[2] M. J. Holst, M. W. Licht (2018). *Geometric transformation of finite element methods: Theory and applications*. arXiv preprint. arXiv:1809.10354.

Distributional curvature approximations with applications to shells

Michael Neunteufel[1], Jay Gopalakrishnan[2], Joachim Schöberl[1], and Max Wardetzky[3]

[1]Institute of Analysis and Scientific Computing, TU Wien.
[2]Maseeh Department of Mathematics + Statistics, Portland State University.
[3]Institute of Numerical and Applied Mathematics, University of Göttingen.
michael.neunteufel@tuwien.ac.at

Abstract

To compute the Gaussian or mean curvature of a surface embedded in $\mathbb{R}^3$ in weak sense, a C^1-surface is required. For a piece-wise affine triangulation this assumption is no longer fulfilled. The approximation of curvature quantities on discrete surfaces is still a field of intensive research in discrete differential geometry (DDG).

The Hellan–Herrmann–Johnson (HHJ) method avoids C^1-conforming finite elements for the biharmonic plate equation, $\Delta^2 w = f$, by means of a mixed method discretizing the bending moments, $\sigma = \nabla^2 w$, by tensor valued elements, where only the normal-normal component is globally continuous [1]. Regge finite elements, which are matrix-valued and solely tangential-tangential continuous, turned out to be the appropriate space for discretizing strain and metric fields [2].

In this talk we combine DDG with HHJ and Regge finite elements to introduce well-defined (high-order) distributional curvature quantities and discuss their convergence [5]. We apply this framework to nonlinear Koiter and Naghdi shells for the bending energy [3] and show how the problem of membrane locking can be mitigated [4]. We demonstrate the performance of the method by means of benchmark examples implemented in the finite element software NGSolve (`www.ngsolve.org`).

Keywords: finite element method, discrete differential geometry, distributional curvatures, shells, locking

References

[1] M. Comodi (1989). *The Hellan-Herrmann-Johnson method: Some new error estimates and post-processing*. Math. Comput., 52, 17–29.

[2] L. Li (2018). *Regge finite elements with applications in solid mechanics and relativity*. PhD thesis. University of Minnesota.

[3] M. Neunteufel, J. Schöberl (2019). *The Hellan–Herrmann–Johnson method for nonlinear shells*. Computers & Structures, 225, 106109.

[4] M. Neunteufel, J. Schöberl (2021). *Avoiding membrane locking with Regge interpolation*. Comput. Methods Appl. Mech. Eng., 373, 113524.

[5] J. Gopalakrishnan, M. Neunteufel, J. Schöberl, M. Wardetzky. *Analysis of curvature approximations via covariant curl and incompatibility for Regge metrics*. arXiv preprint. arXiv:2206.09343.

Solving higher-order tensor-valued partial differential equations on curved and deforming surfaces

Daniel-Santos-Oliván[1], Alejandro Torres-Sanchez[1], Guillermo Vilanova[2], and Marino Arroyo[2,3,4]

[1]European Molecular Biology Laboratory (EMBL-Barcelona), 08003 Barcelona, Spain.
[2]Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology, 08028 Barcelona, Spain.
[3]Universitat Politècnica de Catalunya-BarcelonaTech, 08034 Barcelona, Spain.
[4]Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE), 08034 Barcelona, Spain.
daniel.santos@embl.es

Abstract

Fluid surfaces are common in cell and tissue biology, ranging from lipid membranes that enclose the cell and many of its organelles, to epithelial tissues that line most of our organs. There has been an increasing interest in studying their mechanics and in particular their out-of-equilibrium behavior, which emerges, for instance, from active processes. Solving numerically the governing equations for this kind of fluid surfaces involves several challenges. On the one hand, these equations often involve higher-order derivatives of the surface parametrization, such as those stemming from the Helfrich energy in lipid membranes. They also involve vector- and tensor-valued partial differential equations (PDEs), such as those involved to represent nematic surfaces such as the actin cytoskeleton. Finally, they often involve saddle-point problems, such as those that emerge from imposing incompressibility in the well-known Stokes equations or inextensibility in lipid membranes.

Here we present different methods based on Loop subdivision surfaces, which provide a smooth parametrization of the surface and can therefore deal with higher-order derivatives. To treat vector- and tensor-valued PDEs we introduce a local Monge parametrization (LMP) method [1] where the surface is covered by a collection of local Monge parametrizations for each node of the mesh. The main idea is to construct maps between the element parametrizations, given naturally by the subdivision-surfaces discretization, and the local Monge parametrization around each node. In contrast to other methods, such as the representation of tensors by their Cartesian components or the Hodge decomposition for vector fields, the LMP method uses an optimal number of degrees of freedom to represent a tensor, is general with regards to the topology of the surface, and does not increase the order of the PDEs governing the tensor fields. To handle saddle-point problems using subdivision surfaces, we introduce a framework based on a macro-element approach in which the Lagrange multiplier field is discretized on a coarser mesh. We show that this method satisfies the discrete LBB condition in a range of problems, geometries and topologies.

Keywords: PDEs, tensor-valued PDEs, biological surfaces

References

[1] A. Torres-Sánchez, Daniel Santos-Oliván, Marino Arroyo (2020). *Approximation of tensor fields on surfaces of arbitrary topology based on local Monge parametrizations.* JoCP 405, 109–168.

Finding equilibrium states of fluid membranes

Maxim Olshanskii[1]

[1]Department of Mathematics, University of Houston.
maolshanskiy@uh.edu

Abstract

In this talk we are interested in finding equilibrium configurations of inextensible elastic membranes exhibiting lateral fluidity. Differential equations governing the mechanical equilibrium will be derived using a continuum description of the membrane motions given by the surface Navier–Stokes equations with bending forces. Equilibrium conditions that are found appear to be independent of lateral viscosity and relate tension, pressure and tangential velocity of the fluid. These conditions yield that only surfaces with Killing vector fields, such as axisymmetric shapes, can support non-zero stationary flow of mass. A shape equation will be derived that extends a classical Helfrich model with area constraint to membranes of non-negligible mass. We will introduce a simple numerical method to compute solutions of this highly non-linear equation. The numerical method is then applied a diverse family of equilibrium configurations. This is an exposition of results reported in [1].

Keywords: fluid membrane, surface Navier-Stokes equations, Helfrich model

References

[1] M. A. Olshanskii (2023). *On equilibrium states of fluid membranes.* arXiv preprint. arXiv:2303.16882.

An Eulerian finite element method for tangential Navier-Stokes equations on evolving surfaces

Paul Schwering*[1], Prof. Dr. Maxim A. Olshanskii†[2], and Prof. Dr. Arnold Reusken[1]

[1]Institut für Geometrie und Praktische Mathematik, RWTH Aachen University
[2]Department of Mathematics, University of Houston
schwering@igpm.rwth-aachen.de

4.9.2023

Abstract

The motion of an inextensible viscous fluid layer represented by a material surface can be described by the evolving surface Navier-Stokes equations. We introduce a method for the numerical solution of a simplified problem consisting of tangential surface Navier-Stokes equations (TSNSE) posed on a passively evolving smooth closed surface embedded in $\mathbb{R}^3$. For discretization of the TSNSE, we consider a geometrically unfitted finite element method known as TraceFEM. The TraceFEM applies to a fully Eulerian formulation of the problem and does not require a surface triangulation, which makes it convenient for deforming surfaces. In TraceFEM, one uses standard (bulk) finite element spaces to approximate unknown quantities on the surface $\Gamma(t)$ which propagates through a given triangulation of an ambient volume Ω, i.e. $\Gamma(t) \subset \Omega$ for all times t. The discrete formulation does not need a surface parametrization and uses tangential calculus in the embedding space $\mathbb{R}^3$. For scalar PDEs on evolving surfaces, variants of TraceFEM are known in the literature e.g. in [2]. For the TSNSE we choose a hybrid (finite difference in time - finite elements in space) approach since it is more flexible in terms of implementation and the choice of elements. We use a BDF scheme for the time-discretization and a stable Taylor-Hood pair of finite elements in space. To represent the surface, we use a level-set description and a higher-order method to calculate integrals on the surface approximation. Theoretical results from [1] show the optimal order of convergence. In this presentation, we explain the method and present numerical experiments that illustrate the optimality of the convergence.

Keywords: surface Navier–Stokes system, surface PDEs, evolving surfaces, TraceFEM

References

[1] Maxim A. Olshanskii, Arnold Reusken, and Paul Schwering (2023). *An Eulerian finite element method for tangential Navier-Stokes equations on evolving surfaces.* arXiv:2302.00779

[2] C. Lehrenfeld, M. A. Olshanskii, and X. Xu (2018). *A stabilized trace finite element method for partial differential equations on evolving surfaces.* SIAM Journal on Numerical Analysis, 56, pp. 1643-1672.

*A. Reusken and P. Schwering thank the German Research Foundation (DFG) for financial support within the Research Unit "Vector- and tensor valued surface PDEs" (FOR 3013) with project no. RE 1461/11-2.
†The author M.Olshanskii was partially supported by US National Science Foundation (NSF) through DMS-2011444

MS22 - Model reduction and efficient linear algebra techniques for direct and inverse problems

A rational Krylov subspace method for ill-posed problems

Volker Grimm[1]

[1]Department of Mathematics, Karlsruhe Institute of Technology (KIT)
volker.grimm@kit.edu

Abstract

We discuss a rational Krylov subspace method for the solution of ill-posed operator equations

$$Tx = y^\delta,$$

where the operator acts continuously between Hilbert spaces. The right-hand side y^δ is a perturbation of the exact data y. The rational Krylov subspace method is an optimal order regularisation scheme when Morozov's discrepancy principle is used as a stopping rule (cf. [1]). The rational method might be seen as an acceleration of the popular method of conjugated gradients. In addition, it is shown that the method preserves its good properties for the discretised operator which usually is a huge system of linear equations. An a posteriori stopping rule is introduced such that the scheme applied to the discretised operator provides approximations that are optimal with respect to the noise and with respect to the discretisation error. The findings are illustrated by numerical experiments.

Keywords: Inverse problems, rational Krylov subspace methods, regularisation.

References

[1] V. Grimm (2020). *A conjugate-gradient-type rational Krylov subspace method for ill-posed problems.* Inverse Problems, 36, 015008, 19 pp.

Preconditioning of LSQR for the solution of large-scale discrete inverse problems

Eva Havelková[1] and Iveta Hnětynková[1]

[1]Department of Numerical Mathematics, Charles University, Prague
[1]eva.havelkova@karlin.mff.cuni.cz

Abstract

Large-scale discrete inverse problems of the form $Ax \approx b$ arise in many practical applications. Iterative regularization methods such as LSQR are commonly used for the solution of these problems. Preconditioning is often applied to Krylov subspace methods to accelerate their convergence and improve efficiency. It can be also used to impose additional conditions such as non-negativity on the computed approximates. In such cases, iteration-dependent preconditioners are often required. Incorporating iteration-dependent preconditioners to Krylov subspace methods typically affects orthogonality properties of the computed bases and re-orthogonalization strategies need to be considered.

Here, we first overview approaches to preconditioning of LSQR with fixed preconditioner. Then we focus on a variant of preconditioned LSQR with an iteration-dependent preconditioner. We explain the orthogonalization strategy applied in the algorithm, describe its key properties and relations to CGLS and other algorithms. Numerical experiments will be used for illustration and comparison.

Keywords: Krylov subspace methods, Preconditioning, LSQR, Regularization

References

[1] C. C. Paige, M. Saunders (1982). *LSQR: An Algorithm for Sparse Linear Equations and Sparse Least Squares*. ACM Transactions on Mathematical Software, 8, 43–71.

[2] S. Arridge, M. Betcke, L. Harhanen (2014). *Iterated preconditioned LSQR method for inverse problems on unstructured grids*. Inverse Problems, 30, 075009.

[3] S. Gazzola, Y. Wiaux (2017). *Fast Nonnegative Least Squares Through Flexible Krylov Subspaces*. SIAM Journal on Scientific Computing, 39.2, A655–A679.

The finite element method with neural networks to reconstruct the mechanical properties of an elastic medium

Rafael Henriques[1] and Sílvia Barbeiro[1]

[1]Department of Mathematics, University of Coimbra, Portugal
rafael.henrikes97@gmail.com; silvia@mat.uc.pt

Abstract

In this work we investigate a mathematical model to reconstruct the mechanical properties of an elastic medium, for the optical coherence elastography imaging modality. To this end, we propose machine learning tools by exploring neural networks to solve the inverse problem of elastography. In our framework, we analyze the relative error between the exact function and the neural network for the case of noise free data and noisy data. The direct problem is used to define the cost function. Our algorithm updates the parameters combining the backpropagation technique with the ADAM optimizer to minimize a cost function that takes into account the error of using neural networks in the fully discretized scheme of the direct problem. We report several computational results using fabricated data with and without noise.

Keywords: Linear elasticity, Inverse problem, Mechanical properties reconstruction, Neural networks, Finite element method, Optical coherence elastography.

Acoustic full-waveform inversion for density and velocity variations using a FFT-accelerated scattering approach

Morten Jakobsen*[1,2] and Kui Xiang†[1]

[1]Department of Earth Science, University of Bergen
[2]Center for Modeling of Coupled Subsurface Dynamics, University of Bergen
morten.jakobsen@uib.no

Abstract

We present an iterative nonlinear inverse scattering algorithm for high-resolution acoustic imaging of density and velocity variations. To solve the multi-parameter nonlinear direct scattering problem, the acoustic wave equation for inhomogeneous media in the frequency domain is transformed into a vectorial integral equation of the Lippmann-Schwinger type for the combined pressure and pressure-gradient field[1]. We solve this vectorial integral equation using a FFT-accelerated Krylov subspace method. We discuss how the memory requirements and the computational cost in principle may be reduced below N and $N \log N$ by using various domain decomposition method and (sparsifying) preconditioning techniques[1,2]. To solve the multi-parameter nonlinear inverse scattering problem, we use the Newton-Kantorovich method in conjunction with matrix-free representations of the Frechet derivative operators and their adjoints[3]. The approximate Hessian information that is accounted for in our iterative solution of the (nonlinear) multi-parameter inverse scattering problem is essential for the mitigation of multi-parameter cross-talk effects. We assimilate data for different frequencies in a sequential manner to reduce the computational cost and to mitigate the cycle-skipping (local minimum) problem. Numerical examples related to seismic and medical ultrasound breast imaging illustrate the performance of the new algorithm for multi-parameter acoustic imaging. For models where multi-parameter cross-talk effects are expected to be important, we compare inversion results obtained using the Newton-Kantorovich method, the conjugate gradient method and the L-BFGS (quasi-Newton) method. The Newton-Kantorovich method always gives the best inversion results, but the other iterative methods are typically faster. By using approximate Frechet derivatives and adjoints, we can accelerate all these iterative methods without sacrificing too much inversion quality or resolution.

Keywords: Vectorial integral equations, large linear systems, Krylov subspaces, convolution, FFT, domain decomposition, preconditioner, data assimilation, multi-parameter cross-talk, approximate Hessian information

References

[1] K. Xiang, K. Eikrem, M. Jakobsen, G. Nævdal (2021). *Homotopy scattering series for seismic forward modelling with variable density and velocity.* Geophysical Prospecting, 70, 3–18.

[2] M. Jakobsen, R.S. Wu, X. Huang (2020). *Convergent scattering series solution of the inhomogeneous Helmholtz equation via renormalization group and homotopy continuation approaches.* Journal of Computational Physics, 409, 109343.

[3] K. Xiang, M. Jakobsen, K. Eikrem, G. Nævdal (2022). *A matrix-free variant of the distorted Born iterative method for seismic full-waveform inversion.* Geophysical Prospecting, 71, 431–442.

*Morten Jakobsen thanks VISTA CSD for funding.
†Kui Xiang thanks CSC for funding.

Stable low-rank tensor representation and approximation for the efficient discretization and solution of PDE problems

Vladimir Kazeev[1]

[1]Faculty of Mathematics, University of Vienna
vladimir.kazeev@univie.ac.at

Abstract

Low-rank tensor decompositions, based on techniques of numerical linear algebra and optimization, realize adaptive low-parametric approximation for PDE problems and are capable of dramatically reducing the complexity of numerical solvers. One such a decomposition was proposed under the names of *matrix product states* (MPS) in computational quantum physics and *tensor train* (TT) in computational mathematics. In particular, the *multilevel* MPS-TT representation, building on the classical idea of Kronecker-product multilevel approximation, allows to handle generic but extravagantly large discretizations and leads to data-driven computations based on effective discretizations adapted to the data instead of problem-dependent discretizations (approximation spaces) designed analytically. This approach has been shown, both theoretically and experimentally, to result in the efficient approximation of functions with algebraic singularities and of highly oscillatory solutions to multiscale diffusion problems, achieving root-exponential convergence with respect to the total number of representation parameters.

In this talk, we present recent results on the use of the multilevel MPS-TT representation for the numerical solution of elliptic and parabolic problems. Low-rank tensor approximation, based on the matrix SVD or alternative techniques for low-dimensional approximation, serves to realize adaptivity (instead of local refinement, which is typical for standard adaptive FEM approaches) and to construct quasi-optimal discretization subspaces in an online fashion (instead of offloading the task to a computation-intensive offline phase, as in standard model-order reduction). The most important regime is that of extremely fine discretizations and hence of large numbers of factors in the tensor decompositions involved. In this regime, two notions of stability come into play: not only the standard matrix conditioning of the discretized differential operator but also the stability of long ("deep") tensor factorizations. We address these with a novel low-rank tensor frame representation, building upon the standard multilevel MPS-TT representation.

Keywords: Low-rank tensor approximation, matrix-product states, tensor train, multilevel preconditioning, multilevel frames

Time-limited Balanced Truncation for Data Assimilation Problems

Melina A. Freitag[1] and Josie König[1]

[1]Institut für Mathematik, Universität Potsdam
{melina.freitag, josie.koenig}@uni-potsdam.de

Abstract

Balanced truncation is a well-established model order reduction method in system theory that has been applied to a variety of problems. When solving Bayesian inference problems, the forward model computation in the likelihood term can be very expensive in high dimensions. For linear problems with Gaussian prior and Gaussian noise in the observations, the concept of Balanced truncation was investigated in [2] and [1] (in the variational data assimilation setting). The approach is restricted to stable linear problems and so-called prior-compatible covariances. We show how to extend the method to unstable linear systems and how arbitrary prior covariances as reachability Gramians can be used. Numerical results show how the method performs particularly well for short assimilation windows.

Keywords: Time-limited Balanced truncation, Bayesian inference, data assimilation, 4D-Var, model order reduction

References

[1] D. Green (2019). *Model order reduction for large-scale data assimilation problems.* Dissertation, University of Bath.

[2] E. Qian, J.M. Tabeart, C. Beattie, S. Gugercin, J. Jiang, P.R. Kramer, A. Narayan (2022). *Model reduction for linear dynamical systems via balancing for Bayesian inference.* J. Sci. Comput. 91(29).

Parametric PDE solvers for parameter estimation and Uncertainty Quantification.

Miguel Fernández[1], Damiano Lombardi[1], and Sébastien Riffaud[1]

[1]Sorbonne Université and Inria Paris, 2 rue Simone Iff, 75012 Paris
{miguel.fernandez, damiano.lombardi, sebastien.riffaud}@inria.fr

Abstract

Parameter estimation and Uncertainty Quantification tasks involve a significant computational burden. We propose a numerical method which enables the use of Markov Chain Monte Carlo (MCMC) methods when the system is governed by time dependent parametric PDEs. To this end, we introduce a parametric solver, based on tensor methods, which approximates the solution of a system of parametric PDEs considering the parameters as extra variables. The solution represented in tensor format is used to build an efficient interpolator. This is based on a projection based Reduced Order Model (ROM) and makes it possible to use an MCMC method to adapt the discretisation in the parameter space. The method can be considered as a parsimonious discretisation of a Bayesian filter. The interplay between the tensor solver and the ROM-built interpolator, resulting in a significant speed-up and alleviation of the memory used, will be illustrated by several numerical examples on parameter estimation in fluid-structure interaction problems.

Keywords: Model Reduction, Parameter Estimation, Uncertainty Quantification

Leveraging low-rank approximation and interpolation in parallel-in-time integration

Daniel Kressener[1], Stefano Massei[2], and Junli Zhu[3]

[1]EPFL
[2]University of Pisa
[3]Lanzhou University
daniel.kressner@epf.ch; stefano.massei@unipi.it; zhujl18@lzu.edu.cn

Abstract

This work is concerned with linear matrix equations that arise from the space-time discretization of time-dependent linear partial differential equations (PDEs). Such matrix equations have been considered, for example, in the context of parallel-in-time integration leading to a class of algorithms called ParaDiag. We develop and analyze two novel approaches for the numerical solution of such equations. Our first approach is based on the observation that the modification of these equations performed by ParaDiag in order to solve them in parallel has low rank. Building upon previous work on low-rank updates of matrix equations, this allows us to make use of tensorized Krylov subspace methods to account for the modification. Our second approach is based on interpolating the solution of the matrix equation from the solutions of several modifications. Both approaches avoid the use of iterative refinement needed by ParaDiag and related space-time approaches in order to attain good accuracy. In turn, our new algorithms have the potential to outperform, sometimes significantly, existing methods. This potential is demonstrated for several different types of PDEs.

Keywords: Parallel-in-time, ParaDiag, Low-rank updates, Sylvester equations

References

[1] M. J. Gander, J. Liu, S. L. Wu, X. Yue, T. Zhou, (2020). *Paradiag: Parallel-in-time algorithms based on the diagonalization technique.* arXiv preprint arXiv:2005.09158.

[2] D. Kressner, S. Massei, J. Zhu (2022). *Improved ParaDiag via low-rank updates and interpolation.* arXiv preprint arXiv:2204.03073.

[3] E. McDonald, J. Pestana, A. Wathen (2018). *Preconditioning and iterative solution of all-at-once systems for evolutionary partial differential equations.* SIAM Journal on Scientific Computing, 40(2), A1012–A1033.

Geometry-based approximation of waves propagating through complex domains

Monica Nonino*[1], Davide Pradovera[1], and Ilaria Perugia† [1]

[1]Department of Mathematics, University of Vienna
{monica.nonino, davide.pradovera, ilaria.perugia}@univie.ac.at

Abstract

The focus of this talk is on wave propagation problems in space and time, in 2-dimensional domains with piecewise-linear boundaries, possibly including polygonal scatterers. I will present a surrogate model for the approximation of the propagating wave. In the model, the wave is approximated by the sum of some nonlinear space-time functions: each term in this sum represents a ray, which models either a reflection or a diffraction effect. I will show how it is possible to identify these rays automatically, based on the geometry of the domain. Several numerical examples will showcase the potential of the proposed methodology.

Keywords: wave propagation, model reduction, scattering, geometrical optics, diffraction

References

[1] D. A. McNamara, C. W. Pistorius, J. Mahlerbe (1990). *Introduction to the uniform geometrical theory of diffraction*. Artech House Norwood.

[2] D. Pradovera, M. Nonino, I. Perugia (2023). *Geometry-based approximation of waves propagating through complex domains*. arXiv.

[3] S. F. Potter, M. K. Cameron, R. Duraiswami (2022). *Numerical geometric acoustics: an eikonal-based approach for modeling sound propagation in* 3*D environments*. arXiv.

*M. Nonino thanks the FWF funding through project F 65 "Taming Complexity in Partial Differential Systems".
†I. Perugia thanks the FWF funding through project F 65 "Taming Complexity in Partial Differential Systems".

Sketched and truncated polynomial Krylov subsapce methods

Davide Palitta[1], Marcel Schweitzer[2], and Valeria Simoncini[1]

[1]Dipartimento di Matematica and AM^2, Alma Mater Studiorum - Università di Bologna,Piazza di Porta S. Donato 5, 40123 Bologna, Italy
[2]School of Mathematics and Natural Sciences, Bergische Universität Wuppertal, 42097 Wuppertal, Germany
{davide.palitta, valeria.simoncini}@unibo.it; marcel@uni-wuppertal.de

Abstract

Sketching can be seen as a random dimensionality reduction able to preserving the main features of the original problem with probabilistic confidence. Such kind of techniques is emerging as one of the most promising tools to boost numerical computations and it is quite well-known by theoretical computer scientists. Nowadays, sketching is getting popularity also in the numerical linear algebra community ([1, 2, 4, 3]) even though its use and understanding are still limited. In this talk we present the main concepts related to sketching and how the latter can be combined with Krylov subspace methods. We will focus on the solution of large-scale linear systems as model problem. On the other hand, thanks to the novel sketched Arnoldi relation we will illustrate, the results discussed in this talk can be extended to a panel of diverse algebraic problems ranging from the numerical evaluation of matrix functions to the solution of matrix equations.

Keywords: Sketching, Krylov methods, Large-scale linear systems

References

[1] O. Balabanov, L. Grigori (2022). *Randomized Gram-Schmidt process with application to GMRES.* SIAM Journal on Scientific Computing, 44 (3), A1450–A1474.

[2] S. Güttel, M. Schweitzer (2022). *Randomized sketching for Krylov approximations of large-scale matrix functions.* ArXiv Preprint: 2208.11447.

[3] A. Cortinovis, D. Kressner, Y. Nakatsukasa (2022). *Speeding up Krylov subspace methods for computing $f(A)b$ via randomization.* ArXiv Preprint: 2212.12758.

[4] Y. Nakatsukasa, J. A. Tropp (2021). *Fast & Accurate Randomized Algorithms for Linear Systems and Eigenvalue Problems.* ArXiv Preprint: 2111.00113.

Balanced truncation for Ensemble Kalman Inversion

Elizabeth Qian[1]

[1]School of Aerospace Engineering, Georgia Institute of Technology
eqian@gatech.edu

Abstract

The Ensemble Kalman filter is a classical method for solving data assimilation problems in which a stream of incoming data is used to update the underlying state of a model sequentially in time. The Ensemble Kalman Inversion (EKI) approach re-interprets the ensemble Kalman filter as a method for solving more general inverse problems. For high-dimensional smoothing problems (where the state to be inferred is the unknown initial condition and the indirect measurements are taken at times $t > 0$), a high-dimensional ODE must be solved for each particle at each iteration of the EKI approach. Because the EKI error scales at the Monte Carlo rate $N^{-\frac{1}{2}}$ (where N is the number of particles in the ensemble), this cost can be prohibitive. Balanced truncation for Bayesian inference (BTBI) is a recently introduced model reduction method for linear dynamical systems tailored to the Bayesian smoothing problem. This talk will introduce EKI and BTBI and describe how their union leads to efficient solution of the smoothing problem.

Keywords: Model reduction, inverse problems, data assimilation

Dynamical adaptive state estimation of Hamiltonian systems

Federico Vismara[1], Olga Mula[1], and Cecilia Pagliantini[2]

[1]Eindhoven University of Technology, Netherlands
[2]University of Pisa, Italy
{f.vismara, o.mula}@tue.nl; cecilia.pagliantini@unipi.it

Abstract

This talk focuses on the inverse problem of reconstructing an unknown function u from a finite set of measurements, under the assumption that u is the output of a parameterized partial differential equation with unknown input parameters. Typically, the target function u belongs to an infinite-dimensional Hilbert space and the geometry of the solution set $\mathcal{M}$ is not known *a priori*. Moreover, if $\mathcal{M}$ evolves over time, suitably adapting the position of the sensors is crucial to ensuring an accurate reconstruction at all times. One way to reduce the complexity of the problem is to approximate $\mathcal{M}$ by a linear, finite dimensional subspace V *via* model order reduction techniques, and to search for an approximation $u^* \in V$ to the state u. In order to enhance the quality of the estimation, dynamical low-rank approximation techniques can be employed to adapt the reduced space V. This introduces additional challenges whenever the system is characterized by a Hamiltonian structure, which must be preserved in the reduction step. In this talk we will discuss how to address inverse problems for Hamiltonian systems by combining a structure-preserving, adaptive model order reduction strategy with dynamical placement of the sensors.

Keywords: Model order reduction, Hamiltonian systems, Inverse problems, Dynamical low-rank approximation

MS23 - Multiscale methods for wave propagation problems

Towards a matrix-free parallel scalable multi-level deflation preconditioning for heterogeneous time-harmonic wave problems

Jinqiang Chen[1], Vandana Dwarka[1], and Cornelis Vuik[1]

[1]Delft Institute of Applied Mathematics, Delft University of Technology
{J.Chen-11, V.N.S.R.Dwarka, C.Vuik}@tudelft.nl

Abstract

We propose a matrix-free parallel scalable multi-level deflation preconditioned method for heterogeneous time-harmonic wave problems, including the Helmholtz and elastic wave equations. Building on recent advances in two-level deflation preconditioning [1], and multilevel deflation methods [2] for highly indefinite time-harmonic waves, we adapt these techniques for parallel implementation in the context of solving large-scale heterogeneous problems with minimized pollution error. Our proposed method integrates the geometric multigrid-based Complex Shifted Laplacian preconditioner (CSLP) with deflation approaches, employing higher-order deflation vectors and re-discretization schemes derived from Galerkin coarsening approach for a matrix-free implementation. This yields wavenumber-independent convergence for two-level deflation preconditioning. Numerical experiments demonstrate the effectiveness of our approach for increasingly complex model problems. The matrix-free implementation of the preconditioned Krylov subspace methods reduces memory consumption, and the parallel framework exhibits satisfactory parallel performance and weak parallel scalability. This work represents a significant step towards developing efficient, scalable, and parallel multi-level deflation preconditioning methods for large-scale, real-world applications in wave propagation.

Keywords: Time-harmonic wave, Helmholtz equations, Matrix-free, Parallel computing, Deflation, Scalability

References

[1] V. Dwarka, C. Vuik (2020). *Scalable convergence using two-level deflation preconditioning for the Helmholtz equation.* SIAM Journal on Scientific Computing, 42(2), A901–A928.

[2] V. Dwarka, C. Vuik (2022). *Scalable multi-level deflation preconditioning for highly indefinite time-harmonic waves.* Journal of Computational Physics, 469, 111327.

Efficient discretization of nonlinear Schrödinger equations by localized orthogonal decomposition

Christian Döding[1], Patrick Henning[1], and Johan Wärnegård[2]

[1]Department of Mathematics, Ruhr-Universität Bochum
[2]Department of Applied Physics and Applied Mathematics, Columbia University
christian.doeding@rub.de

Abstract

The Gross-Pitaevskii equation (GPE) is a nonlinear Schrödinger equation which is used in quantum physics to model the dynamics of Bose-Einstein condensates (BECs). It is well known that this equation has important time invariants such as the total energy of the system. Preserving the energy under numerical discretization can be of great significance in many practical situations. In this talk we consider numerical approximations of the GPE based on multiscale approaches. To be more precise, we choose a generalized finite element space which is based on the localized orthogonal decomposition method and which allows to capture the energy with a 6th order accuracy. Paired with energy-preserving time integrators we demonstrate how such an approach can lead to an efficient solver for the GPE and thus for the simulation of the dynamics of BECs on larger time scales.

Keywords: nonlinear Schrödinger equation, Gross-Pitaevskii equation, Bose-Einstein condensate, localized orthogonal decomposition, multiscale discretization

An extension of the approximate component mode synthesis method to the heterogeneous Helmholtz equation

Elena Giammatteo*[1], Alexander Heinlein†[2], and Matthias Schlottbom[1]

[1]Department of Applied Mathematics, University of Twente
[2]Delft Institute of Applied Mathematics, Delft University of Technology
{e.giammatteo, m.schlottbom}@utwente.nl; a.heinlein@tudelft.nl

Abstract

We present an extension of the approximate component mode synthesis (ACMS) method to the heterogeneous Helmholtz equation. The ACMS framework has originally been introduced by Hetmaniuk and Lehoucq as a multiscale approach to solve elliptic partial differential equations. The ACMS method uses a domain decomposition to separate the numerical approximation by splitting the variational problem into two independent parts: local Helmholtz problems and a global interface problem. While the former are naturally local and decoupled such that they can be easily solved in parallel, the latter requires the construction of suitable local basis functions relying on local eigenmodes and suitable extensions. We show error estimates focusing on the case where the domain decomposition is kept fixed, but the number of eigenfunctions is increased.

Keywords: multiscale method, approximate component mode synthesis (ACMS), Helmholtz equation, heterogeneous media

References

[1] U. Hetmaniuk, A. Klawonn (2014). *Error estimates for a two-dimensional special finite element method based on component mode synthesis.* Electron. Trans. Numer. Anal, 41, 109—132.

[2] U. Hetmaniuk, R. Lehoucq (2010). *A special finite element method based on component mode synthesis.* ESAIM: Mathematical Modelling and Numerical Analysis, 44, 401—420.

*EG and MS acknowledge support by the Dutch Research council (NWO) via grant OCENW.GROOT.2019.071.
†AH and MS acknowledge support by the 4TU.AMI SRI *Bridging Numerical Analysis and Machine Learning.*

Perfectly Matched layers for wave propagation problems with heterogeneous microstructure

Filip Marttala[1], Doghonay Arjmand[1], and Gunilla Kreiss[1]

[1]Department of Information Technology, Uppsala University
{filip.marttala, doghonay.arjmand, gunilla.kreiss}@it.uu.se

Abstract

Simulating propagation of waves in unbounded domains is computationally infeasible and a truncation of the infinite domain is needed in computations. Truncating the domain, however, results in reflections from the boundary, which is not present in the original infinite domain problem. One widely adopted methodology is to use perfectly matched layers (PML)[1], which are bounded buffer zones around the computational domain, over which the outgoing waves will be attenuated and no reflections will be seen in the interior. PML is known to perform very well if the wave speed is constant on the interface between the interior domain and the PML. The present work centers mainly on the development of a multiscale PML, based on the Heterogeneous Multiscale Method (HMM)[6], which is accurate also for problems with rapidly varying wave speeds over the interface. A secondary goal is to discuss several ways of constructing local problems[2,3,4], in our multiscale PML algorithm, and present our recent progress in developing an open source automated multiscale solver in the FeniCs environment[5].

Keywords: Perfectly mathed layer, Heterogeneous multiscale methods, Numerical homogenization

References

[1] J. P. Berenger (1994). *A perfectly matched layer for the absorption of electromagnetic waves.* Journal of computational physics, 114(2), 185–200.

[2] D. Arjmand, O. Runborg (2016). *A time dependent approach for removing the cell boundary error in elliptic homogenization problems.* Journal of Computational Physics, 314, 206–227.

[3] A. Gloria (2011). *Reduction of the resonance error—Part 1: Approximation of homogenized coefficients.* Mathematical Models and Methods in Applied Sciences, 21(08), 1601–1630.

[4] A. Abdulle, D. Arjmand, E. Paganoni (2019). *Exponential decay of the resonance error in numerical homogenization via parabolic and elliptic cell problems.* Comptes Rendus Mathematique, 357(6), 545–551.

[5] A. Logg, K. A. Mardal, G. Wells (Eds.). (2012). *Automated solution of differential equations by the finite element method: The FEniCS book.* Vol. 84. Springer Science & Business Media.

[6] E. Weinan, B. Engquist (2003). *The heterognous multiscale methods.* Communications in Mathematical Sciences, 1(1), 87–132.

Preconditioning with locally harmonic spectral coarse spaces

Arne Strehlow*[1], Chupeng Ma[2], and Robert Scheichl[1]

[1]Department of Mathematics, University of Heidelberg
[2]Faculty of Sciences, Great Bay University
{arne.strehlow, r.scheichl}@uni-heidelberg.de; chupeng.ma@gbu.edu.cn

Abstract

The multiscale spectral generalized finite element method (MS-GFEM, [1], [2]) employs locally harmonic spectral coarse spaces to approximate solutions of PDEs with heterogeneous coefficient, and has recently been extended to the Helmholtz equation [3]. The method is cast in an approximation framework, but also lends itself to the construction of a preconditioner. In this talk we will investigate the latter viewpoint. We lay out how the use of local particular functions in MS-GFEM naturally leads to a restricted, multiplicative two-level Schwarz preconditioner. We analyse convergence and condition number, point out similarities and differences to other spectral coarse space methods, and test our preconditioner on typical applications such as the Marmousi problem.

Keywords: Helmholtz equation, Preconditioning, Heterogeneous Coefficient, Domain Decomposition

References

[1] Ivo Babuska, Robert Lipton (2014). *Optimal Local Approximation Spaces for Generalized Finite Element Methods with Application to Multiscale Problems.*

[2] Chupeng Ma, Robert Scheichl, Tim Dodwell (2021). *Novel design and analysis of generalized FE methods based on locally optimal spectral approximations.*

[3] Chupeng Ma, Christian Alber, Robert Scheichl (2022). *Wavenumber explicit convergence of a multiscale generalized finite element method for heterogeneous Helmholtz problems.*

[4] Arne Strehlow, Chupeng Ma, Robert Scheichl (work in progress). *Multiscale Generalized Finite Elements as a Two Level Schwarz Preconditioner.*

*Arne Strehlow thanks to Christian Albers for providing his Matlab implementation of MsGFEM.

MS24 - Structure-preserving unfitted finite element discretizations

Bound-preserving cut discontinuous Galerkin methods for hyperbolic conservation laws

Pei Fu[1], Gunilla Kreiss[2], and Sara Zahedi[3]

[1]Department of Mathematics, Nanjing University of Aeronautics and Astronautics
[2]Department of Information Technology, Uppsala University
[3]Department of Mathematics, KTH Royal Institute of Technology
fu.pei@nuaa.edu.cn; gunilla.kreiss@it.uu.se; sara.zahedi@math.kth.se

Abstract

In this talk, I will present a family of high order cut discontinuous Galerkin (DG) methods for hyperbolic conservation laws. To avoid the small cut cell problem, we use ghost penalty stabilization to stabilize the scheme [1]. The strong stability preserving Runge-Kutta method is used for time discretization and the time step is independent of the size of the cut elements. The proposed unfitted methods have similar stability and accuracy properties as standard DG-methods on a regular mesh. To obtain a bound-preserving approximate solution, we reconstruct a solution on a macro-element partitioning of the mesh and apply the bound-preserving limiter [2, 3]. We prove that our method is bound-preserving for scalar conservation laws and the Euler equations. Numerical examples demonstrate that the proposed schemes are high order accurate for smooth problems and can keep the maximum principle for scalar problems, and positivity of density and pressure for Euler equations.

Keywords: Hyperbolic conservation laws, Cut discontinuous Galerkin methods, Bounded-preserving property

References

[1] P. Fu, G. Kreiss (2021). *High order cut discontinuous Galerkin methods for hyperbolic conservation laws in one space dimension.* SIAM Jour. Sci. Comput., 43, A2404–A2424.

[2] X. Zhang, C-W Shu (2010). *On maximum-principle-satisfying high order schemes for scalar conservation laws.* Jour. Comput. Phys., 229(9), 3091–3120.

[3] X. Zhang, C-W Shu (2010). *On positivity-preserving high order discontinuous Galerkin schemes for compressible Euler equations on rectangular meshes.* Jour. Comput. Phys., 229(9), 8918–8934.

Cut FEM meets Finite Differences

Gunilla Kreiss[1]

[1]Department of Information Technology, Uppsala University

Abstract

There is a cut-FEM methodology with ghost penalty stabilization, which can be applied to hyperbolic conservation laws. Explicit time-stepping is preferable for hyperbolic problems, but even the standard DG and CG metods suffer from increasingly severe time-step restrictions as the order of the method increases. For high order finite difference methods the time-step restriction is not at all as severe. In this talk we will explore possibilities of applying the cut-FEM methodology to finite difference methods. The goal is to formulate a finite difference method that can be seen as a Galerkin method. Applying the cut-FEM methodology will then yield an immersed boundary finite difference metod.

Keywords: Cut Finite Difference Galerkin metod

Divergence preserving Cut Finite Element Methods for the Stokes flow

Thomas Frachon[1], Erik Nilsson[1], and Sara Zahedi[1]

[1]Department of Mathematics, KTH
erikni6@kth.se

Abstract

We have developed mixed cut finite element methods which preserve the mass balance equation of Stokes flow [1]. This is achieved by using $\mathbf{H}^{\mathrm{div}}$-conforming elements for the velocity field and new mixed ghost penalty stabilization terms. These stabilization terms retain the saddle point structure of the system while providing control of the condition number of the matrix assosciated with the discrete problem. In this talk we will present two unfitted methods for the Stokes problem that result in pointwise divergence-free velocity approximations, discuss the challenge of handling Dirichlet boundary conditions, and show numerical results.

Keywords: Stokes equations, Fictitious domain problems, Mixed finite element methods, Cut finite element method, Lagrange multipliers

References

[1] T. Frachon, E. Nilsson, S. Zahedi (2023). *Divergence-free cut finite element methods for Stokes flow.* https://arxiv.org/abs/2304.14230.

Unfitted finite element methods for axisymmetric two-phase flow

Harald Garcke[1], Robert Nürnberg[2], and Quan Zhao[1]

[1]Fakultät für Mathematik, Universität Regensburg, Germany
[2]Dipartimento di Mathematica, Università di Trento, Italy
{harald.garcke, quan.zhao}@ur.de; robert.nurnberg@unitn.it

Abstract

We propose and analyze unfitted finite element approximations for the two-phase incompressible Navier–Stokes flow in an axisymmetric setting. The discretized schemes are based on an Eulerian weak formulation for the Navier–Stokes equation in the 2d-meridian halfplane, together with a parametric formulation for the generating curve of the evolving interface. We use lowest order Taylor–Hood and piecewise linear elements for discretizing the Navier–Stokes formulation in the bulk and the moving interface, respectively. We discuss a variety of schemes, amongst which is a linear scheme that enjoys an equidistribution property on the discrete interface and good volume conservation. An alternative scheme can be shown to be unconditionally stable and to conserve the volume of the two phases exactly. Numerical results are presented to show the robustness and accuracy of the introduced methods for simulating both rising bubble and oscillating droplet experiments.

Keywords: two-phase flow, axisymmetry, finite element method, stability, volume preservation, XFEM

A cut finite-element method for fracture and contact problems in large-deformation solid mechanics

Mikhail Poluektov[1]

[1]Department of Mathematics, School of Science and Engineering, University of Dundee, Dundee DD1 4HN, UK
mpoluektov001@dundee.ac.uk

Abstract

There is a variety of numerical methods to handle problems with interfaces in solid mechanics. Most methods can be classified into two groups: the diffuse-interface methods and the sharp-interface methods. There is an important class of methods within the latter group – the fictitious domain methods, to which the CutFEM approach belongs. This class of methods allows the interface to cut through the elements and to avoid any kind of mesh generation that conforms to the mesh. This is extremely convenient from the practical point of view when non-stationary interfaces are considered, as the interfaces can move independently of the mesh. Initially, the CutFEM method has been proposed for linear PDEs [1, 2]. Recently, a generalisation of the CutFEM method to large deformations and arbitrary constitutive behaviour of materials in solid mechanics has been performed [3].

In this talk, the results of [3] are further generalised to cases when the interface represents a more complex physical behaviour – fracture, i.e. separation of the interface, and contact between the separated surfaces [4]. The starting point is the case of the simple solid-solid phase boundary (e.g. a discontinuity in material behaviour), which is first generalised to fracture (crack opening), then generalised to contact. The contact case is considered separately and provides an additional challenge because the contact points might not coincide in the reference configuration of the material. From the numerical point of view, two goals are addressed here. The first goal is to ensure that any incremental generalisation of the approach contains a prior approach as a particular case, i.e. the phase boundary problem is a particular case of the fracture problem, while the latter can become a particular case of the contact problem under certain specific conditions. The second goal is to ensure that the weak form obtained for the contact problem is symmetric with respect to the choice of the contact surfaces for the integration. The presentation of the method is followed by a number of numerical examples highlighting the applicability of the approach.

Keywords: cut finite element method; fictitious domain method; sharp interface method; contact mechanics; large deformation mechanics; unbiased contact formulation; large deformation contact; crack propagation

References

[1] A. Hansbo, P. Hansbo (2002). *An unfitted finite element method, based on Nitsche's method, for elliptic interface problems*. Comput. Methods Appl. Mech. Eng., 191, 5537–5552.

[2] E. Burman, P. Hansbo (2012). *Fictitious domain finite element methods using cut elements: II. A stabilized Nitsche method*. Appl. Numer. Math., 62(4), 328–341.

[3] M. Poluektov, Ł. Figiel (2019). *A numerical method for finite-strain mechanochemistry with localised chemical reactions treated using a Nitsche approach*. Comput. Mech., 63(5), 885–911.

[4] M. Poluektov, Ł. Figiel (2022). *A cut finite-element method for fracture and contact problems in large-deformation solid mechanics*. Comput. Methods Appl. Mech. Eng., 388, 114234.

A cut finite element method based on Hermite interpolation polynomials

Ivy Weber[1] and Gunilla Kreiss[1]

[1]Department of Information Technology, Uppsala University
ivy.weber@it.uu.se

Abstract

In previous studies of the cut finite element method for wave systems [1, 2] solved using standard Lagrange elements and explicit time-stepping, it was found that increasing the order of the method with the polynomial degree would lead to similar restrictions on the time-step as for the non-cut method applied on the background mesh. This means that the time-step usually needs to be taken as $\mathcal{O}(p^{-2})$ for polynomial degree p, which leads to significant computational costs for simulating the system for a fixed duration. More recent work, see [3], using Hermite interpolation polynomials as basis functions has indicated that the maximum stable time-step reduces more slowly $\mathcal{O}(p^{-1})$ rather than $\mathcal{O}(p^{-2})$ for Hermite finite elements than Lagrange finite elements on a fixed cartesian grid.

We will present numerical experiments, were we solve the second order wave equation using a mesh that is unfitted to the domain, and Hermite elements. The experiments have three aims:

- Verify that Hermite elemets are a viable option for the cut finite element framework,
- Test the time-step stability constraints, and compare them to the constraints for the non-cut method,
- Test the order of accuracy of the method to ensure it performs correctly at higher orders.

Keywords: Cut FEM, wave equation, Hermite elements

References

[1] S. Sticko, G. Kreiss (2019). *High Order Cut Finite Elements for the Wave Equation.* Journal of Scientific Computing 80, 1867.

[2] S. Sticko, G. Ludvigsson, G. Kreiss (2020). *High Order Cut Finite Elements for the Elastic Wave Equation.* Advances in Computational Mathematics 46, 45.

[3] I. Weber, G. Kreiss, M. Nazarov (2022). *Stability analysis of high order methods for the wave equation.* Journal of Computational and Applied Mathematics 404, 113900.

MS25 - Transport at multiple scales in medical processes: from modelling to simulation

Multi-dimensional modelling of drug resistance & therapeutic outcomes in melanoma

Arran B J Hodgkinson[1]

[1]Department of Mathematics and Statistics, University of Exeter, United Kingdom
A.B.J.Hodgkinson@exeter.ac.uk

Abstract

Resistance to targeted therapies continues to pervade the treatment of cancers and requires a quantitative approach to provide meaningful solutions. Cancer is, however, a complicated disease, comprising spatio-temporal processes at the scale of the tumour and cell, as well as in metabolic and genetic cellular function. To tackle this problem, we construct a higher-dimensional partial differential equation (PDE) modelling framework, in order to analyse and interpret single-cell RNA sequencing data from in vivo primary derived xenograft tumours, which can recapitulate both the pathogenic tumour growth and its response to targeted BRAF inhibitor therapies. By allowing for higher-dimensional dynamics simultaneously in time, space, and RNA expression profile, we are able to observe co-evolution across these domains and to make quantitative predictions which generate important biological hypotheses. Firstly, given the data-driven tumour analysis, we found that spatial heterogeneity may play a major role in allowing the tumour to grow during the resistance phase, in particular by secreting cancer cells which remain sensitive to drugs within a protective ring of resistant cells. Secondly, using computer-generated virtual experiments, we tested the outcome of several proposed therapeutic approaches *in silico*: To begin, we looked at the case wherein two drug candidates exist, initially effective BRAF inhibitors alongside a drug (called 'drug X') which targets less fundamental metabolic pathways and which appears less effective, overall. In this case, counterintuitive results are observed, wherein treatment with drug X prior to BRAF inhibitors actually depletes the tumour to a greater extend and for a longer time period. Next, we observed that the primary effect of increasingly popular phased therapies (wherein drugs are given periodically) appears to be the increase of intra-tumour heterogeneity and reduced responsiveness to therapy, in the long-term. Although, ultimately, none of these strategies proved conclusive, these studies provide important mathematical tools as well as insights into the dynamics of drug resistance in response to numerous therapeutic approaches.

Keywords: Structured Dynamics, Tumour Heterogeneity, Melanoma Modelling

Hybridized discontinuous Galerkin/hybrid mixed methods for a multiple network poroelasticity model with application in biomechanics

Johannes Kraus*[1], Philip Lederer[2], Maria Lymbery[3], Kevin Osthues[4], and Joachim Schöberl[5]

[1]Faculty of Mathematics, University Duisburg-Essen, Germany
[2]Department of Applied Mathematics, University of Twente, The Netherlands
[3]Institute for Artificial Intelligence in Medicine, University Duisburg-Essen, Germany
[4]Faculty of Mathematics, University Duisburg-Essen, Germany
[5]Institute for Analysis and Scientific Computing, TU Wien, Austria
{johannes.kraus, maria.lymbery, kevin.osthues}@uni-due.de; p.l.lederer@utwente.nl; joachim.schoeberl@tuwien.ac.at

Abstract

The quasi-static multiple network poroelastic theory (MPET) model, first introduced in the context of geomechanics, [1], has recently found new applications in biomechanics [2]. The parameters in the MPET equations in practice may vary over several orders of magnitude which makes their stable discretization and fast solution a challenging task. Here, a new efficient parameter-robust hybridized discontinuous Galerkin method, which features fluid mass conservation, is proposed for the MPET model. The uniform well-posedness of the discrete model is established by means of a new pratical framework for the stability analysis of perturbed saddle-point problems [3]. Thereby a constructive norm-fitting technique is applied that guides also the construction of parameter-robust norm-equivalent preconditioners. We present a series of comparative numerical tests for a 4-network MPET model of a human brain which demonstrate the performance of the new algorithms.

Keywords: MPET model, strongly mass-conserving high-order discretizations, parameter-robust LBB stability, norm-equivalent preconditioners, hybrid discontinuous Galerkin methods, hybrid mixed methods

References

[1] G.I. Barenblatt, G.I. Zheltov, I.N. Kochina (1960). *Basic concepts in the theory of seepage of homogeneous liquids in fissured rocks [strata].* J. Appl. Math. Mech., 24(5), 1286–1303.

[2] J. Lee, E. Piersanti, K.-A. Mardal, M. Rognes (2019). *A mixed finite element method for nearly incompressible multiple-network poroelasticity.* SIAM J. Sci. Comput., 41, A722–A747.

[3] Q. Hong, J. Kraus, M. Lymbery, F. Philo (2023). *A new practical framework for the stability analysis of perturbed saddle-point problems and applications.* Math. Comp., 92, 607–634.

*The first author acknowledges the funding by the German Science Fund (DFG) - project "Physics-oriented solvers for multicompartmental poromechanics" under grant number 456235063.

A fast front-tracking approach for a temporal multiscale blood flow problem with a fractional boundary growth

Ping Lin[1]

[1]Division of Mathematics, University of Dundee, United Kingdom
plin@dundee.ac.uk

Abstract

In the talk we consider a blood flow problem coupled with a slow plaque growth at the artery wall. In the model, the micro (fast) system is the Navier-Stokes equation with a periodically applied force and the macro (slow) system is a fractional reaction equation, which is used to describe the plaque growth with memory effect. We construct an auxiliary temporal periodic problem and an effective time-average equation to approximate the original problem and analyze the approximation error of the corresponding linearized PDE (Stokes) system, where the simple front-tracking technique is used to update the slow moving boundary. An effective multiscale method is then designed based on the approximate problem and the front tracking framework. We also present a temporal finite difference scheme with a spatial continuous finite element method and analyze its temporal discrete error. Furthermore, a fast iterative procedure is designed to find the initial value of the temporal periodic problem and its convergence is analyzed as well. Our designed front-tracking framework and the iterative procedure for solving the temporal periodic problem make it easy to implement the multiscale method on existing numerical PDE software. The numerical method is implemented by a combination of the finite element platform COMSOL Multiphysics and the mainstream software MATLAB, which significantly reduce the programming effort and easily handle the fluid-structure interaction, especially moving boundaries with more complex geometries.

Keywords: Front-Tracking, Temporal Multiscale, Blood Flow Modelling

The interplay between cross-adhesion and cross-diffusion in cancer dynamics

Zhihao Tao[1]

[1]Division of Mathematics, University of Dundee, United Kingdom
zytao@dundee.ac.uk

Abstract

In this talk we focus on establishing an extensive computational modelling and analysis framework for the invasion of a solid tumour in the human body that accounts for the interplay between the cross-adhesion and cross-diffusion cells sub-populations processes that are involved within the underlying cancer cells migration. Specifically, we will explore the non-local spatio-temporal evolution of an invading tumour that assumes two cancer cells sub-populations (namely, a primary cancer cell population as well as a mutated one) that proliferate and at the same time exercise both random movement and directed migration. In particular, the directed movement is assumed to be driven here by the naturally arising interplay between cell-adhesion and cross-diffusion cells populations processes, and in this context, this talk will explore three cell migration scenarios. These will be accompanied by numerical simulation (based on finite volume) as well as a novel functional analysis approach for the cross-diffusion parameters sensitivity.

Keywords: Cancer Modelling, Cross-Adhesion, Cross-Diffusion

Exploring the Multiscale Dynamics of Cancer Invasion in Fibrous Environment in the Presence of Tumour Associated Macrophages

Dumitru Trucu[1], Szabolcs Suveges[1], and Raluca Eftimie[2]

[1]Division of Mathematics, University of Dundee,Dundee, United Kingdom
[2]Laboratoire Mathématiques de Besançon, UMR-CNRS 6623, Université de Franche-Comté, Besancon, France
trucu@maths.dundee.ac.uk

Abstract

Cancer invasion of the human tissue is a complex multiscale process, which is accomplished through a cascade of interlinked macro- and micro- processes, including the secretion and spatial transport of various types of matrix-degrading enzymes, cell proliferation, and adhesive interactions both between the migrating cells and between the cells and the surrounding fibrous environment. In this context, one of the most abundant types of immune cells in the tumour microenvironment, the macrophages get involved in the tumour spread process, not only through the secretion of proteolytic enzymes that degrade the surrounding extracellular matrix, but also through the promoting or inhibiting effects that different sub-classes of macrophages have upon the spreading tumour. Indeed, notable here is that these tumour-associated macrophages (TAMs) have a tumour promoting phenotype (M2), contributing to tumour proliferation and spread. However, the plasticity of the macrophages makes it possible to re-polarise them into an anti-tumoral phenotype (M1), making their re-education an attractive future potential strategy in immunotherapy. Building upon a previous multi-scale moving-boundary mathematical model that we proposed for cancer invasion within fibrous environment, we now consider here also the multi-scale effects of tumour-associated macrophages as well as their re-polarisation. Numerical investigation of this new model shows the importance of the interactions between TAMs and the fibrous extracellular matrix (ECM), highlighting the impact of the fibres on the spatial structure of solid tumours. These also enable us to explore the role that macrophages play in a series of hypothetical situations aimed at slowing down the tumour growth and spread by re-polarising the pro-tumoral phenotype (M2).

Keywords: Cancer Invasion, Multiscale Moving Boundary Modelling, Macrophages Dynamics

References

[1] S. Suveges, R. Eftimie, D. Trucu (2020). *Directionality of macrophages movement in tumour invasion: a multiscale moving boundary approach*. Bulletin of Mathematical Biology. Vol. 82, 148, 1–50, https://doi.org/10.1007/s11538-020-00819-7.

[2] S. Suveges, R. Eftimie, D. Trucu (2022). *Re-polarisation of Macrophages Within Collective Tumour Cell Migration: A Multiscale Moving Boundary Approach, Frontiers*. In Applied Mathematics and Statistics, Section Dynamical Systems. Vol. 7, Article 799650, 1–27, https://doi.org/10.3389/fams.2021.799650.

An adaptive solution strategy for Richards' equation

Jakob S. Stokke[1], Koondanibha Mitra[2], Erlend Storvik[1,3], Jakub W. Both[1], and Florin A. Radu[1]

[1]Center for Modeling of Coupled Subsurface Dynamics, Department of Mathematics, University of Bergen
[2] Computational Mathematics group, Hasselt University
[3]Department of Computer science, Electrical engineering and Mathematical sciences, Western Norway University of Applied Sciences
{jakob.stokke, jakub.both, florin.radu}@uib.no; koondanibha.mitra@uhasselt.be; erlend.storvik@hvl.no

Abstract

Flow in variably saturated porous media is typically modelled by Richards' equation, a nonlinear elliptic-parabolic equation, which is notoriously challenging to solve numerically. Common linearization techniques like Newton's or Picard's methods may not converge, while more robust methods like the L-scheme may converge unacceptably slow.

In this work, we propose a robust and efficient switching algorithm for Richards' equation. The algorithm is based upon the L-scheme and Newton's method, thus utilizing the robustness of the L-scheme and quadratic convergence of Newton's method. For the switching criteria in the algorithm we derive reliable *a posteriori* indicators. The algorithm's performance is illustrated through realistic numerical examples and compared to the L-scheme and Newton's method in terms of number of iterations and computational time.

Keywords: Iterative linearization, Adaptivity, L-scheme, Newton's method, Richards'equation, Nonlinear degenerate diffusion

References

[1] J. S. Stokke, K. Mitra, E. Storvik, J. W. Both, F. A. Radu (2023). *An adaptive solution strategy for Richards' equation*. DOI: 10.48550/ARXIV.2301.02055.

[2] F. List, F.A. Radu (2016). *A study on iterative methods for solving Richards' equation*. Computational geosciences 20, 341–353.

MS26 - Multiscale and reduced-order modeling for poroelasticity

Multiscale immersed modelling of vascular tissues

Camilla Belponer*[1,2], Alfonso Caiazzo[1], and Luca Heltai[3]

[1]Centre for Advanced Analytics and Predictive Sciences, University of Augsburg, Germany
[2]Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Germany
[3]International School for Advanced Studies (SISSA), Italy
camilla.belponer@uni-a.de; caiazzo@wias-berlin.de; luca.heltai@sissa.it

August 31, 2023

Abstract

We present a multiscale computational approach for the efficient simulation of vascularized tissues. The work is motivated by the solution of inverse problems in the context of tissue imaging, where available medical data (such as those obtained via Magnetic Resonance Elastography) have a limited resolution, typically at the scale of an effective - macro scale - tissue, and cannot resolve the microscale of quantities of interests related, for instance, to the tissue vasculature. Our model is based on a geometrical multiscale 3D (elastic) -1D (fluid) formulation combined with an immersed method.

At the tissue-fluid interface we impose a trace-averaged boundary condition whose goal is to impose only a local Dirichlet boundary condition – driven by vessel deformation – allowing the enforcement of a pure normal displacement at the fictional vessel boundary. In order to decouple the discretization of the elastic tissue from the vessel boundary, the boundary condition on is imposed via a Lagrange multiplier, modelling the fluid vessels as immersed singular sources for the elasticity equation (see, e.g., [1,2]).

Next, to efficiently handle the multiscale nature of the problem, the problem is formulated as a mixed-dimensional PDE using the recently proposed framework of reduced Lagrange multipliers on a space of co-dimension 2. In this talk, we present the numerical analysis of the obtained formulation and we discuss accuracy properties and convergences of the method, validating it in several numerical examples. Finally, we present perspectives for the coupling with a one-dimensional flow model defined on the vascular network and for the numerical upscaling of the tissue model.

Keywords: Elasticity, Immersed boundary, coupled problems

References

[1] L. Heltai, A. Caiazzo (2019). *Multiscale modeling of vascularized tissues via non-matching immersed methods*. International Journal for Numerical Methods in Biomedical Engineering, 35.12: e3264.

[2] L. Heltai, A. Caiazzo, L.O. Müller (2021). *Multiscale Coupling of One-dimensional Vascular Models and Elastic Tissues*. Ann Biomed Eng. 49, 3243—3254.

[3] L. Heltai, P. Zunino (2023). *Reduced Lagrange multiplier approach for non-matching coupling of mixed-dimensional domains*. arXiv, 303.10600.

*Camilla Belponer gratefully acknowledges funding from the German Research Foundation (DFG) under the grants CA 1159/4-1 and PE 2143/6-1

A Novel Iterative Time Integration Scheme for Linear Poroelasticity

Matthias Deiml[1] and Robert Altmann[1]

[1]Department of Mathematics, University of Augsburg, Germany
{matthias.deiml, robert.altmann}@uni-a.de

Abstract

The equations of poroelasticity appear in various application fields such as in geomechanics or medicine. They are composed of an equation for the elastic deformation of the solid and a second equation for the flow of the liquid and, hence, form a coupled elliptic–parabolic problem.

We focus on the time discretization of the spatially discretized poroelasticity model [1]. For this, the application of fully implicit methods exhibits inefficiency due to the high dimensionality of the coupled problem. As such we consider two *semi-explicit* approaches, meaning that the mechanics and flow equations are solved sequentially rather than at once. On one hand, *iterative methods* such as the fixed-stress scheme [2] try to approximate the fully implicit solution through an iterative matrix splitting, often introducing relaxation to achieve universal convergence. These approaches, however, usually lack a rigorous analysis for a fixed number of inner iterations. On the other hand, the recently introduced *semi-explicit Euler method* [3] only needs to solve the mechanics and flow equations exactly once, but it is only stable if the coupling between the two equations is sufficiently *weak*.

Within this talk, we introduce a novel time integration scheme which combines the iterative idea with the semi-explicit Euler approach. More precisely, we consider an iterative scheme with an a priori specified number of inner iteration steps depending on the coupling strength of the elastic and the flow equation. The construction of the scheme, however, is based on the semi-explicit Euler scheme extended with an inner fixpoint iteration and an additional relaxation step. While the convergence of the scheme for an unlimited number of inner iteration steps can be shown easily, we also present an explicit upper bound for the number of iterations needed to guarantee first-order convergence. Finally, we compare all three approaches using an example taken from medical literature.

Keywords: poroelasticity, semi-explicit time discretization, decoupling

References

[1] M. F. Wheeler, X. Gai (2007). *Iteratively coupled mixed and Galerkin finite element methods for poro-elasticity*. Numer. Meth. Part. D. E., 23(4), 785—797.

[2] J. Kim, H. A. Tchelepi, R. Juanes (2011). *Stability and convergence of sequential methods for coupled flow and geomechanics: fixed-stress and fixed-strain splits*. Comput. Methods Appl. Mech. Engrg., 200(13-16): 1591—1606.

[3] R. Altmann, R. Maier, B. Unger (2021). *Semi-explicit discretization schemes for weakly-coupled elliptic-parabolic problems*. Math. Comp., 90(329), 1089—1118.

Semi-explicit time discretization schemes for poroelasticity problems

Robert Altmann[1], Roland Maier[2], and Benjamin Unger[3]

[1]Department of Mathematics, University of Augsburg, Germany
[2]Institute of Mathematics, Friedrich Schiller University Jena, Germany
[3]Stuttgart Center for Simulation Science, University of Stuttgart, Germany
robert.altmann@math.uni-augsburg.de; roland.maier@uni-jena.de;
benjamin.unger@simtech.uni-stuttgart.de

Abstract

We consider the time discretization of coupled elliptic-parabolic problems as they arise, for instance, in the context of poroelasticity. We introduce semi-explicit time-stepping schemes for such problems that may be applied if the coupling of the equations is rather weak. The main advantage of such schemes is that they decouple the equations and therefore allow for faster computations. Theoretical convergence results are presented that rely on a close connection of the semi-explicit schemes to partial differential equations that include delay terms. First-order as well as higher-order discretizations are discussed and numerical experiments are shown that confirm the theoretical findings.

Keywords: poroelasticity, semi-explicit time discretization, delay PDE, decoupling

References

[AMU21] R. Altmann, R. Maier, B. Unger (2021). *Semi-explicit discretization schemes for weakly-coupled elliptic-parabolic problems.* Math. Comp., 90, 1089–1118.

[AM22] R. Altmann, R. Maier (2022). *A decoupling and linearizing discretization for poroelasticity with nonlinear permeability.* SIAM J. Sci. Comput., 44(3), B457–B478.

[AMU22] R. Altmann, R. Maier, B. Unger (2022). *Semi-explicit integration of second order for weakly coupled poroelasticity.* ArXiv Preprint, 2203.16664.

Multilevel methods for nearly-singular problems in mixed dimensions

Ludmil T Zikatanov[1], Ana Budiša[2], Xiaozhe Hu[3], Miroslav Kuchta[4], and Kent-Andre Mardal[5]

[1]Department of Mathematics, Penn State, USA
[2]Simula Research Laboratory, Norway
[3]Department of Mathematics, Tufts University, USA
[4]Simula Research Laboratory, Norway
[5]Department of Mathematics, University of Oslo, Simula Research Laboratory, Norway
ludmil@psu.edu; xiaozhe.hu@tufts.edu; {ana, miroslav}@simula.no;
kent-and@math.uio.no

Abstract

We consider nearly singular problems, that is, problems with operators that are small, but nonsingular perturbations of singular operators. Discretizations of such problems lead to matrices with condition numbers of the system growing rapidly with mesh size and model parameters. This results in slow convergence even when using preconditioners which are optimal when the nonsingular perturbation dominates. To design efficient preconditioners we follow the theory of the method of subspace corrections and construct block Schwarz smoothers for the underlying multilevel solution method. The blocks are chosen specifically to cover the supports of the vectors/functions spanning the kernel of the singular part of the operator. We demonstrate key features of such solvers on a mixed-dimensional model of electrodiffusion in brain tissue.

Keywords: multilevel methods, operator preconditioning, nearly-singular operators

MS27 - Novel numerical methods for the solution of nonlinear hyperbolic PDE's

Semi-implicit fully well-balanced schemes for the 1D shallow-water system

C. Caballero-Cárdenas[1], M.J. Castro[1], C. Chalons[2], T. Morales de Luna[1], and M.L. Muñoz-Ruiz[1]

[1]Departamento de Análisis Matemático, Estadística e IO y Matemática Aplicada, Universidad de Málaga
[2]Department of Mathematics, Université Versailles Saint-Quentin-en-Yvelines
{celiacaba, mjcastro, tmorales, mlmunoz}@uma.es; christophe.chalons@uvsq.fr

Abstract

In this work we present a first order semi-implicit numerical scheme for the shallow-water equations based on a splitting technique. Specifically, an approximation of the relaxed system for the pressure is first considered, and then the transport step is performed. This strategy is inspired on the Lagrange-Projection technique proposed in [1], although the approach presented here avoids the use of Lagrangian coordinates. One of the advantages of this approach is that the pressure step can be done either explicitly or implicitly, and the latter allows us to consider larger time steps since it has a less restrictive CFL condition. Indeed, for small Froude numbers, the main restriction on the time step is driven by the pressure term. The fully well-balanced character of the scheme is achieved by considering the time fluctuations with respect to a local steady state at each cell, frozen at time t^n as proposed in [2] and the use of a exactly well-balanced reconstruction operator [3]. Moreover, the resulting scheme is also positive-preserving for the water depth, under some natural assumptions on the exactly well-balanced reconstruction operator and CFL like condtions. Finally, some numerical examples are presented.

Keywords: Shallow-water, Fully well-balanced, Semi-implicit scheme

References

[1] M.J. Castro, C. Chalons, T. Morales de Luna (2018). *A fully well-balanced Lagrange–projection-type scheme for the shallow-water equations.* SIAM J. Numer. Anal., 56 (5), 3071–3098.

[2] I. Gómez-Bueno, S. Boscarino, M. J. Castro, C. Parés, G. Russo (2023). *Implicit and semi-implicit well-balanced finite-volume methods for systems of balance laws.* Applied Numerical Mathematics, 184, 18–48.

[3] M.J. Castro, C. Parés (2020). *Well-balanced high-order finite volume methods for systems of balance laws.* Journal of Scientific Computing, 82 (2).

A New Locally Divergence-Free Path-Conservative Central-Upwind Scheme for Ideal and Shallow Water Magnetohydrodynamics

Alina Chertock[1], Alexander Kurganov[2], Michael Redle[1], and Kailiang We[3]

[1]Department of Mathematics, North Carolina State University
[2]Department of Mathematics, SUSTech International Center for Mathematics, and Guangdong Provincial Key Laboratory of Computational Science and Material Design, Southern University of Science and Technology
[3]Department of Mathematics and SUSTech International Center for Mathematics, Southern University of Science and Technology, and National Center for Applied Mathematics Shenzhen (NCAMS)
chertock@math.ncsu.edy; alexander@sustech.edu.cn; mtredle@ncsu.edu; wukl@sustech.edu.cn

Abstract

In this talk, we present a new second-order unstaggered semi-discrete path-conservative central-upwind (PCCU) scheme for ideal and shallow water magnetohydrodynamics (MHD) equations. The new scheme possesses several important properties: it locally preserves the divergence-free constraint, it does not rely on any (approximate) Riemann problem solver, and it robustly produces high-resolution and non-oscillatory results. The derivation of the scheme is based on the Godunov-Powell nonconservative modifications of the studied MHD systems. The local divergence-free property is enforced by augmenting the modified systems with the evolution equations for the corresponding derivatives of the magnetic field components. These derivatives are then used to design a special piecewise linear reconstruction of the magnetic field, which guarantees a non-oscillatory nature of the resulting scheme. In addition, the proposed PCCU discretization accounts for the jump of the nonconservative product terms across cell interfaces, thereby ensuring stability. We test the proposed PCCU scheme on several benchmarks for ideal and shallow water MHD systems. The obtained numerical results illustrate the performance of the new scheme, its robustness, and its ability not only to achieve high resolution but also to preserve the positivity of computed quantities such as density, pressure, and water depth.

Keywords: Ideal magnetohydrodynamics, shallow water magnetohydrodynamics, divergence-free constraints, path-conservative the central-upwind scheme, nonconservative hyperbolic systems of nonlinear PDEs

Discontinuous Galerkin on curved boundary domain: the Reconstruction Off-site Data (ROD) method

Stéphane Clain[1], Milene Santos[1], Adérito Araújo[1], and Sílvia Barbeiro[1]

[1]Centre of Mathematics, University of Coimbra
clain@mat.uc.pt; {milene,alma,silvia}@umat.uc.pt

Abstract

Very high order method on curved boundary domains represents a critical issue where one has to preserve the optimal convergence order. DG methods are essentially based on a local transformation onto curved element (isoparametric element, NURBS [1]). Very recently, two new technologies were developed using a local polynomial reconstruction coupling the solution in the domain and the boundary condition: the shifted method [2, 3] and the ROD method [4, 5, 6]. Both of them provide a mechanism to transfer the data from the real frontier to the nodes on the computational domain.
We present the ROD method in the DG context and show that we manage to guarantee very high-order of accuracy for two-dimensional geometries with curved interface both with Dirichlet or Neumann conditions.
The advantages of the method are: (1) no curved elements or geometrical transformation is required, we just use an approximate polygonal domain which simplifies mesh procedure of the domain; (2) the ROD procedure is implemented as a black box independently of the equations of the interior domain; (3) one can achieved any order of accuracy in function of the polynomial degree used in the ROD procedure; (4) we only need a DG solver involving Dirichlet conditions, independently of the boundary conditions, since the ROD procedure translate any Robin conditions into an equivalent Dirichlet one.

Keywords: Very High Order, Curved boundary problems, ROD method

References

[1] R. Duvigneau (2020). *Cad-consistent adaptive refinement using a nurbs-based discontinuous Galerkin method*. Int. J Numer Methods Fluids, 92, 1096-–1117.

[2] N.M. Atallah, C. Canuto, G. Scovazzi (2022). *The high-order Shifted Boundary Method and its analysis*, Computer Methods in Applied Mechanics and Engineering 394, 114885.

[3] L. Nouveau, M. Ricchiuto, G. Scovazzi (2019). *High-order gradients with the shifted boundary method: an embedded enriched mixed formulation for elliptic PDEs*, J.Comput.Phys. 398, 108898.

[4] R. Costa, S. Clain, R. Loubère, G. J. Machado (2018). *Very high-order accurate finite volume scheme on curved boundaries for the two-dimensional steady-state convection-diffusion equation with Dirichlet condition*, Appl. Math Model, 54, 752-–767.252.

[5] R. Costa, J. M. Nóbrega, S. Clain, G. J. Machado, R. Loub'ere (2019). *Very high-order accurate finite volume scheme for the convection-diffusion equation with general boundary conditions on arbitrary curved boundaries*. Int. J. Numer. Methods Engrg, 117(2), 188—220.

[6] S. Clain, D. Lopes, R.M.S. Pereira (2021). *Very high-order Cartesian-grid finite difference method on arbitrary geometries*, J. Comput.Phys. 434, 110217.

Well balanced discontinuous Galerkin schemes with aposteriori sub-cell limiter on moving Voronoi meshes with topology changes

Elena Gaburro*[1]

[1]Inria center at the University of Bordeaux, France
elena.gaburro@inria.fr

Abstract

In this talk we present a novel family of high order accurate numerical schemes for the solution of hyperbolic partial differential equations (PDEs) which combines several geometrical and physical structure preserving properties. Indeed, first, we settle in the Lagrangian framework, where each element of the mesh evolves following as close as possible the local fluid flow, so to *reduce* the *numerical dissipation* at contact waves and moving interfaces and to respect the *Galilean and rotational invariance* of the studied PDEs system. In particular, we choose the direct Arbitrary-Lagrangian-Eulerian setting which, in order to always guarantee the *high quality of the moving mesh*, allows to combine the Lagrangian motion with mesh optimization techniques. The employed Voronoi tessellation is thus regenerated at each time step, the previous one is connected with the new one by space-time control volumes, including hole-like sliver elements in correspondence of topology changes, over which we integrate a space-time divergence form of the original PDEs through a *high order* accurate ADER discontinuous Galerkin (DG) scheme [**?**, **?**]. Mass *conservation* and the respect of the *GCL condition* are guaranteed by construction thanks to the integration over closed control volumes, and *robustness* over shock discontinuities is ensured by the use of an *a posteriori* sub-cell finite volume (FV) limiter. On the top of this effective moving mesh framework, we have also made, for the first time in literature, the full ADER DG scheme with *a posteriori* sub-cell FV limiter *well balanced*, by assuring that any projection, reconstruction and integration procedures were always performed by summing up the exact value of the equilibria plus the high order accurate evolution of the fluctuations [**?**]. The presentation is closed by a wide set of numerical results, including simulations of Keplerian disks, which demonstrate all the claimed properties and the increased accuracy and robustness of our novel family of schemes.

Keywords: Hyperbolic equations, High order discontinuous Galerkin schemes, Well balanced methods, direct Arbitrary-Lagrangian-Eulerian methods, Voronoi tessellations, topology changes

References

[1] E. Gaburro, W. Boscheri, S. Chiocchetti, M. Dumbser, C. Klingenberg, V. Springel (2020). *High order direct Arbitrary-Lagrangian-Eulerian schemes on moving Voronoi meshes with topology changes.* Journal of Computational Physics. Vol. 407, 109167.

[2] E. Gaburro, S. Chiocchetti (2023). *High-order Arbitrary-Lagrangian-Eulerian schemes on crazy moving Voronoi meshes.* Numerical aspects of hyperbolic balance laws and related problems, Sema Simai, Springer.

[3] E. Gaburro (2023). *High order well balanced Arbitrary-Lagrangian-Eulerian ADER Discontinuous Galerkin scheme on moving Voronoi meshes.* In preparation.

*E. Gaburro gratefully acknowledges the support received from the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie Individual Fellowship *SuPerMan*, grant agreement No. 101025563.

High-order methods that preserve all the hydrostatic stationary solutions for Ripa model and Euler with gravity

I. Gómez-Bueno[1], M.J. Castro[1], and C. Parés[1]

[1]Departamento de Análisis Matemático, Estadísica e I.O. y Matemática Aplicada, Universidad de Málaga
{igomezbueno, mjcastro, pares}@uma.es

Abstract

In the previous work [1], two of the authors introduced a general technique to design high-order finite volume numerical methods that exactly preserve a two-parameter family of non-moving stationary solutions for the Euler equations of gas dynamic with gravitational forces. In this work we consider different fluid models expressed as systems of balance laws of the form

$$\begin{cases} \rho_t + (\rho u)_x = 0, \\ (\rho u)_t + \left(\rho u^2 + p\right)_x = S_2 H_x, \\ E_t + (u\Psi)_x = S_3 H_x, \end{cases} \tag{1}$$

where ρ, u, and E are the unknowns, $q = \rho u$ is the momentum or the discharge; $H(x)$ is a continuous known function and p, S_i, $i = 2, 3$, and Ψ are functions of (ρ, q, E). Two well-known examples of the previous system are the one-dimensional compressible Euler system with gravity source term and the Ripa model. Our goal is to design a general procedure to obtain high-order finite volume numerical methods that preserve all the stationary solutions that represent fluid at rest, i.e. $u = 0$, which satisfy

$$p_x = S_2 H_x. \tag{2}$$

Note that, given an arbitrary locally integrable density function, ρ, (2) gives an ordinary differential equation for p:

$$\frac{dp}{dx} = G(x, \rho, p), \tag{3}$$

where

$$G(x, \rho, p) = S_2(\rho, E(\rho, 0, p))H_x. \tag{4}$$

This ODE will be assumed to have a 1-parameter family of solutions. Therefore, there are infinitely many hydrostatic stationary solutions. A methodology to design methods which preserve all of them will be presented, performing a number of numerical tests to check the well-balancedness of the methods: the numerical results confirm the theoretical ones.

Keywords: Well-balanced methods, Euler equations, Ripa model, hydrostatic stationary solutions

References

[1] M.J. Castro, C. Parés (2020). Well-balanced high-order finite volume methods for systems of balance laws *Journal of Scientific Computing*, 82, Article number: 48.

Well-Balanced High-Order Discontinuous Galerkin Methods for Systems of Balance Laws

E. Guerrero Fernández[1], C. Escalante[2], and M. J. Castro Díaz[2]

[1]National Oceanographic and Atmospheric Administration (NOAA), US.
[2]University of Málaga, Spain.
ernesto.g.fernandez@noaa.gov

Abstract

This work introduces a general strategy to develop well-balanced high-order Discontinuous Galerkin (DG) numerical schemes for systems of balance laws. The essence of our approach is a local projection step that guarantees the exactly well-balanced character of the resulting numerical method for smooth stationary solutions. The strategy can be adapted to some well-known different time marching DG discretisations. Particularly, in this article, Runge–Kutta DG and ADER DG methods are studied. Additionally, a limiting procedure based on a modified WENO approach is described to deal with the spurious oscillations generated in the presence of non-smooth solutions, keeping the well-balanced properties of the scheme intact. The resulting numerical method is then exactly well-balanced and high-order in space and time for smooth solutions. Finally, some numerical results are depicted using different systems of balance laws to show the performance of the introduced numerical strategy.

Keywords: systems of balance laws; exactly well-balanced; high-order methods; discontinuous Galerkin methods; ADER; Runge–Kutta; WENO; reconstruction operators

References

[Castro and Parés(2020)] M.J.Castro, C. Parés (2020). *Well-balanced high-order finite volume methods for systems of balance laws. Journal of Scientific Computing, 82, 48.*

[Parés and Parés-Pulido(2021)] C. Parés, C. Parés-Pulido (2021). Well-balanced high-order finite difference methods for systems of balance laws. Journal of Computational Physics, 425, 109880.

[Bermúdez and Vázquez(1994)] A. Bermúdez; M. E. Vázquez (1994). Upwind methods for hyperbolic conservation laws with source terms. Computers & Fluids, 23, 1049–1071.

Relation between Riemann based schemes and additional diffusive terms in Smoothed Particle Hydrodynamics

Tomáš Halada*[1] and Luděk Beneš[1]

[1]Department of Mathematics, Faculty of Mechanical Engineering, Czech technical university in Prague
{tomas.halada, ludek.benes}@fs.cvut.cz

Abstract

The widely used weakly compressible variant of Smoothed Particle Hydrodynamics (SPH) method suffers from density oscillations and hence pressure oscillations. This is due to the particle Lagrangian nature of the SPH method in combination with weakly compressible assumption, explicit time scheme and that the SPH approximation of the differential operators is inherently central. There are two common strategies how to suppress these issues. One of them is to use numerical diffusive term which is added in the continuity equation in order to suppress the spurious oscillations on density field. The second option is to describe the particle-particle interaction in terms of Riemann problem and use Riemann solver, which provides numerical dissipation, to handle particle interactions. In our work, we deal with the relation between these two approaches. For the piecewise constant reconstruction and for the piecewise linear reconstruction we show that the usage of Riemann solvers is due to its intrinsic numerical viscosity equivalent to usage of diffusive terms based on even derivatives, with the difference that the Riemann solvers lead to significantly higher value of coefficient of numerical diffusion, then is used in case of standard diffusive terms. Moreover we show, how this affects the conservation properties. We also discuss the usage of limiters in case we work with the piecewise linear reconstruction of the solution. We demonstrate the properties and relations between these two approaches on standard SPH test cases.

Keywords: Smoothed Particle Hydrodynamics, Diffusive terms, Riemann solver, Pressure oscillations

References

[1] M. Antuono, A. Colagrossi, S. Marrone (2012). *Numerical diffusive terms in weakly-compressible SPH schemes*. Comput. Phys. Commun., 183.

[2] J.P. Vila (1999). *On the weighted methods and SPH*. Mathematical Models and Methods in Applied Sciences, 9(1999), 161–209.

[3] C. Zhang, X.Y. Hu, N.A. Adams (2017). *A weakly compressible SPH method based on a low-dissipation Riemann solver*. Journal of Computational Physics, 335 (2017), 605–620.

*Author to whom correspondence should be addressed.

Upwind schemes for numerical approximation of the eikonal equation enhanced with a small curvature term

Katarína Lacková*[1] and Peter Frolkovič[2]

[1,2]Department of Mathematics and Descriptive Geometry, Faculty of Civil Engineering, STU Bratislava, Slovakia.
{katarina.lackova, peter.frolkovic}@stuba.sk

Abstract

Level set methods are effective techniques for implicitly describing the evolution of interfaces. We deal with a general nonlinear form of the level set equation in 2D given by

$$\partial_t \psi + s|\nabla \psi| = 0\,, \quad s = a - \epsilon\kappa\,, \quad \psi(x,0) = \psi^0(x)\,, \quad x \in R^2, \tag{1}$$

where the zero level set of the unknown function $\psi = \psi(x,t)$ represents the evolution of the said interface, κ denotes the mean curvature of the level sets, and $\epsilon = \epsilon(\kappa) \geq 0$ is a small parameter. The interface advances in the normal direction of the level sets at a speed s dictated by the prescribed velocity $a = a(x) > 0$ with the mean curvature playing the role of a small regularization term [1].

We aim to propose a fully upwinded numerical scheme for the approximation of the eikonal equation regularized by small mean curvature term inspired by a semi-Lagrangian type of scheme for mean curvature flows [2, 3] and advection-diffusion equations [4]. By using upwind discretization, the resulting discrete algebraic system can be efficiently solved using solvers that take advantage of the upwind schemes' causality principle, allowing for fast convergence with a small number of iterations. Moreover, to allow for more general settings without restriction on ϵ, we investigate possibilities to extend the upwind scheme in a spirit of Weighted Essentially Non-Oscillatory (WENO) approximations [5].

Keywords: upwind numerical approximation, eikonal equation, mean curvature

References

[1] Lacková, Katarína, Frolkovič, Peter (2023). *Efficient numerical methods for models of evolving interfaces enhanced with a small curvature term.* Submitted.

[2] Carlini, Elisabetta, Falcone, Maurizio, Ferretti, Roberto (2011). *Convergence of a large time-step scheme for mean curvature motion.* Interfaces and Free Boundaries. Vol. 12(4), 409–441.

[3] Carlini, Elisabetta, Ferretti, Roberto (2017). *A semi-Lagrangian scheme with radial basis approximation for surface reconstruction.* Computing and Visualization in Science. Vol. 18(2), 103–112.

[4] Bonaventura, Luca, Calzola, Elisa, Carlini, Elisabetta, Ferretti, Roberto (2021). *Second order fully semi-Lagrangian discretizations of advection-diffusion-reaction systems.* Journal of Scientific Computing. Vol. 88(1), 1–29.

[5] Zhang, Yong-Tao, Hong-Kai Zhao, Jianliang Qian (2006). *High Order Fast Sweeping Methods for Static Hamilton–Jacobi Equations.* Journal of Scientific Computing. Vol. 29(1), 25-56.

*The work is supported by the grant VEGA 1/0314/23 and APVV-19-0460.

A well-balanced all-Mach scheme for compressible multiphase flow

Sandro Malusà[1,2] and Alessandro Alaia[2]

[1]Department of Applied Science and Technology, Politecnico di Torino
[2]Optimad srl
sandro.malusa@optimad.it; alessandro.alaia@optimad.it

Abstract

In this work, we propose an all-Mach finite volume scheme for the compressible multiphase Baer and Nunziato model [1]. In many industrial applications such as, trickle-bed reactors, sedimentation flows and reactive flows in porous media, the characteristic velocity of the mean flow can be orders of magnitude smaller than the characteristic speed of acoustic perturbations. As a consequence in the low-Mach regime, explicit finite volume schemes suffer from stringent time-step limitations due to the stiff contribution of acoustic waves.

In order to solve model equations efficiently and accurately in the low-Mach regime, we split the convective term in a stiff part associated to fast acoustic waves, and a non-stiff part corresponding to mean flow advection. An Implicit-Explicit Runge-Kutta (IMEX-RK) method (see [2]) is then used to integrate the stiff part implicitly, while non-stiff terms are treated explicitly. By linearizations of time and space derivatives in the energy equation, we derive a predictor-corrector scheme where the contribution of pressure waves is accounted for by solving a system of non-linear elliptic equations for the phasic pressures. This approach generalizes that in [3] to non-isentropic flows. A well-balanced discretization of non-conservative terms is also introduced in order to preserve steady-states, including the so-called "lake-at-rest" condition. The resulting numerical scheme is stable under a CFL condition based on the macroscopic velocity. We also prove that our numerical scheme is asymptotic-preserving. Finally, numerical results demonstrate the capabilities of our numerical scheme to correctly capture shocks in the high-Mach regime as well as to efficiently simulate flows at low Mach numbers.

Keywords: Compressible multiphase flow, All-Mach schemes, IMEX Runge-Kutta, Well-balanced schemes

References

[1] M. R. Baer and J. W. Nunziato (1986). *A two-phase mixture theory for the deflagration-to-detonation transition (ddt) in reactive granular materials.* International Journal of Multiphase Flow 12.6, pp. 861–889.

[2] L. Pareschi and G. Russo (2010). *Implicit-explicit Runge-Kutta schemes and applications to hyperbolic systems with relaxation.* arXiv:1009.2757 [math.NA].

[3] M. Lukacova-Medvidova, G. Puppo and A. Thomann (2022). *An all Mach number finite volume method for isentropic two-phase flow.* arXiv:2202.01577 [math.NA].

High-order In-cell Discontinuous Reconstruction path-conservative methods for non conservative hyperbolic systems - DR.MOOD

Ernesto Pimentel-García*[1], Manuel J. Castro[1], Christophe Chalons[2], Tomás Morales de Luna[1], and Carlos Parés[1]

[1]Departamento de Análisis Matemático, Estadística e Investigación Operativa, y Matemática aplicada, Universidad de Málaga, Bulevar Louis Pasteur, 31, 29010, Málaga, Spain
[2]Laboratoire de Mathématiques de Versailles, UVSQ, CNRS, Université Paris-Saclay, 78035 Versailles, France
erpigar@uma.es

Abstract

We are interested in the numerical approximation of discontinuous solutions in non conservative hyperbolic systems. Due to the lack of control of numerical viscosity, standard path-conservative methods converge, in general, to weak solutions with wrong jump conditions (see [1]). In [3] a new strategy based on in-cell discontinuous reconstructions which deal with this challenging topic was developed. Next, in [4] the authors extended this strategy to second-order accuracy. In this work we present an extension to high-order accuracy. It is based on the combination of the first-order in-cell discontinuous reconstruction with the MOOD philosophy [2]. The first-order strategy allows in particular to capture exactly the isolated shocks and this new high-order extension keep this property and improve the results when dealing with more than one shock. Several numerical tests are proposed to validate the methods.

Keywords: Non conservative systems, high-order methods, MOOD, shock-capturing methods

References

[1] M. J. Castro, P. G. LeFloch, M. L. Muñoz-Ruiz, C. Parés (2008). Why many theories of shock waves are necessary: Convergence error in formally path-consistent schemes. *J. Comput. Phys.*, 227 (17), 8107–8129.

[2] S. Clain, S. Diot, R. Loubère (2011). *A high-order finite volume method for systems of conservation laws—Multi-dimensional Optimal Order Detection (MOOD)*. J. Comput. Phys, 230 (10), 4028–4050.

[3] C. Chalons (2020). *Path-conservative In-cell Discontinuous Reconstruction schemes for non conservative hyperbolic systems*, Commun. Math. Sci., 18(1), 1–30.

[4] E. Pimentel-García, M. J. Castro, C. Chalons, T. Morales de Luna, C. Parés (2022). *In-cell Discontinuous Reconstruction path-conservative methods for non conservative hyperbolic systems – Second-order extension*, J. Comput. Phys, 459, 111152.

*E. P. G. thanks the European Regional Development Fund (ERDF), the Regional Government of Andalusia (RGA), and the University of Málaga (UMA) through the projects of reference RTI2018-096064-B-C21 (SG-ERDF), UMA18-Federja-161 (RGA-ERDF-UMA), and P18-RT-3163 (RGA-ERDF).

An all-speed IMEX scheme for two-fluid flows

Andrea Thomann[1], Ilya Peshkov[2], Mária Lukáčová-Medvid'ová[3], and Gabriella Puppo[4]

[1]Université de Strasbourg, CNRS, Inria, IRMA, F-67000 Strasbourg, France.
[2]Department of Civil, Environmental and Mechanical Engineering, Trento University, Italy.
[3]Institut für Mathematik, Johannes-Gutenberg-Universität Mainz, Germany.
[4]Dipartimento di Matematica, La Sapienza Università di Roma, Italy.
andrea.thomann@inria.fr; ilya.peshkov@unitn.it; lukacova@mathematik.uni-mainz.de; gabriella.puppo@uniroma1.it

Abstract

We are interested in the numerical simulation of liquid-gas mixtures, where the sound speed of the liquid phase is consistently faster than the one of the gas phase. If in addition, the material wave is significantly slower than the individual acoustic waves, the system can exhibit three different scales of wave speeds. In these regimes, which are characterized by small, potentially different phase Mach numbers, using an explicit scheme requires a time step that scales with the smallest appearing Mach number. This is especially problematic when phenomena are monitored over a long time period. Moreover, the main interest often lies on a sharp resolution of slow dynamics which would allow for a much larger time step. Therefore, we use implicit-explicit (IMEX) time integrators where fast waves are treated implicitly leading to a CFL condition which is restricted only by the local flow velocity.

In this talk, we present an all-speed finite volume scheme for two-phase flows based on a symmetric hyperbolic thermodynamically compatible model given in [1, 2]. Since the flow regimes can range from compressible for gases to almost incompressible for some liquids, a consistent discretisation of the limit equations in the singular Mach number limit is important. This so called asymptotic preserving (AP) property together with the correct numerical viscosity are essential for the simulation of weakly-compressible flows. Since the flow regime of the two-phase flow model from [1, 2], is characterized by two potentially distinct phase Mach numbers, different singular Mach number limits can be obtained which depend on the constitution of the mixture. The AP property of our IMEX scheme is obtained by using a reference solution approach based on the profound knowledge of well-prepared initial data. Further, the reference state is used to linearise pressure based quantities avoiding the necessity for nonlinear implicit solvers, see [3]. The consistency with single phase flow, accuracy and the approximation of material waves in different Mach number regimes is illustrated in numerical simulations.

Keywords: All-speed scheme, IMEX method, reference state strategy, two-fluid flow, AP property, SHTC model

References

[1] E. Romenski, E. F. Toro (2004). *Compressible Two-Phase Flows: Two-Pressure Models and Numerical Methods*. Comput. Fluid Dyn. J., 13, 403–416.

[2] E. Romenski, D. Drikakis, E. F. Toro (2010). *Conservative Models and Numerical Methods for Compressible Two-Phase Flow*. J. Sci. Comput., 42, 68–95.

[3] M. Lukácová-Medvid'ová, G. Puppo, A. Thomann (2023). *An all Mach number finite volume method for isentropic two-phase flow*. J. Numer. Math., in press. doi: https://doi.org/10.1515/jnma-2022-0015.

Quinpi: Implicit High-Order Schemes for Hyperbolic Systems

Gabriella Puppo[1], Matteo Semplice[2], and Giuseppe Visconti[1]

[1]Department of Mathematics, Sapienza University of Rome
[2]Department of Science and High Technology, University of Insubria
{gabriella.puppo, giuseppe.visconti}@uniroma1.it; matteo.semplice@uninsubria.it

Abstract

This talk is concerned with the challenges of devising high-order implicit schemes for systems of m hyperbolic conservation laws

$$\frac{\partial}{\partial t}\mathbf{u}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{u}(x,t)) = \mathbf{0}. \tag{1}$$

The eigenvalues $\{\lambda_j(\mathbf{u}(x,t))\}_{j=1}^m$ of the Jacobian of $\mathbf{f}$ provide the characteristic speeds, which describe the speed propagation of waves in the system.

When solving hyperbolic systems, a source of difficulty is represented by stiff problems that occur when the speeds span different orders of magnitude. In this case, implicit schemes may become convenient for the numerical treatment of (1). In fact, it is well-known that the explicit time integration of (1) requires to choose a time step $\Delta t = \min\{\Delta t_{\text{acc}}, \Delta t_{\text{stab}}\}$ where Δt_{acc} is fixed by accuracy constraints, and Δt_{stab} is due to the CFL stability condition, with

$$\Delta t_{\text{stab}} \leq C\frac{h}{\max_{j=1,\dots,m}|\lambda_j(\mathbf{u})|}, \quad C \leq 1.$$

Therefore, the stability constraint is more demanding than accuracy when $\max_{j=1,\dots,m}|\lambda_j(\mathbf{u})| \gg 1$. In contrast, implicit schemes are not constrained to the CFL condition and, thus, can be used to set up larger time step sizes. However, implicit methods may be more computationally expensive than explicit ones, since they require the solution of a system of equations, in general nonlinear, at each time step.

Here, we deal with an efficient formulation of implicit high-order finite volume schemes. While first order implicit schemes are fully linear and the only source of non-linearity is due to the nonlinear flux function, they produce large dissipation errors. Achieving high-order accuracy allows to cure the low-resolution, but it typically requires to employ non-linear space reconstructions to prevent spurious oscillations. The use of such space-limiting procedures introduces an additional source of non-linearity which becomes computationally challenging when using implicit schemes. The novel idea of [1] is to use an implicit first order scheme to pre-compute the non-linearities of the space-limiting procedure. This approach, named *Quinpi*, is tailored to the third order implicit approximation of (1), achieved by using a third order DIRK for the time integration and a third order CWENO reconstruction for the space discretization. The first order implicit scheme is a composite backward Euler, used to freeze the nonlinear weights of the CWENO reconstruction making the resulting third order implicit scheme nonlinear just because of the non-linearity of the flux function.

Keywords: Implicit methods, Essentially non-oscillatory schemes, Finite volumes

References

[1] G. Puppo, M. Semplice, G. Visconti (2023). *Quinpi: integrating conservation laws with CWENO implicit methods*. Commun. Appl. Math. Comput., 5, 343–369.

MS28 - Reduced-order modeling and learning of parameterized dynamical systems: state-of-the-art vs. avant-garde methods

Order reduction of dissipative parameterized LTI systems via constrained multivariate rational fitting

Tommaso Bradde[1] and Stefano Grivet-Talocia[1]

[1]Department of Electronics and Telecommunications, Politecnico di Torino
{tommaso.bradde, stefano.grivet}@polito.it

Abstract

We present a constrained multivariate rational fitting framework for generating reduced order models (ROMs) of dissipative LTI systems depending on a set of external parameters. Denoting with $\boldsymbol{\vartheta} \in \Theta \subset \mathbb{R}^d$ the vector of such parameters and with s the Laplace variable, we assume that the parameterized transfer function of the underlying system, $\breve{H}(s, \boldsymbol{\vartheta}) \in \mathbb{C}^{P\times P}$, is known at discrete frequency-parameter configurations $s_k = j\omega_k,\ k = 1 \dots K,\ \boldsymbol{\vartheta}_m,\ m = 1 \dots M$. A multivariate fitting approach is applied to synthesize a reduced order transfer function fulfilling the fitting condition $\mathsf{H}(j\omega_k, \boldsymbol{\vartheta}_m) \approx \breve{H}(j\omega_k, \boldsymbol{\vartheta}_m)$, based upon the rational model structure

$$\mathsf{H}(s,\boldsymbol{\vartheta}) = \frac{\mathsf{N}(s,\boldsymbol{\vartheta})}{\mathsf{D}(s,\boldsymbol{\vartheta})} = \frac{\sum_{i=0}^{\bar{n}} R_i(\boldsymbol{\vartheta})\,\varphi_i(s)}{\sum_{i=0}^{\bar{n}} r_i(\boldsymbol{\vartheta})\,\varphi_i(s)},\quad \begin{cases} \varphi_0(s) = 1, \quad \varphi_{i>0}(s) = (s-q_i)^{-1}, \quad \Re\{q_i\} < 0. \\ R_i(\boldsymbol{\vartheta}) = \sum_{\boldsymbol{\ell}\in\mathcal{I}_{\bar{\boldsymbol{\ell}}}} R_{i,\boldsymbol{\ell}}\, b^{\bar{\boldsymbol{\ell}}}_{\boldsymbol{\ell}}(\boldsymbol{\vartheta}), \quad r_i(\boldsymbol{\vartheta}) = \sum_{\boldsymbol{\ell}\in\mathcal{I}_{\bar{\boldsymbol{\ell}}}} r_{i,\boldsymbol{\ell}}\, b^{\bar{\boldsymbol{\ell}}}_{\boldsymbol{\ell}}(\boldsymbol{\vartheta}). \end{cases} \tag{1}$$

In (1), the functions $b^{\bar{\boldsymbol{\ell}}}_{\boldsymbol{\ell}}(\boldsymbol{\vartheta})$ are multivariate Bernstein polynomials of degree $\bar{\boldsymbol{\ell}} = (\bar{\ell}_1, \dots, \bar{\ell}_d)$, and the set $\mathcal{I}_{\bar{\boldsymbol{\ell}}}$ contains all the multi-indices identifying the basis components. The coefficients $R_{i,\boldsymbol{\ell}} \in \mathbb{R}^{P\times P}$, $r_{i,\boldsymbol{\ell}} \in \mathbb{R}$ are the model unknowns, that are found enforcing the fitting condition in least-squares sense, through an iteratively re-weighted linearized estimation process, known as PSK iteration [2]. As proved in [1], a ROM with transfer function $\mathsf{H}(s,\boldsymbol{\vartheta})$ structured as in (1) is dissipative (positive/bounded real, depending on the system representation) when the following conditions are concurrently satisfied $\forall\omega \in \mathbb{R}, \forall\boldsymbol{\vartheta} \in \Theta$

$$\Re\{\mathsf{D}(j\omega,\boldsymbol{\vartheta})\} > 0 \quad \text{and} \quad \begin{cases} \mathsf{N}(j\omega,\boldsymbol{\vartheta})\mathsf{D}^\star(j\omega,\boldsymbol{\vartheta}) + \mathsf{N}^\star(j\omega,\boldsymbol{\vartheta})\mathsf{D}(j\omega,\boldsymbol{\vartheta}) \succeq 0 & \text{(positive real)}, \\ \mathsf{N}^\star(j\omega,\boldsymbol{\vartheta})\mathsf{N}(j\omega,\boldsymbol{\vartheta}) - \mathbb{I}\cdot\mathsf{D}^\star(j\omega,\boldsymbol{\vartheta})\mathsf{D}(j\omega,\boldsymbol{\vartheta}) \preceq 0 & \text{(bounded real)}, \end{cases} \tag{2}$$

where $\mathbb{I}$ is the identity matrix of dimension P and superscript * denotes Hermitian transposition. Making use of the Kalman-Yakubovich-Popov lemma, both conditions in (2) are rewritten equivalently in terms of Linear Matrix Inequalities (LMIs) in the model coefficients, that are required to hold uniformly over Θ. By systematically applying the properties of the Bernstein polynomials, we show that such convex yet infinite-dimensional constraints are implied by the fulfillment of two finite-dimensional LMIs. We incorporate these LMIs in the fitting process, thus concurrently enforcing the model-data fitting and the ROM dissipativity conditions. The effectiveness of the resulting constrained rational fitting approach is demonstrated over test-cases of practical relevance in the field of electronic CAD.

Keywords: Multivariate rational fitting, Parameterized model order reduction, Dissipative systems

References

[1] T. Bradde, S. Grivet-Talocia, A. Zanco, G.C. Calafiore (2022). *Data-Driven Extraction of Uniformly Stable and Passive Parameterized Macromodels*. IEEE Access, 10, 15786–15804

[2] P. Triverio, S. Grivet-Talocia, M.S. Nakhla (2009). *A parameterized macromodeling strategy with uniform stability test*. IEEE Transactions on Advanced Packaging, 32, 205–215.

Data-driven parametric reduced-order modeling in the Loewner framework: some new considerations

Ion Victor Gosea[1], Charles Poussot-Vassal[2], and Athanasios C. Antoulas[3]

[1]CSC Group, Max Planck Institute, Magdeburg, Germany
[2]Department of Information Processing and Systems, Onera, Toulouse, France
[3]Department of Electrical and Computer Engineering, Rice University, Houston, USA
gosea@mpi-magdbeurg.mpg.de; charles.poussot-vassal@onera.fr; aca@rice.edu

Abstract

Data-driven methods for learning reduced-order models of dynamical systems from measurements are an important category of model reduction methods [1]. In this talk, data are composed of frequency response measurements, i.e., samples of the transfer function of the unknown model, sampled at particular interpolation points. Out of a plethora of data-driven methods for approximating dynamical systems (see [1]), we mention here the Loewner framework (LF) originally introduced in [2]. It is a data-driven system identification and complexity reduction methodology that constructs models from frequency response data by means of interpolation. To compute a reduced-order model, one first computes data matrices $\mathbb{L}$ and $\mathbb{L}_s$ which respectively denote the Loewner and the shifted Loewner matrix associated to the data. Then, one uses the decay of the singular values of the Loewner pencil $\zeta\mathbb{L} - \mathbb{L}_s$ to make an a priori decision on what dimension should the reduced model have. In the last decade, the LF has been extended to the problem of approximating data by multivariate rational functions [3, 4]. This is closely connected to reduced-order modeling of parametric dynamical systems, as shown in [4], where the parametric Loewner framework (pLF) was introduced. This method is effective, but does not inherit some important properties of LF, and it is challenging to be extended to more than 2 parameters (the explicit computation of barycentric forms in higher dimensions becomes tedious or even unfeasible). In the current work, we discuss a modification of pLF that allows expressing the parametric Loewner matrices as solutions of nested (linear) Sylvester equations. This circumvents the need of explicitly using barycentric forms, and incorporates least-squares fit into the process. Additionally, we discuss ways of circumventing one bottleneck associated to the pLF: scalability with the number of parameters. We show that by using the Sylvester equation formulation, it is possible to directly extend this new framework to multiple dimensions, in an elegant and straightforward manner. This is done by having to (approximately) solve k nested Sylvester equations, where k is the the total number of variables.

Keywords: Parametric dynamical systems, Rational approximation, Loewner framework, Sylvester equations.

References

[1] A. C. Antoulas, C. Beattie, S. Gugercin (2020). *Interpolatory methods for model reduction.* Computational Science and Engineering 21. SIAM, Philadelphia.

[2] A. J. Mayo, A. C. Antoulas (2007). *A framework for the solution of the generalized realization problem.* Linear Algebra Appl., 425(2–3), 634–662, Special Issue in honor of P. A. Fuhrmann.

[3] A. C. Antoulas, A. C. Ionita, S. Lefteriu (2012). *On two-variable rational interpolation.* Linear Algebra Appl., 436, 2889–2915.

[4] A.C. Ionita, A.C. Antoulas (2014). *Data-driven parametrized model reduction in the Loewner framework.* SIAM Journal on Scientific Computing, 36(3), A984–A1007.

Point-set registration-based model applied to parametrized porous media flows

Birgul Koc[1], Guillaume Enchéry[2], Angelo Iollo[3], and Tommaso Taddei[4]

[1]IFPEN & INRIA-Memphis
[2]IFPEN
[3]Institut de Mathématiques de Bordeaux
[4]Inria Bordeaux Sud-Quest
[1]{birgul.koc,angelo.iollo,tommaso.taddei}@inria.fr; guillaume.enchery@ifpen.fr

Abstract

We build a nonlinear registration-based model reduction procedure to obtain new outputs from available solutions of parametrized porous-media flow problems. The point-set model, which is independent of the underlying equation, is made of two main steps: (i) determine displacement; (ii) build a bijective mapping. To obtain displacement, we consider deforming the point clouds in the point-set registration model.

We present the results of this methodology in cases of single and two-phase flows.

Keywords: optimal transport, registration, porous-media

References

[1] A. Iollo, T. Taddei (2022). *Mapping of coherent structures in parameterized flows by learning optimal transportation with Gaussian models.* Journal of Computational Physics, 471, 111671.

[2] T. Taddei (2022). *An optimization-based registration approach to geometry reduction.* arXiv preprint arXiv:2211.10275.

[3] B. Battisti, T. Blickhan, G. Enchery, V. Ehrlacher, D. Lombardi, O. Mula (2022). *Wasserstein model reduction approach for parametrized flow problems in porous media.*

Parametric Reduced-order Modeling via Nonlinear Least Squares

Serkan Güğercin[1,2] and Petar Mlinarić[1]

[1]Department of Mathematics, Virginia Tech
[2]Division of Computational Modeling and Data Analytics, Academy of Data Science, Virginia Tech
{gugercin, mlinaric}@vt.edu

Abstract

In this talk, we consider reduced-order modeling for (parametric) linear time-invariant systems based on nonlinear least-squares. We show how this problem is a special case of the more general $\mathcal{L}_2$-optimal parametric reduced-order modeling problem and corresponds to a proper choice of the measure space. By exploiting this theoretical connection, we propose a gradient-based optimization algorithm for finding locally optimal reduced-order models. We discuss how our framework relates to (and differ from) the vector fitting method for rational least-squares reduced-order modeling of linear time-invariant systems. Furthermore, we present the necessary optimality conditions in the interpolation form, analogous to the interpolatory $\mathcal{H}_2$-optimality conditions. Finally, we demonstrate the results on a number of numerical examples.

Data-driven adaptive approximation of parametric dynamical systems with pole bifurcations

Davide Pradovera[1], Fabio Nobile[2], and Alessandro Borghi[3]

[1]Department of Mathematics, University of Vienna, Austria
[2]CSQI, EPF Lausanne, Switzerland
[3]Modeling, Simulation, and Optimization of Real Processes, TU Berlin, Germany
davide.pradovera@univie.ac.at; fabio.nobile@epfl.ch; borghi@tu-berlin.de

Abstract

We describe an MOR approach for parametric frequency-response problems, where the high-fidelity problem is used to model not only the impact of the frequency $z \in \mathbb{C}$ on the system response, but also that of additional (e.g., design or uncertain) parameters $\mathbf{p} \in \mathbb{R}^n$, $n \geq 1$.

Our proposed MOR method relies on minimal rational interpolation [1] for the surrogate modeling of the frequency dependence, for few fixed values of the parameters $\mathbf{p}$. In this step, only the dependence on z is taken into account, and the resulting surrogates are a collection of rational functions of frequency only. The different z-surrogates are then combined to obtain a global approximation with respect to both frequency and parameters [2].

Our approach is non-intrusive, i.e., we do not require access to the matrices/operators defining the underlying problem. This is of practical interest, for instance, when the (e.g., finite element) solver that computes the frequency response is a black box, which happens when closed-source proprietary code is used. Moreover, since we do not assume the high-fidelity problem to have a specific structure, our method can easily be applied even when nonlinearities are present.

We also describe how, in the interest of making our approach more accurate and efficient, one can select the sample points adaptively, still within a non-intrusive framework. This is achieved by using *locally adaptive sparse grids* over $\mathbf{p}$-space. This approach, among other benefits, is also able to weaken the curse of dimension that is incurred if many parameters are present ($n \gg 1$).

Finally, we describe some of the issues that one encounters if the poles and residues of the system do not depend smoothly on the parameters. We describe how our method can be adapted to tackle this case more effectively. Specifically, one first identifies the locations of potential singularities via an *a posteriori* indicator. Then, higher-order approximations of poles and residues are introduced locally around such locations. In most cases, this refinement step does not entail any extra computational cost.

Keywords: Parametric dynamical systems, Adaptive rational approximation, Locally adaptive sparse grids, Bifurcations

References

[1] D. Pradovera (2020). *Interpolatory rational model order reduction of parametric problems lacking uniform inf-sup stability*. SIAM J. Num. Anal., 58(4), 2265–2293.

[2] F. Nobile, D. Pradovera (2021). *Non-intrusive double-greedy parametric model reduction by interpolation of frequency-domain rational surrogates*. ESAIM: M2AN, 55(5), 1895–1920.

Model reduction for stochastic systems with nonlinear drift

Martin Redmann*[1]

[1] Institute of Mathematics, Martin Luther University Halle-Wittenberg
martin.redmann@mathematik.uni-halle.de

Abstract

In this talk, we study dimension reduction techniques for large-scale controlled stochastic differential equations (SDEs). The drift of the considered SDEs contains a polynomial term satisfying a one-sided growth condition. Such nonlinearities in high dimensional settings occur, e.g., when stochastic reaction diffusion equations are discretized in space. We provide a brief discussion around the stability of solutions. (Almost) stability then is the basis for new concepts of Gramians that we introduce and study in this work. With the help of these Gramians, dominant subspace are identified leading to a balancing related highly accurate reduced order SDE. We provide an algebraic error criterion and an error analysis of the propose model reduction schemes. The talk is concluded by applying our method to spatially discretized reaction diffusion equations.

Keywords: Model order reduction, nonlinear stochastic systems, Gramians, Lévy processes

*This project is supported by the DFG via the individual grant "Low-order approximations for large-scale problems arising in the context of high-dimensional PDEs and spatially discretized SPDEs"– project number 499366908.

A parametric data-driven time-domain one- or two-sided moment matching method

Giordano Scarciotti[1] and Junyu Mao[1]

[1]Department of Electrical and Electronic Engineering, Imperial College London, London SW7 2AZ, U.K.
{g.scarciotti,junyu.mao18}@imperial.ac.uk

Abstract

The availability of mathematical models is essential for the analysis, control and design of modern technological devices. As the computational power has advanced, the complexity of these mathematical descriptions has increased. This has kept the computational needs at the top or over the available possibilities. A solution to this problem is represented by model reduction which consists in finding a simplified mathematical model which maintains some key properties of the original description.

In this presentation, methods to obtain parametric reduced order models by moment matching from input/output data generated by system interconnections are presented. Algorithms for the estimation of the moments of linear and nonlinear parametric systems are proposed by extending the results in [1]. Collecting time-snapshots of the input and output of the system at a given sequence of time instants t_k, algorithms to define parametric families of reduced order models at each instant of the iteration t_k are devised. These models asymptotically match the moments of the unknown parametric system to be reduced. Conditions to enforce additional properties, e.g. matching with prescribed eigenvalues, upon the reduced order model are provided and discussed.

Additional results are presented for linear systems. On the one hand, the free parameters are exploited to obtain a constrained optimal model that minimizes the error of the transient response, extending the results in [2]. On the other hand, a method to obtain two-sided moment matching at arbitrarily selected interpolation points is developed based on collecting time-snapshots of the input of and output of an interconnection of the system with two signal generators. Some discussion about the impact of noise is provided [3].

References

[1] G. Scarciotti, A. Astolfi (2017). *Data-driven model reduction by moment matching for linear and nonlinear systems*. Automatica, Vol. 79, 340–351.

[2] G. Scarciotti, Z.-P. Jiang, A. Astolfi (2020). *Data-driven constrained optimal model reduction*. European Journal of Control, Vol. 53, 68–78.

[3] J. Mao, G. Scarciotti (2023). *Data-Driven Model Reduction by Two-Sided Moment Matching*. Submitted.

Parametric Low-Order State-Space Modeling of MIMO Systems in the Loewner Framework

Tea Vojkovic[1], David Quero[2], Charles Poussot-Vassal[3], and Pierre Vuillemin[3]

[1]Delft Center for Systems and Control, Delft University of Technology
[2]Institute of Aeroelasticity, German Aerospace Center
[3]ONERA/DTIS, Université de Toulouse
[1]T.Vojkovic@tudelft.nl

Abstract

In this talk, we present a novel data-driven method for identifying parametric MIMO generalized state-space or descriptor systems of low order that accurately capture the frequency and time domain behavior of large-scale linear dynamical systems. The low-order parametric descriptor systems are identified from transfer matrix samples by means of two-variable Lagrange rational matrix interpolation. This is done within the Loewner framework by deploying the new matrix-valued barycentric formula given in both right and left matrix fraction form, which enables construction of minimal descriptor systems for rectangular transfer matrices. The developed method allows the reduction of order and parameter dependence complexity of the constructed system. Stability of the system is preserved by the post-processing technique based on the flipping signs of unstable poles. The developed methodology is illustrated with a few academic examples and applied to low-order parametric state-space identification of an aerodynamic system.

Keywords: Parametric model-order reduction, low-order system identification, two-variable rational matrix interpolation, parametric state-space realization

MS29 - Efficient numerical methods in computational biomechanics

Numerical approximations for solid Tumor growth model

Sonia Seyed Allaei[1] and Adélia Sequeira [2]

[1,2]CEMAT (Center for Computational and Stochastic Mathematics), Instituto Superior Técnico, University of Lisbon, Portugal
[1]sonia.seyedallaei@tecnico.ulisboa.pt

Abstract

A numerical algorithm for a multiscale diffuse interface model describing the evolution of a tumor inside a host tissue is elaborated in 2D. The model consists of fourth-order nonlinear advection-reaction-diffusion equations (of Cahn-Hilliard-type) for the cell-species coupled with reaction-diffusion equations for the substrate components [3, 2]. Due to the high non linearity of the coupling system, and to its numerical stiffness the numerical solution of the model is challenging.

Our goal is to use a stabilized method, to obtain an unconditionally stable linear scheme with second-order accuracy in both time and space derived from a modification of the Crank-Nicolson scheme for time discretization and a quadratic Lagrange finite element method (P2 element) for discretization in space [1]. Due to the diffuse interface structure of the model, the system will have solutions with sharp steep in the tumor/host interface [3]. An adaptive time algorithm will be used for increasing the accuracy and reducing the number of iterations. Some numerical simulations are reported that accurately and efficiently reproduce the progression of tumors with complex morphologies.

Keywords: advection diffusion equations, coupled system, numerical approximation, diffuse interface model, solid tumor growth

References

[1] D. Wang, X. Wang, R. Zhang, H. Jia (2022). *An unconditionally stable second-order linear scheme for the Cahn-Hilliard-Hele-Shaw system.* Appl Numer Math., 171, 58–75.

[2] S. M. Wise a, J. S. Lowengrub, V. Cristini (2011). *An adaptive multigrid algorithm for simulating solid tumor growth using mixture models.* Math Comput Model., 53, 1–20.

[3] S. M. Wise, J. S. Lowengrub, H. B. Frieboes, V. Cristini. *Three-dimensional multispecies nonlinear tumor growth-I: model and numerical method*, J. Theoret. Biol., 253, 524–543.

Flux-based error control for a Cahn-Hilliard system modelling tumour growth

Fleurianne Bertrand [1]

fleurianne.bertrand@mathematik.tu-chemnitz.de
[1]TU Chemnitz

Abstract

In this talk, a diffuse interface model for tumour growth is considered, with a Cahn-Hilliard equation for the tumour cells. A finite element approximation of the model is introduced, and the importance of the dual quantities is demonstrated. As these fluxes are not $H(div)$ conforming, several dual approaches are investigated and a particular focus lies on the adaptive error control. Finally, we present some numerical results.

Keywords: Cahn-Hilliard, flux reconstruction, mixed finite element method

References

[1] L. T. Biegler, G. P. Crespo, K. Martini, L. A. Barba (2019). *A phase-field model for tumour growth subject to nutrient deprivation and chemotherapy treatment.* Journal of Mathematical Biology, 78(3), 887–920.

[2] B. Merlet, M. J. Schinner, L. M. R. Villada (2015). *A Cahn-Hilliard Navier-Stokes Model for Multiphase Flows with Large Density Variations: Application to Tumor Growth.* SIAM Journal on Applied Mathematics, 75(2), 593–615.

[3] J. W. Cahn, J. E. Hilliard (1958). *Free energy of a nonuniform system. I. Interfacial free energy.* The Journal of Chemical Physics, 28(2), 258–267.

[4] A. Ern, M. Vohralik (2013). *H1 and H(div) polynomial extensions for polynomial-degree-robust potential and flux reconstruction.* SIAM Journal on Numerical Analysis, 51(2), 1188–1211.

Numerical modeling of cardiac derived stem cells and isogeometric simulation of an engineered tissue

Sofia Botti[1,2], Chiara Bartolucci[4], Alessandro Reali[5], Stefano Severi[4], Michele Torre[5], Luca F. Pavarino[2], and Rolf Krause[1,3]

[1]Euler Institute, Università della Svizzera Italiana
[2]Department of Mathematics "Felice Casorati", University of Pavia
[3]Faculty of Mathematics and Informatics, FernUni, Brig
[4]Department of Electrical, Electronic, and Information Engineering "Guglielmo Marconi", University of Bologna
[5]Department of Civil Engineering and Architecture, University of Pavia
sofia.botti@usi.ch

Abstract

Recent advances in regenerative cardiology recently have been employing induced stem cells [1], and *in silico* numerical models can help experimental techniques studying the electronic maturation toward the expression of an adult cardiac phenotype [4]. We present a numerical model based on a reaction-diffusion system coupled with stem cells ionic models, yielding a novel and highly accurate simulation of the action potential propagation in an engineered 3D cardiac tissue.

Our model is based on a 3D non-linear reaction-diffusion partial differential equation, known as cardiac *Monodomain* equation, describing the space-time evolution of the electrical transmembrane potential. This equation is coupled with a stiff system of ordinary differential equations for stem cells, known as ionic model, describing the dynamic of gating variables and ionic concentrations through the myocyte's membrane. The cardiac model is then discretized using an operator splitting technique, and then employing Isogoemetric Analysis in space and semi-implicit finite differences in time. The resulting numerical solver is then applied to assess the accuracy of the simulation of the action potential propagation in a cardiac fiber. The solver is then applied to investigate the 3D action potential propagation in an engineered ventricle model, calibrated as in [3]. Our results demonstrate the feasibility of virtual representations of innovative derived stem cells ventricle, indicating an *in silico* low-cost approach to stem cells tissue investigations [5].

References

[1] K. Takahashi, S. Yamanaka (2006). *Induction of Pluripotent Stem Cells from Mouse Embryonic and Adult Fibroblast Cultures by Defined Factors.* Cell 126.4, 663—676.

[2] A. O. Verkerk, C. C. Veerman, R. Wilders et al. (2017). *Patch-clamp (...) characteristics through dynamic clamp.* Journal of Molec. Sc. 18(9).

[3] L. MacQueen et al (2018). *A tissue-engineered scale model of the heart ventricle.* Nat. Biomed. Eng. 2.1, 930—941.

[4] S. Botti, C. Bartolucci, R. Krause, L.F. Pavarino, S. Severi (2023). *An in silico Study of Cardiac (...) by Dynamic Clamp.* In *Functional Imaging and Modeling of the Heart - FIMH 2023.* To appear

[5] S. Botti, M. Torre (2023). *Isogeometric simulation of a derived stem cell engineered ventricle.* Submitted.

Modeling of Patient-specific Blood Flows and Clinical Validation

Xiao-Chuan Cai[1]

[1]Department of Mathematics, University of Macau, Macau, China
xccai@um.edu.mo

Abstract

In this talk, we present some applications of domain decomposition based implicit finite element methods in the simulation of blood flows in the human artery at the full-body and individual organ scales. Several mathematical, clinical, bio-mechanical, and supercomputing issues will be discussed in detail.

Keywords: Navier-Stokes equations, blood flow problems, domain decomposition

Modelling Spacial Heterogeneity in 3D tumour growth driven by oxygen mediated phenotypic changes

Cicely K. MacNamara[1], Alfonso Caiazzo[2], and Tommaso Lorenzi[3]

[1]University of Glasgow, UK
[2]WIAS Berlin, Germany
[3]Politecnico di Torino, Italy
cicely.macnamara@glasgow.ac.uk; alfonso.caiazzo@wias-berlin.de;
tommaso.lorenzi@polito.it

Abstract

Cancer growth is a complex phenomenon due to the interaction of different biological and physical processes, as well as the presence of multiple spatial and temporal scales. This research focuses on 3D individual-based (agent-based) models, in which each agent (a single cell, for example) is fully realized within the model, and interactions are primarily governed by mechanical forces between elements.

This work builds on the individual-based model recently introduced in [1, 2], which allows acounting for mechanical interaction, interaction with microcirculation, and the presence of fibrous extracellular matrix, by introducing different types of agents (cells with different phenotypes, tissue fibers, and blood vessels) and considering the coupling of the cancer growth model with an immersed finite element method for modeling the oxygen concentration within the tissue.

In particular, we introduce general oxygen-mediated phenotypic changes by describing the phenotype of each cell with a discrete value in the interval $[0, 1]$ (where 0 corresponds to a normoxic state and 1 to a hypoxic state). Phenotypic mutations are modeled by a uniform probability function depending on the availability of nutrients for the particular cell, following the approach introduced for a continuum (PDE-based) model by [3].

We show preliminary numerical simulations to validate the results of the individual-based model against the expected values from the corresponding continuum description, discussing also different aspects of the linkage between agent-based and PDE-based simulations.

Keywords: Cancer modeling, Agent-based model, Continuum model, Oxygen phenotypes

References

[1] A. Caiazzo, I. Ramis-Conde (2015). *Multiscale modelling of palisade formation in gliobastoma multiforme.* J Theor Biol, 383: 145–156

[2] C. K. Macnamara, A. Caiazzo, I. Ramis-Conde, M. A. J. Chaplain (2020). *Computational modelling and simulation of cancer growth and migration within a 3d heterogeneous tissue: The effects of fibre and vascular structure.* J Comp Sci, 40:101067.

[3] C. Villa, M. A. J. Chaplain, T. Lorenzi (2021). *Modeling the emer- gence of phenotypic heterogeneity in vascularized tumors.* SIAM J Appl. Math, 81(2), 434–453.

Temporal homogenisation and parallelisation for the numerical simulation of atherosclerotic plaque growth

Stefan Frei[1], Alexander Heinlein[2], and Thomas Richter[3]

[1]University of Konstanz, Germany
[2]Delft University of Technology, The Netherlands
[3]Otto-von-Guericke-University Magdeburg, Germany
stefan.frei@uni-konstanz.de; A.Heinlein@tudelft.nl; thomas.richter@ovgu.de

Abstract

The numerical simulation of atherosclerotic plaque growth is computationally prohibitive, since it involves a complex cardiovascular fluid-structure interaction (FSI) problem with a characteristic time scale of milliseconds to seconds, as well as a plaque growth process governed by convection-diffusion-reaction equations, which takes place over several months or years. A resolution of the fast (*micro*) scale over this period can easily require more than a billion time steps, each corresponding to the solution of a computationally expensive FSI problem.

To tackle this problem, we combine a temporal homogenisation approach with parallelisation in time. First, a temporal two-scale approach is developed, which separates the problem in an FSI problem on the micro scale and a convection-diffusion-reaction problem on the macro scale. Second, a parallel time-stepping approach based on the parareal algorithm is applied on the macro scale of the homogenised system. We investigate modifications in the coarse propagator of the parareal algorithm to further reduce the number of expensive micro problems to be solved and test the numerical algorithms in detailed numerical studies.

Keywords: Atherosclerotic plaque growth; Temporal homogenisation; Temporal parallelisation; Fluid-structure interactions

References

[1] S. Frei, T. Richter (2020). *Efficient approximation of flow problems with multiple scales in time.* SIAM Multiscale Model Simul 18(2), 942–969.

[2] S. Frei, A. Heinlein, T. Richter (2021). *On temporal homogenization in the numerical simulation of atherosclerotic plaque growth.* PAMM 21:e202100055.

[3] S. Frei, A. Heinlein (2022). Towards parallel time-stepping for the numerical simulation of atherosclerotic plaque growth. submitted journal article, preprint: `http://arxiv.org/abs/2203.06526`.

Modeling Simulation Behavior: Error Balancing in a Multi-Scale Muscle Simulation using Bayesian Optimization

Felix Huber[1], Dominik Göddeke[1,3], and Miriam Schulte[2,3]

[1]Department of Mathematics, University of Stuttgart
[2]Department of Computer Science, University of Stuttgart
[3]Stuttgart Center for Simulation Science, University of Stuttgart
{felix.huber, dominik.goeddeke}@mathematik.uni-stuttgart.de;
miriam.schulte@ipvs.uni-stuttgart.de

Abstract

Simulations, such as the muscle simulation framework OpenDiHu [3], consist of many numerical components that affect the simulation accuracy and the required resources. Components such as models, discretization, solvers and floating point accuracy, all influence the simulation behavior. However, finding an optimal combination of these components that balances accuracy and computational resources can be a difficult and time-consuming process. Model-based Bayesian optimization is a useful tool to tackle such problems [2]. Many existing optimization approaches treat the optimization function as a black-box. We present a Bayesian approach that uses prior knowledge of the simulation components to optimize the temporal discretizations on multiple scales of the simulation. In each step of the Bayesian optimization, a model for the simulation error and the run time is improved. This model uses already known data of the simulation properties and incorporates prior knowledge of the simulation such as a priori convergence orders and run time scaling of the components. Based on the model a new set of simulation parameters is selected, for which the simulation is run. A new simulation run should not only help to approach the optimum of the objective problem, but also improve the models that are used for the optimization. Further it has to take the cost of each possible simulation run into account, which depend on the discretization parameters and thus vary significantly. We discuss our optimization approach, how a priori knowledge is used in the model and how simulation costs can be integrated.

Keywords: Bayesian optimization, Constrained optimization, Multi-scale simulation

References

[1] Bradley, C.P., Emamy, N., Ertl, T., Göddeke, D., Hessenthaler, A., Klotz, T., Krämer, A., Krone, M., Maier, B., Mehl, M., Rau, T. and Röhrle, O. (2018). Enabling Detailed, Biophysics-Based Skeletal Muscle Models on HPC Systems. *Frontiers in Physiology*, 9, 816.

[2] Gardner, J.R., Kusner, M.J., Xu, Z.E., Weinberger, K.Q. and Cunningham, J.P. (2014). Bayesian Optimization with Inequality Constraints. In: *Proceedings of the 31st International Conference on Machine Learning*, 32, 937–945.

[3] Krämer, A., Maier, B., Rau, T., Huber, F., Klotz, T., Ertl, T., Göddeke, D., Mehl, M., Reina, G. and Röhrle, O. (2021). Multi-Physics Multi-Scale HPC Simulations of Skeletal Muscles. *High Performance Computing in Science and Engineering '20 – Transactions of the High Performance Computing Center.*

Numerical Simulation of Effective Models for Transport Processes in Deformable Porous Media within Mixed Eulerian/Lagrangian Framework

Jonas Knoch[1,2], Markus Gahn[1,2], Maria Neuss-Radu[1,2], and Nicolas Neuß[1]

[1]Friedrich-Alexander-Universität Erlangen-Nürnberg
[2]Ruprecht-Karls-Universität Heidelberg
jonas.knoch@fau.de; markus.gahn@iwr.uni-heidelberg.de; {maria.neuss-radu, neuss}@math.fau.de

Abstract

We present in this talk an effective model for transport processes in periodically perforated elastic media, taking into account also cyclic elastic deformation as it occurs e.g. in lung tissue due to respiratory movement. The underlying microscopic problem consists of a linear elasticity equation for the displacement within the Lagrangian framework, posed on a fixed domain and a diffusion equation for the concentration within the Eulerian framework, posed on the current deformed domain. After a transformation of the diffusion equation onto the fixed domain, we derive the upscaled model by means of a formal asymptotic expansion. The system is nonlinearly coupled through effective coefficients, which also take into account the periodic microstructure. We develop and study numerical methods for our problem and perform simulations that are inspired by a bioengineered microdevice which is able to reconstitute critical lung functions (Lung-On-A-Chip). The simulations shed light into the sensitivity of the model with respect to several experimental parameters such as frequency or magnitude of the cyclic mechanical strain.

Keywords: Perforated elastic medium, Evolving microstructure, Diffusive transport, Two-scale expansion, Finite-element method

References

[1] J. Knoch, M. Gahn, M. Neuss-Radu, N. Neuß (2023). *Multi-Scale Modeling and Simulation of Transport Processes in an Elastically Deformable Perforated Medium.* Transport in Porous Media, 1–31.

Calibration of Windkessel parameters for 1D-0D coupled blood flow models using kernel methods and quantum algorithms

Tobias Köppl[1], Gabriele Santin[2], and Ilie-Daniel Gheorge-Pop[3]

[1]Faculty of Science, Mathematics and Statistics, University of Hasselt, Hasslet, Belgium
[2]Fondazione Bruno Kessler, Center for Information and Communication Technology, Trento, Italy
[3]Fraunhofer Institute for Open Communication Systems (FOKUS), Berlin, Germany
tobias.koeppl@uhasselt.be; gsantin@fbk.eu;
ilie-daniel.gheorghe-pop@fokus.fraunhofer.de

Abstract

In this talk, we present a model for simulating blood flow within a network consisting of the largest arteries branching out of the heart. In order to decrease the computational effort one-dimensional (1D) Navier-Stokes equations are used to describe the flow field within this network. Since only large arteries are modeled by means of the 1D Navier-Stokes equations, appropriate boundary conditions have to be imposed at the outlets of the considered network. One way to account for the missing vessels is to use systems of ordinary differential equations incorporating the resistance and capacity of the omitted vessels. Since they exhibit no space variable they are indicated as 0D models. All in all, this results in a 1D-0D coupled blood flow model [1, 3]. Parameters of the 0D models have to be chosen in a careful way to produce realistic simulation data. Using measurements of blood pressure curves, these parameters are calibrated by means of appropriate minimization problems. To avoid expensive evaluations of the respective cost functionals, kernel methods are considered [1, 2] to approximate the cost functionals. For the solution of the minimization problems, we apply two different types of approaches: The first one is a classical optimization method, while the second one exploits features of a quantum annealer. In case of the second approach, we discuss new algorithmic aspects [4]. The performance of both algorithms is illustrated by several numerical tests.

Keywords: Blood flow modeling, dimension reduced models, machine learning, quantum computing

References

[1] T. Koeppl, G. Santin, B. Haasdonk,R. Helmig (2018). *Numerical modelling of a peripheral arterial stenosis using dimensionally reduced models and kernel methods.* International journal for numerical methods in biomedical engineering, 34, 8, e3095, Wiley Online. Library.

[2] G. Santin, B. Haasdonk (2019). *Kernel methods for surrogate modeling.* Model Order Reduction, 1, 311–354.

[3] J. P. K. H. Alastruey, K. H. Parker, J. Peiró, S. M. Byrd, S. J. Sherwin (2007). *Modelling the circle of Willis to assess the effects of anatomical variations and occlusions on cerebral flows.* Journal of biomechanics, 40(8), 1794–1805.

[4] Endre Boros, Peter L Hammer, Gabriel Tavares (2007). *Local search heuristics for quadratic unconstrained binary optimization (QUBO).* Journal of Heuristics, 13, 99–132, Springer.

Computationally efficient simulation of multiple moving cells that release diffusing compounds in their environment

Qiyao Peng[1] and Sander C. Hille[1]

[1]Mathematical Institute, Leiden University
{q.peng, shille}@math.leidenuniv.nl

Abstract

In biomedical applications, there are many interactions between single objects and the direct environment, and one of the most important interactions is conducted by the diffusion of the compounds, such as signalling molecules. For example, in the wound healing, immune cells releases cytokines to attract the skin cells migrate towards the wound region; in drug delivery, the microbubbles release the drug molecules to the targeted region.

For the sake of computational efficiency, in mathematical modelling and for theoretical purposes, the Dirac Delta distributions are often utilized as a replacement for cells or vesicles, since the size of cells or vesicles is much smaller than the size of the surrounding tissues. Here, we consider the scenario that the cell or the vesicle releases the diffusive compounds to the immediate environment, which is modelled by the diffusion equation. Typically, one separates the intracellular and extracellular environment and uses homogeneous Neumann boundary condition for the cell boundary (so-called spatial exclusion approach), while the point source approach neglects the intracellular environment. We show that extra conditions are needed such that the solutions to the two approaches are consistent. We prove a necessary and sufficient condition for the consistency. Suggested by the numerical results, we conclude that an initial condition in the form of Gaussian kernel in the point source approach compensates for a time-delay discrepancy between the solutions to the two approaches in the numerical solutions. Various approaches determining optimal amplitude and variance of the Gaussian kernel have been discussed; see [1] for more details.

For the homogeneous flux density from the cell membrane, one can easily replace each cell by one Dirac point at the cell center. However, for inhomogeneous flux density, for instance, the sinusoidal function, multiple Dirac points are needed besides the cell center to represent the cell, which forms a dipole or tripole system — similar to the cases in electromagnetism.

Keywords: Diffusion equation, Dirac delta distributions, Point source, Gaussian kernel, Numerical analysis

References

[1] Q. Peng, S.C. Hille (2023). *Quality of approximating a mass-emitting object by a point source in a diffusion model.* ArXiv.

Numerical approximation of a viscoelastic Cahn–Hilliard model for tumour growth

Dennis Trautwein[1] and Harald Garcke[1]

[1]Department of Mathematics, University of Regensburg
{Dennis.Trautwein, Harald.Garcke}@ur.de

Abstract

In this talk, we present a phase-field model for tumour growth, where a diffuse interface separates a tumour from the surrounding host tissue. In our model, we consider transport processes by an internal, non-solenoidal velocity field and biological effects like chemotaxis. We include viscoelastic effects with a general Oldroyd-B type description with possible relaxation, stress sources by growth and additional stress diffusion. We discuss the numerical approximation with a fully-practical, stable and converging finite element scheme in two and three space dimensions, which preserves the physical properties of the model. As the discretization parameters tend to zero, we pass to the limit in the numerical scheme and show (subsequence) convergence towards a global-in-time weak solution in two and three space dimensions. Finally, we illustrate the practicability of the discrete scheme with the help of numerical simulations.

Keywords: Finite element approximation, Cahn–Hilliard, viscoelasticity, tumour growth

Efficient Monolithic Methods for Fluid-Structure Interaction Applied to Flapping Membranes

Daniel Jodlbauer[1], Ulrich Langer[2], and Thomas Wick[3]

[1]Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences, Altenberger Str. 69, 4040 Linz, Austria
[2]Johannes Kepler University Linz, Institute of Numerical Mathematics, Altenberger Str. 69, 4040 Linz, Austria
[3]Leibniz University Hannover, Institute of Applied Mathematics, Welfengarten 1, 30167 Hannover, Germany
daniel.jodlbauer@ricam.oeaw.ac.at; ulanger@numa.uni-linz.ac.at;
thomas.wick@ifam.uni-hannover.de

Abstract

This presentation is devoted to the efficient solution of variational-monolithic fluid-structure interaction (FSI) initial-boundary value problems [1]. Due to the interface coupling conditions, the development of robust scalable parallel solvers remains a challenging task. The main purpose of this work consists in further numerical studies of the solver, developed in [2, 3], for a benchmark problem that is motivated by hemodynamic applications. Specifically, we consider channel flow with elastic membranes and elastic solid walls. This situation is challenging because of the thin elastic flaps and was the motivation for fluid-structure interaction models such as immersed methods in the past. We employ arbitrary Lagrangian-Eulerian coordinates, because of the high accuracy of the coupling conditions as the interface is tracked. For a careful evaluation of the performance of our physics-based block FSI preconditioner from [3], we use sparse direct solvers for the mesh, solid, and fluid subproblems. These sparse direct solvers should be replaced by iterative solvers in the case of large-scale problems with a high number of degrees of freedom. Therein, the flow part with well-known saddle-point structure becomes very critical, which was not yet the case for our solver applied to some FSI benchmarks. The performance of our block FSI preconditioner and overall linear GMRES solver is evaluated in terms of iteration numbers as well as memory storage. Moreover, iteration numbers of the nonlinear Newton solver are monitored. Finally, a compu- tational convergence analysis for flap tip displacements, drag and lift for different spatial mesh levels is conducted.

Keywords: Monolithic Framework, Scalable Parallel Solution, Fluid-Structure Interaction, Flapping Membranes

References

[1] D. Jodlbauer, U. Langer, T. Wick (2023). *Efficient monolithic solvers for fluid-structure interaction applied to flapping membranes.* In *Domain Decomposition Methods in Science and Engineering XXVI*, 327–335, Springer.

[2] D. Jodlbauer (2021). *Parallel Multigrid Solvers for Nonlinear Coupled Field Problems.* Dissertation, Johannes Kepler University Linz.

[3] D. Jodlbauer, U. Langer, T. Wick (2019). *Parallel block-preconditioned monolithic solvers for fluid-structure interaction problems.* Int. J. Num. Meth. Eng. Vol. 117 (6), 623–643.

MS30 - Robust Numerical Methods for Nonlinear and Coupled Diffusion Problems in Biology

A numerical method for simulating cell membrane and cytosolic dynamics

Davide Cusseddu[1,2] and Anotida Madzvamuse[3]

[1]Grupo de Física-Matematica Universidade de Lisboa, Portugal
[2]CMAT, Universidade do Minho, Portugal
[3]Mathematics Department, University of British Columbia, Canada
davide.cusseddu@gmail.com

Abstract

The *bulk-surface wave-pinning (BSWP) model* is a reaction-diffusion system given by

$$\begin{cases} u_t = D_u \Delta u, & x \in \Omega \subset \mathbb{R}^3, \\ -D_u \mathbf{n} \cdot \nabla u = f(u,v) & x \in \partial\Omega, \\ v_t = D_v \Delta_\Gamma v + f(u,v), & x \in \partial\Omega, \end{cases}$$

where Δ_Γ indicates the Laplace-Beltrami operator and the reaction function is

$$f(u,v) = \left(\alpha + \frac{\beta v^\gamma}{K^\gamma + v^\gamma}\right) u - \delta v.$$

Such system constitutes one of the simplest model of cell polarisation and describes the switching between active (v) and inactive (u) state of a representative protein from the GTPase family. Since GTPase active proteins are generally bounded to the cell membrane, and inactive proteins are generally found in the cytosol, the bulk-surface framework naturally allows us to define u and v on different domains, respectively $\partial\Omega$ and $\overline{\Omega}$. Interactions are described by the nonlinear reaction term $f(u,v)$ at the surface. Cell polarisation arises as the surface component develops specific patterns. The surface reaction-diffusion equation promotes propagating front solutions with non-constant speed, which eventually get pinned. In this way, the surface will finally be characterised either by areas with low or areas with high levels of v.
Following some test examples presented in our recent work [1], I will present and discuss the bulk-surface finite element method, which we use for solving the system numerically, over simple and complex geometries, showing pattern formation due to propagation and pinning dynamics. The generality of our mathematical and computational framework is suitable for the study of more complex biochemical reactions and biomechanical properties associated with cell polarisation in multi-dimensions.

Keywords: bulk-surface system, bulk-surface finite element method, wave-pinning, pattern formation

References

[1] D. Cusseddu, A. Madzvamuse (2022). *Numerical investigations of the bulk-surface wave pinning model*. Mathematical Biosciences. 354: 108925.

Discontinous Galerkin methods on polytopal grids for multiphysics modeling of the cerebrospinal fluid

Ivan Fumagalli[*‡1], Paola F. Antonietti[*†‡1], Mattia Corti[‡1], and Nicola Parolini[*†‡1]

[1]MOX, Department of Mathematics, Politecnico di Milano, Italy
{ivan.fumagalli, paola.antonietti, mattia.corti, nicola.parolini}@polimi.it

Abstract

The modeling of the dynamics the Cerebrospinal Fluid (CSF) in the brain intrinsically entails different physics, since the CSF both filtrates through the cerebral tissue and it flows in three-dimensional neuron-free regions such as the brain ventricles and the subarachnoid space. Moreover, the generation of CSF is strictly coupled with blood perfusion in the brain. Motivated by this, we introduce a multiphysics model encompassing dynamic Multiple-Network Poroelastic (MPE) equations for the poromechanics of the tissue [1] and Navier-Stokes equations for the 3D modeling of the CSF flow in the neuron-free regions. The MPE model accounts for multiple scales of blood vessels and the extracellular component of the CSF, while the interface conditions between the physical domain describe the physiological exchange of mass and stress [2].

We present a discontinuous Galerkin method for the space discretization of this coupled problem, based on polytopal grids for an accurate representation of the extremely complex geometry of the interface between the two physical domains. Through a priori analysis, we provide stability results and error bounds for the semi-discrete problem on polygonal/polyhedral elements of general shapes. Combining a Newmark β-method and θ-methods, we introduce a second-order temporal discretization of the system. The verification of the method is carried out by convergence tests in simplified and realistic geometries, and a three-dimensional patient-specific simulation is carried out on a domain reconstructed from magnetic resonance images.

Keywords: Navier-Stokes equations, multiple-network poroelastic theory, a priori analysis, polygonal/polyhedral mesh

References

[1] M. Corti, P. F. Antonietti, L. Dede', A. Quarteroni (2023). *Numerical modelling of the brain poromechanics by high-order discontinuous Galerkin methods*, Math. Mod. Meth. Appl. Sci.. In press.

[2] M. Causemann, V. Vinje, M.E. Rognes (2022). *Human intracranial pulsatility during the cardiac cycle: a computational modelling framework*. Fluids Barriers CNS 19, 84.

*IF, PA and NP acknowledge the funding by the Italian Research Center on High Performance Computing, Big Data and Quantum Computing (ICSC), under the NextGenerationEU project.

†PA and NP acknowledge the funding by MUR for the PRIN 2020 research grant n. 20204LN5N5 "Advanced polyhedral discretisations of heterogeneous PDEs for multiphysics problems".

‡All the authors are members of GNCS-INdAM.

Discrete and continuum modeling of robust biological transportation networks

Jan Haskovec[1], Clarissa Astuto[1], and Peter Markowich[1]

[1]King Abdullah University of Science and Technology, Thuwal, KSA
{jan.haskovec, clarissa.astuto, peter.markowich}@kaust.edu.sa

Abstract

Motivated by recent results on formation and adaptation of biological transport networks [1], in particular leaf venation in plants, we study a discrete model consisting of an energy consumption function constrained by a linear system on a graph. We discuss how structural properties of the optimal network patterns, like sparsity and (non)existence of loops, depend on the convexity/concavity of the metabolic part of the energy functional. We then introduce robustness of the network in terms of algebraic connectivity of the graph and explain its impact on the network structure. Passing to the continuum limit as the number of edges and nodes of the graph tends to infinity, we recover a nonlinear system of PDEs. This elliptic-parabolic system consists of a Darcy's type equation for the pressure field and a reaction-diffusion equation for the network conductance. We explain how the robustness property is reflected on the level of the PDE description. We give both analytical results and systematic numerical simulations for the PDE system, providing interesting insights into the mechanisms of network formation and adaption in biological context.

Keywords: Biological transportation networks, algebraic connectivity, continuum limit.

References

[1] D. Hu, D. Cai (2013). *Adaptation and Optimization of Biological Transport Networks.* Physical Review Letters. Vol. 111, No. 13.

On Efficient Implementation of Trigonometric Integrators in Molecular Dynamics

Tobias Kliesch[1], Volker Grimm[1], and Marlis Hochbruck[1]

[1]Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology
{tobias.kliesch, volker.grimm, marlis.hochbruck}@kit.edu

Abstract

In classical molecular dynamics, interactions between bonded particles introduce high frequencies to the system and render the solution highly oscillatory. With a suitable linearisation this nonlinear problem can be formulated as a semilinear problem. In this case, trigonometric integrators are well-known to allow for long time steps by using matrix-valued trigonometric functions (e.g., [1, Chap. XIII] and [2]). The efficiency of these integrators depends strongly on the evaluation of the product of the matrix-valued trigonometric functions with a vector. Krylov subspace approximations are a good choice for this task [3]. We also discuss an alternative approach based on Chebychev polynomials proposed in [4], where the trigonometric functions are approximated by appropriate polynomials. The resulting leapfrog-Chebychev scheme can be seen as a particular implementation of the trigonometric integrator.

We present a parallel implementation of a trigonometric integrator and a leapfrog-Chebychev scheme in the molecular dynamics software package LAMMPS [5]. We demonstrate the efficiency on selected examples ranging from solids to gases. Depending on the system, our implementation is up to 3 times faster than the highly optimized implementation of the standard Verlet integrator.

Keywords: Molecular Dynamics, Trigonometric Integrators, Leapfrog-Chebychev Schemes

References

[1] E. Hairer, G. Wanner, C. Lubich (2010). *Geometric Numerical Integration*. Vol 2. Springer.

[2] M. Hochbruck, A. Ostermann (2010). *Exponential integrators*. Acta Numer. 19, 209–286.

[3] M. Hochbruck, C. Lubich (1997). *On Krylov subspace approximations to the matrix exponential operator*. SIAM J. Numer. Anal. 34, 1911–1925.

[4] C. Carle, M. Hochbruck, A. Sturm (2020). *On leapfrog-Chebyshev schemes*. SIAM J. Numer. Anal. 58, 2404–2433.

[5] A. P. Thompson et. al. (2022). *LAMMPS — a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales*. Comput. Phys. Commun., 271, 108–171.

A level-set approach for a multiscale cancer invasion model

Ulrike Kochan-Eilers[1], Dumitru Trucu[2], and Thomas Carraro[1]

[1]Chair of Applied Mathematics, Helmut Schmidt University / University of the Federal Armed Forces Hamburg, Germany
[2]Division of Mathematics, University of Dundee, Dundee, United Kingdom.
kochaneu@hsu-hh.de; D.Trucu@dundee.ac.uk; carraro@hsu-hh.de

Abstract

We present a multiscale model for tumor invasion and its implementation with adaptive finite elements using cut cells in a two dimensional domain. The macroscopic dynamics determines the distribution of cancer cell c and extracellular matrix v in the domain $\Omega(t) \subset \mathbb{R}^2$, see equations (1–2), where the time-dependent domain is defined by a transport equation for a level set function $\phi(t)$. The interface dynamics, determined by the velocity of the domain boundary $V(m)$, is governed by the solution of the distribution of matrix degrading enzymes m defined in a microscopic domain ϵY at the boundary of the cancer region (3). In [1] the transport equation for the domain is solved by the stream line diffusion finite element method. Here, we present a propagation of the domain according to a computed velocity field, where the Fast Marching algorithm solves the eikonal equation (4) in a time step ΔT of the macroscopic problem. We discuss some aspects of the numerical implementation and show numerical results.

Macroscopic model component:

$$\frac{\partial c}{\partial t} = D_1 \Delta c - \eta \nabla \cdot (c \nabla v) + \mu_1 c(1 - c - v) \qquad \text{in } \Omega(t) \times [0, T], \tag{1}$$

$$\frac{\partial v}{\partial t} = -\alpha c v + \mu_2 (1 - c - v) \qquad \text{in } \Omega(t) \times [0, T]. \tag{2}$$

Microscopic model component:

$$\frac{\partial m}{\partial t}(y, t') = D_2 \Delta m(y, t') + F_x(c) \quad (y, t') \text{ in } \epsilon Y \times [0, T']. \tag{3}$$

Transport of domain boundary:

$$V(m) \cdot \|\nabla \phi\| = 1, \quad \text{in } \Omega' \times (0, \Delta T]. \tag{4}$$

Keywords: Mathematical Biology, Multiscale Model, Finite Element Method, Adaptive Grid, Cut Cells, Fast Marching Method

References

[1] T. Carraro, S. E. Wetterauer, A. V. Ponce Bobadilla, D. Trucu (2021). *A level set approach for a multi-scale cancer invasion model.* Math. Appl. Sci. Eng., 2, 32–54.

Preliminary numerical results in the optimization of bioenergy-intended raceway ponds

Aurea Martínez*[1], Lino J. Alvarez-Vázquez[1], Carmen Rodríguez[2], and Miguel E. Vázquez-Méndez[3]

[1]Departamento Matemática Aplicada II, EI Telecomunicación, Universidade de Vigo, 36310 Vigo, Spain
[2]Departamento Matemática Aplicada, Facultad Matemáticas, Universidade de Santiago de Compostela, 15782 Santiago, Spain
[3]CITMAGA, 15782 Santiago de Compostela, Spain; and Departamento Matemática Aplicada, EPS, Universidade de Santiago de Compostela, 27002 Lugo, Spain
{aurea,lino}@dma.uvigo.es; {carmen.rodriguez,miguelernesto.vazquez}@usc.es

Abstract

Most usual algae cultivation systems are the raceway ponds (open channels in the shape of an oval with a rotating paddle wheel to promote the recirculation of the shallow water inside them) [1, 2]. This work deals with the optimization of different characteristics in these raceway ponds: location and speed of the paddlewheel, height of water, etc. [3]. We formulate this real-world problem as an optimal control problem where the state system couples the nonlinear Navier-Stokes equations for hydrodynamics with the 3D convection-reaction-diffusion equations for algae/nitrogen/phosphorus concentrations [4], and the objective function to be maximized represents global algae concentration at the final time of the process, subject to suitable geometric and technological constraints. After a detailed mathematical formulation of the problem, we propose a numerical algorithm for the resolution of the discretized problem. Finally, we show some preliminary computational results related to the numerical modelling of the state system and to the optimization of the discretized problem.

Keywords: Optimal design, Algae-based bioenergy, Raceway, Optimal control of PDEs, Numerical optimization

References

[1] S.K. Bhatia, S. Mehariya, R.K. Bhatia, M. Kumar, A. Pugazhendhi, K. Awasthi, A.E. Atabani, G. Kumar, W. Kim, S.-O. Seo, Y.-H. Yang (2021). *Wastewater based microalgal biorefinery for bioenergy production: Progress and challenges*. Sci. Total Environ., 751, 141599.

[2] J.C.M. Pires, M.C.M. Alvim-Ferraz, F.G. Martins (2017). *Photobioreactor design for microalgae production through computational fluid dynamics: A review*. Renewable Sust. Energy Rev., 79, 248–254.

[3] F. Rayen, B. Taidi, D. Pareau (2019). *Optimization of a raceway pond system for wastewater treatment: A review*. Critical Rev. Biotechnol., 39, 422–435.

[4] L.J. Alvarez-Vázquez, F.J. Fernández, I. López, A. Martínez (2010). *An Arbitrary Lagrangian Eulerian formulation for a 3D eutrophication model in a moving domain*. J. Math. Anal. Appl., 366, 319–334.

*This research was funded by Ministerio de Ciencia e Innovación (Spain) grant number TED2021-129324B-I00.

Multiscale modelling and simulations of plant tissues

Mariya Ptashnyk[1], Arezki Boudaoud *[2], and Annamaria Kiss[3]

[1]Department of Mathematics, Heriot-Watt University, The Maxwell Institute for Mathematical Sciences, Edinburgh, Scotland, UK
[2]LadHyX, CNRS, Ecole Polytechnique, IP Paris, Palaiseau, France
[3]RDP, Univ Lyon, ENS de Lyon, Univ Claude Bernard Lyon 1, CNRS, INRAE, Lyon, France
m.ptashnyk@hw.ac.uk; arezki.boudaoud@polytechnique.edu; annamaria.kiss@ens-lyon.fr

Abstract

Many biological tissues must be structured in such a way as to be able to adapt to two extreme biomechanical scenarios: they have to be strong to resist high pressure and mechanical forces and yet be flexible to allow large expansions and growth. A part of nature's solution to this intriguing problem are the complex microstructures and microscopic (cellular) processes, that modify tissue's elastic properties. To analyse the interplay between the mechanics, microstructure, and the chemistry we derive microscopic models for plant biomechanics, assuming that the elastic properties depend on the chemical processes and chemical reactions depend on the mechanical stresses. The microscopic models constitute strongly coupled systems of reaction-diffusion-convection equations for chemical processes and equations of elasticity or poroelasticity for elastic deformations. Multiplicative decomposition of the deformation gradient into elastic and growth parts is used to model growth of a biological tissue. To analyse the properties and behaviour of plant tissues, the macroscopic models are derived using homogenization techniques. Numerical solutions for macroscopic models demonstrate the impact of the microstructure on tissue deformations and growth.

Keywords: Multiscale analysis and numerics, Tissue growth, Plant modelling

References

[1] A. Boudaoud, A. Kiss, M. Ptashnyk (2023). *Multiscale modelling and analysis of growth of plant tissues*. arXiv:2302.08449.

[2] M. Ptashnyk, B. Seguin (2016). *Multiscale analysis of a system of elastic and reaction-diffusion equations modelling plant cell wall biomechanics*. ESAIM M2AN, 50, 593–631.

[3] M. Ptashnyk, B. Seguin (2017). *Homogenization of a viscoelastic model for plant cell wall biomechanics*. ESAIM: Control, Optimis., Calculus of Variations, 23, 1447–1471.

[4] M. Ptashnyk, B. Seguin (2016). *The impact of microfibril orientations on the biomechanics of plant cell walls and tissues: modelling and simulations*. Bulletin of Mathematical Biology, 78, 2135–2164.

*A. B. thanks the French National Research Agency

Model selection for reaction-diffusion equations using rare data in life-sciences

Cordula Reisch[1] and Hannah Burmester[1]

[1]Institute for Partial Differential Equations, TU Braunschweig
c.reisch@tu-bs.de

Abstract

Modeling biological processes is a highly demanding task because not all processes are yet fully understood. Therefore the mathematical models include terms that abstract from the real micro-scale mechanisms. For these terms, experimental parameter calibration is extremely challenging as the parameter value can not be determined by single experiments.

In this talk, we present ideas on how to overcome these difficulties by using longtime characteristics of solutions for, first, finding abstract mechanisms covering large-scale observations and, second, determining parameter values for the abstract mechanisms. These parameter values are not directly connected to experimental data but serve as link between known mechanisms and observations. The framework combines machine learning techniques with characteristic solution behavior of reaction-diffusion equations. For testing the framework, ordinary differential equations with different complexity are used. This simplified setting gives insight into challenges by using rare data only.

Keywords: Reaction diffusion models, model discovery, multi-scale information

References

[1] C. Reisch, D. Langemann (2022). *Automative model selection and model certification for reaction-diffusion equations*. IFAC-PapersOnLine, 55(20) 16, 73–78, doi: 10.1016/j.ifacol.2022.09.074

PDE modelling and simulation of intracellular signalling pathways

Sofie Verhees[1], Dr. Mariya Ptashnyk [2], and Dr. Chandrasekhar Venkataraman[3]

[1]MAC-MIGS (Maxwell Institute Graduate School) & Heriot-Watt University
[2]The Maxwell Institute for Mathematical Sciences & Heriot-Watt University
[3]University of Sussex
s.b.verhees@sms.ed.ac.uk

Abstract

Communication and interactions between cells happen mostly through intercellular signalling processes. These signalling pathways are important in all physiological activities of the cell, such as cell division, cell movement, immune response, and tissue development. In many of these signalling pathways, the chemical processes and mechanics of the cell work together [1]. However, how exactly these two phenomena communicate is not well known. A common way to model the chemical processes of cell signalling pathways are reaction-diffusion equations [2]. The mechanical properties of the cell are modelled assuming elastic constitutive relationships. Regarding the chemical process, our model includes the diffusion of signalling molecules and membrane receptors, and the reactions between the molecules and receptors. This is coupled to the mechanical properties such that the mechanics of the extracellular matrix influences the interaction between the signalling molecules and the results of the signalling pathways affect the deformation of the cell. To explore this coupling, we model the cell signalling processes involving the Rho signalling molecule, which is known to interact with the mechanical properties of the cell and the extracellular matrix [3]. Simulation results, benchmarking and a comparison to experimental observations will also be presented.

Keywords: Intercellular signalling pathways, reaction-diffusion equations, elasticity, finite element method

References

[1] P. Romani, L. Valcarcel-Jimenez, C. Frezza, S. Dupont (2021). *Crosstalk between mechanotransduction and metabolism.* Nature Reviews Molecular Cell Biology, 22, 22-–38.

[2] M. Ptashnyk, C. Venkataraman (2020). *Multiscale analysis and simultion of signalling process with surface diffusion.* MMS, SIAM Journal, 18, 851–886.

[3] K. E. Scott, S. I. Fraley, P. Rangamani (2021). *A spatial model of YAP/TAZ signaling reveals how stiffness, dimensionality, and shape contribute to emergent outcomes.* Proceedings of the National Academy of Sciences, 118:e2021571118.

A multi-physics reduced order model for the vascular microenvironment

P. Vitullo[1], A. Colombo[1], N. R. Franco[1], A. Manzoni[1], and P. Zunino[1]

[1]MOX, Department of Mathematics, Politecnico di Milano
{piermario.vitullo, alessio.colombo, nicolarares.franco, andrea1.manzoni, paolo.zunino}@polimi.it

Abstract

Multi-physics mathematical models of the vascular microenvironment (VME) provide quantitative insights on the pathophysiology of diseases such as cancer. The full order model (FOM) describes blood flow and oxygen transfer from the microvasculature to the tissue [1] and it consists of a 3D model for the tissue combined to a 1D model in the vascular network, based on parametrized partial differential equations (PDEs). In order reduce the computational cost of the high-fidelity FOM solution $\boldsymbol{u}_h(\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g)$, representing the oxygenation of the microvascular environment, where $\boldsymbol{\mu}_{ph}$ are the physiological parameters and $\boldsymbol{\mu}_g$ describes the architecture of the vascular network, we adopt a non-intrusive and nonlinear model order reduction for PDEs [2]. We propose a reduced order model (ROM) that can handle the dependence on $\boldsymbol{\mu}_{ph}$ and $\boldsymbol{\mu}_g$ in the framework of proper orthogonal decomposition and artificial neural networks (POD-NN) [3]. First, we build the matrix $\mathbb{V}$ of POD basis functions, so that $\boldsymbol{u}_h(\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g) \approx \mathbb{V}\mathbb{V}^T\boldsymbol{u}_h(\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g)$ where $\mathbb{V}^T\boldsymbol{u}_h(\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g)$ are the reduced basis coefficients. We approximate these reduced coefficients using a neural network $\widetilde{\boldsymbol{u}}_{NN}(\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g)$ that combines dense layers for the physical parametrization with a Mesh-Informed Neural Network (MINN) [4] for the geometrical inputs. An augmented POD-NN approach is carried out exploiting a neural closure model based on the geometrical parametrization, in order to retrieve the local nonlinear information and to capture the effect of the subgrid-scale processes. In this context we define the map $\widetilde{\boldsymbol{u}}^C_{NN}(\boldsymbol{\mu}_g, \widetilde{\boldsymbol{u}}_{NN}(\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g; \boldsymbol{\theta}^0_{ph}, \boldsymbol{\theta}^0_g); \boldsymbol{\theta}^C_g) = \mathbb{V}\widetilde{\boldsymbol{u}}_{NN}(\boldsymbol{\mu}_{ph}, \boldsymbol{\mu}_g; \boldsymbol{\theta}^0_{ph}, \boldsymbol{\theta}^0_g) + f^C(\boldsymbol{\mu}_g; \boldsymbol{\theta}^C_g)$ approximating the FOM solution $\boldsymbol{u}_h$. Due to a relevant speed-up and negligible loss in accuracy with respect to the FOM, the proposed ROM is exploited to accelerate the estimation of statistics of oxygen-related quantities of interest, applying a multifidelity Monte Carlo (MFMC) method and developing a robust and reliable Uncertainty Quantification (UQ) analysis. An unbiased estimator of the statistics of the total variation is provided through an optimal balance between the evaluations of the FOM and ROM models.

Keywords: Vascular microenvironment, multi-physics model, ROM, POD-NN, uncertainty quantification

References

[1] L. Possenti, A. Cicchetti, R. Rosati et al. (2021). *A Mesoscale Computational Model for Microvascular Oxygen Transfer*. Annals of Biomedical Engineering, 49(12), 3356–3373.

[2] N. R. Franco, A. Manzoni, P. Zunin (2023). *A deep learning approach to reduced order modelling of parameter dependent partial differential equations*. Mathematics of Computation, 92, 483–524.

[3] J. S. Hesthaven, S. Ubbiali (2018). *Non-intrusive reduced order modeling of nonlinear problems using neural networks*. Journal of Computational Physics. Vol. 363, 55–78.

[4] N. R. Franco, A. Manzoni, P. Zunino (2022). *Learning Operators with Mesh-Informed Neural Networks*. arXiv preprint; arXiv:2203.11648.

MS31 - Advances in polytopal methods for multiphysics problems

Discontinuous Galerkin Methods for Fisher-Kolmogorov Equation with Application to Prionic Proteins' Spreading in Neurodegeneration

Mattia Corti[1], Paola F. Antonietti*‡[1], Francesca Bonizzoni†[1], Luca Dede'‡[1], and Alfio M. Quarteroni‡[1,2]

[1]MOX, Department of Mathematics, Politecnico di Milano, Italy
[2]Institute of Mathematics, École Polytechnique Fédérale de Lausanne, Switzerland
{mattia.corti, paola.antonietti, francesca.bonizzoni, luca.dede, alfio.quarteroni}@polimi.it

Abstract

The spreading of prionic proteins is at the basis of brain neurodegeneration. To study the numerical modelling of the misfolding process, we introduce and analyze a discontinuous Galerkin method for the semi-discrete approximation of the Fisher-Kolmogorov (FK) equation. We employ a PolyDG method for space discretization, which allows us to accurately simulate the wavefronts typically observed in the prionic spreading [1]. For this problem, we prove stability and a priori error estimates for the semi-discrete formulation. After a numerical verification, we carry out realistic simulations of α-synuclein in a three-dimensional patient-specific brain geometry reconstructed from magnetic resonance images. Moreover, we simulate the spreading in a two-dimensional brain slice in the sagittal plane with a polygonal agglomerated grid.

Starting from medical images we construct also reduced-order models based on graph brain connectome, that are useful if the problem needs to be solved many times, for example in uncertainty quantification algorithms. In the FK equation, the reaction coefficient can be modelled as a stochastic random field, taking into account all the many different underlying physical processes, and overcoming its non-measurability. We infer probability distribution by means of the Monte Carlo Markov Chain method applied to clinical data of Amyloid-β concentration. The resulting model is patient-specific and can be employed for predicting the disease's future development. Forward uncertainty quantification techniques (Monte Carlo and sparse grid stochastic collocation) are applied to quantify the impact of the reaction variability on the progression of protein accumulation within the next 20 years [2].

Keywords: Fisher-Kolmogorov equation, Neurodegeneration, Uncertainty quantification

References

[1] M. Corti, P.F. Antonietti, F. Bonizzoni, L. Dede', A.M. Quarteroni (2023). *Discontinuous Galerkin methods for the Fisher-Kolmogorov equation with application to α-synuclein spreading in Parkinson's disease.* ArXiv.

[2] M. Corti, P.F. Antonietti, F. Bonizzoni, A.M. Quarteroni. *Uncertainty quantification for Fisher-Kolmogorov equation on graphs with application to patient-specific Alzheimer disease.* In preparation.

*PFA acknowledges the funding by the Italian Research Center on High Performance Computing, Big Data and Quantum Computing (ICSC), under the NextGenerationEU project.
†FB acknowledges the funding by "INdAM – GNCS Project", codice CUP E53C22001930001
‡PFA, LD and AMQ acknowledge the funding by MUR for the PRIN 2020 research grant n. 20204LN5N5.

Application of hybrid high-order methods to the elasto-acoustic problem

Omar Duran[1] and Inga Berre[1]

[1]Department of Mathematics, University of Bergen
omar.duran@uib.no

Abstract

For the wave equation, hybrid high-order methods (HHO) were developed and analyzed for fitted [1,2] and unfitted [3] meshes. This contribution extends these methods to simulate the elasto-acoustic problem, where the mesh fits the material interface. Both the second-order formulation in time and its reformulation as a first-order system are discussed. The implicit, second-order accurate Newmark scheme is used for the time discretization of the second-order formulation, while diagonally-implicit Runge-Kutta schemes are used for the first-order formulation. The HHO scheme is amenable to static condensation at each time step for both schemes. On the basis of numerical results from test cases involving analytical solutions, it has been shown that the methods can deliver optimal convergence rates.

Keywords: HHO methods, Elasto-acoustics, Polytopal meshes

References

[1] E. Burman, O. Duran, A. Ern (2021). *Hybrid High-Order Methods for the Acoustic Wave Equation in the Time Domain*. In *Communications on Applied Mathematics and Computation*. Vol. 4(2), 597–-633. Springer Science and Business Media LLC. https://doi.org/10.1007/s42967-021-00131-8

[2] E. Burman, O. Duran, A. Ern, M. Steins (2021). *Convergence Analysis of Hybrid High-Order Methods for the Wave Equation*. In *Journal of Scientific Computing*. Vol. 87(3). Springer Science and Business Media LLC. https://doi.org/10.1007/s10915-021-01492-1

[3] E. Burman, O. Duran, A. Ern (2022). *Unfitted hybrid high-order methods for the wave equation*. In *Computer Methods in Applied Mechanics and Engineering*. Vol. 389, 114366. Elsevier BV. https://doi.org/10.1016/j.cma.2021.114366

The Bulk-Surface Virtual Element Method in 3D and applications in battery modeling

Massimo Frittelli[1], Anotida Madzvamuse[2], Ivonne Sgura[1], and Benedetto Bozzini[3]

[1]Department of Mathematics and Physics "E.De Giorgi", University of Salento, Via per Arnesano, Lecce, 73100, Italy
[2]Department of Mathematics, University of British Columbia, 1984 Mathematics Road, Vancouver, BC V6T 1Z2, Canada
[3]Department of Energy, Politecnico di Milano, via Lambruschini 4, Milano, 20156, Italy
{massimo.frittelli, ivonne.sgura}@unisalento.it; am823@math.ubc.ca;
benedetto.bozzini@polimi.it

Abstract

Bulk-Surface Partial Differential Equations (BSPDEs) have quicky become a prominent topic both in numerical analysis and mathematical modeling.

For the numerical approximation of Reaction-Diffusion Systems of Bulk-Surface type (BSRDSs), we present the Bulk-Surface Virtual Element Method (BSVEM) of lowest order. We provide a geometric error analysis of flat polyhedral meshes independent of the method [1]. Then, we provide a full error analysis that holds even in the presence of curved boundaries, provided the exact solution is $H^{2+3/4}$ in the bulk and H^2 on the surface [2]. The method extends the 2D counterpart previously introduced in our work [3].

We present a novel BSRDS model for the simulation of electrodeposition processes taking place in batteries, called BSDIB model, where the surface PDEs model metal growth on the electrodes, while the bulk PDEs model concentrations in the electrolyte. The BSDIB model extends the so-called DIB model previously introduced in [4], by accounting for the space-time dependence of the electrolyte concentrations in a more realistic fashion. For the BSDIB model, simulations are carried out exploiting the geometric flexibility of the BSVEM.

Keywords: Bulk-surface PDEs, polyhedral meshes, bulk-surface virtual element method, convergence, battery modeling, Turing patterns.

References

[1] M.Frittelli, A.Madzvamuse, I. Sgura (2023). *Virtual element method for elliptic bulk-surface PDEs in three space dimensions.* Numer. Methods Partial Differ. Equ., Accepted for publication, doi: 10.1002/num.23040

[2] M.Frittelli, A.Madzvamuse, I. Sgura (2023). *The Bulk-Surface Virtual Element Method for Reaction-Diffusion PDEs: Analysis and Applications.* Commun. Computat. Phys., 33(3), 733–763, doi: 10.4208/cicp.OA-2022-0204

[3] M.Frittelli, A.Madzvamuse, I. Sgura (2021). *Bulk-surface virtual element method for systems of PDEs in two-space dimensions.* Numer. Math., 147(2), 305–348, doi: 10.1007/s00211-020-01167-3

[4] B.Bozzini, D.Lacitignola, I.Sgura (2013). *Spatio-temporal organization in alloy electrodeposition: a morphochemical mathematical model and its experimental validation.* J. Solid State Electrochem., 17, 467–479, doi: 10.1007/s10008-012-1945-7

A polyhedral DivDiv complex

Daniele A. Di Pietro[1] and Marien-Lorenzo Hanot[1]

[1]IMAG, Univ. Montpellier, CNRS, Montpellier, France
{daniele.di-pietro, marien-lorenzo.hanot}@umontpellier.fr

Abstract

We present, following the recent work [1], the first DivDiv complex on polyhedral meshes. This complex can be used for fourth order problems such as the biharmonic equation, or for problems requiring some symmetry (such as symmetric or trace-free tensor fields). Our complex strongly enforces the symmetry constraints at the discrete level. The discretization in 3 dimensions is challenging, and has been recently completed [2] using finite elements on simplicial meshes. On the other hand, our construction follows the Discrete De Rham approach [3], whose flexibility has greatly helped to alleviate these difficulties. We provide an in-depth study of the algebraic properties of the local complex, showing that it is exact on mesh elements with trivial topology. We illustrate the use of the scheme with an a numerical scheme for the approximation of biharmonic problems, for which we provide detailed stability and convergence analyses.

Keywords: divdiv complex, discrete de Rham method, polyhedrla meshes, biharmonic problems

References

[1] D. A. Di Pietro and M. Hanot (2023). *A discrete three-dimensional divdiv complex on polyhedral meshes with application to a mixed formulation of the biharmonic problem.* arXiv preprint 2305.05729 [math.NA].

[2] J. Hu, Y. Liang and R. Ma (2022). *Conforming finite element divdiv complexes and the application for the linearized Einstein–Bianchi system.* SIAM J. Numer. Anal. 60.3, 1307-1330.

[3] D. A. Di Pietro and J. Droniou (2023). *An arbitrary-order discrete de Rham complex on polyhedral meshes: Exactness, Poincaré inequalities, and consistency.* Found. Comput. Math., 23, 85–164.

Multilevel Algorithms and Rational Approximations for Multi-Physics problems

Kent-Andre Mardal[1], Ana Budisa[2], Xiaozhe Hu[3], Miroslav Kuchta[4], and Ludmil Zikatanov[5]

[1]Department of Mathematics, University of Oslo, Simula Research Laboratory
[2]Simula Research Laboratory
[3]Department of Mathematics, Tufts University, USA
[4]Simula Research Laboratory
[5]Department of Mathematics, Penn State, USA
kent-and@math.uio.no

Abstract

In multi-physics problems such as Darcy-Stokes, Biot-Stokes, Extracellular-Membrane-Intracellular models of exitable tissue, 3D-1D coupled problems there is a need for special solvers which treats the couplings in a careful manner [1,2,3]. Here, we will present a number of observations that rely on fractional or metric operators at at the couplings that enable fast solvers either in terms of rational approximations of fractional operators or multigrid methods that treat the near singular operators associated to the interface. The tools are implemented in [2].

Keywords: Multi-physics problems, multigrid, rational approximation, fractional operators

References

[1] A. Budisa, X. Hu, M. Kuchta, K.A. Mardal, L. Zikatanov (2022). *Rational approximation preconditioners for multiphysics problems.* arXiv:2209.11659.

[2] A. Budisa, X. Hu, M. Kuchta, K.A. Mardal, L. Zikatanov (2022). *HAZniCS – Software Components for Multiphysics Problems.* arXiv:2210.13274.

[3] A. Budisa, X. Hu, M. Kuchta, K.A. Mardal, L. Zikatanov (2023). *Algebraic Multigrid Methods for Metric-Perturbed Coupled Problems.* arXiv.

A Mixed Virtual Element Formulation of the Biot Poroelastic Model with Strong Symmetric Stresses

Michele Botti[1], Franco Dassi[2], Alessio Fumagalli[1], Lorenzo Mascotto[2], Daniele Prada[3], Stefano Scialò[4], Anna Scotti[1], Giuseppe Vacca[5], and Michele Visinoni[6]

[1]Politecnico di Milano, Dipartimento di Matematica, MOX
[2]Università degli Studi di Milano Bicocca, Dipartimento di Matematica e Applicazioni
[3]Consiglio Nazionale delle Ricerche, Istituto di Matematica Applicata e Tecnologie Informatiche "Enrico Magenes"
[4]Politecnico di Torino, Dipartimento di Scienze Matematiche "G. L. Lagrange"
[5]Università degli Studi di Bari "Aldo Moro", Dipartimento di Matematica
[6]Università degli Studi di Milano, Dipartimento di Matematica "Federico Enriques"
{michele.botti, alessio.fumagalli, anna.scotti}@polimi.it; {franco.dassi, lorenzo.mascotto}@unimib.it; daniele.prada@imati.cnr.it; stefano.scialo@polito.it; giuseppe.vacca@uniba.it; michele.visinoni@unimi.it

Abstract

We present a mixed Virtual Element Method (VEM) for the approximate solution of the three-dimensional Biot poroelastic model. We propose a low-order scheme with strong symmetric total stresses. At each time step, the semi-discretized coupled problem is solved monolithically. A convergence and stability analysis is developed and confirmed via some numerical tests. Finally, we illustrate our methodology on some real-life applications.

Keywords: Virtual Element Method, Biot poroelasticity, Geoscience, Ophthalmology

References

[1] S.Y. Yi (2014). *Convergence analysis of a new mixed finite element method for biot's consolidation model*. Numer. Methods Partial Differential Eq., 30, 1189–1210.

[2] L. Beirão da Veiga, F. Brezzi, L. D. Marini, A. Russo (2016). *Mixed virtual element methods for general second order elliptic problems on polygonal meshes*. ESAIM: M2AN, 50, 727–747.

[3] F. Dassi, C. Lovadina, M. Visinoni (2020). *A three-dimensional Hellinger-Reissner virtual element method for linear elasticity problems*. Comput. Methods Appl. Mech. Engrg., 364.

Free convection in porous media: the impact of fracture networks

Arash Andrea Roknian[1], Alessio Fumagalli[1], and Anna Scotti[1]

[1]MOX, Department of Mathematics, Politecnico di Milano
arashandrea.roknian@mail.polimi.it; {alessio.fumagalli, anna.scotti}@polimi.it

Abstract

We want to investigate the onset of free convection in fractured porous media. Density changes are here due to the presence of a variable solute concentration, but could be linked to temperature depending on the application of interest. The onset of gravitational instability is linked to the Rayleigh number, which compares the strength of buoyancy and diffusion. A theoretical threshold value can be identified in homogeneous domains [2], and previous studies have shown by means of numerical simulations that the presence of well connected fractures can lower this threshold favoring free convection. Following [1] we aim at characterizing the effect of different fracture configurations by i) direct numerical simulation of the coupled, nonlinear problem and ii) eigenvalue analysis of the linearized, discretized problem. The numerical discretization, based on the PorePy library [4], employs Multipoint Finite Volume Approximation [3] for the Darcy problem and the transport of concentration, to ensure mass conservation and allow for the general grids that can be created to honor fracture networks. The results, in 2D and 3D configurations, are in agreement with existing literature and, moreover, show that the eigenvalues/eigenvectors computation, though expensive, allows us to find the unstable modes without solving a time dependent problem and removing the dependence of the solution on the choice of the initial perturbation.

Keywords: fractured porous media, multipoint finite volumes, instability

References

[1] K. Vujević, T. Graf (2015). *Combined inter- and intra-fracture free convection in fracture networks embedded in a low-permeability matrix*. Advances in Water Resources, 84, 52–63.

[2] E. R. Lapwood (1948). *Convection of a fluid in a porous medium*. Mathematical Proceedings of the Cambridge Philosophical Society ,44-4, 508–521.

[3] M. Starnoni, I. Berre, E. Keilegavlen, J. M. Nordbotten (2019). *Consistent MPFA Discretization for Flow in the Presence of Gravity*. Water Resources Research, 55-12, 10105–10118

[4] E. Keilegavlen et al. (2021). *PorePy: an open-source software for simulation of multiphysics processes in fractured porous media*. Computational Geosciences, 25, 243–265.

Improving high-order VEM stability on badly-shaped elements

Gioana Teora[1], Stefano Berrone[1], and Fabio Vicini[1]

[1]Dipartimento di Scienze Matematiche, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy.
{gioana.teora, stefano.berrone, fabio.vicini}@polito.it

Abstract

The Virtual Element Method (VEM) is a numerical method for the approximation of partial differential equations, which offers a convenient framework to handle challenging geometries and to build high-order methods. However, the resulting system matrix can become ill-conditioned in presence of badly-shaped elements when resorting to the scaled monomial basis in the definition of both the local projectors and the local DOFs yielding to very low-quality results. The use of orthonormal polynomial bases [2, 3] has been found to be efficient in preventing the ill-conditioning of the system matrix, but this approach can be very expensive from a computational point of view, since its overall cost depends on the local polynomial degree.

In this talk, we present an alternative strategy that represents a better trade-off between the need of mitigating the ill-conditioning of the global system matrix and the computational effort required to achieve this goal. This approach consists in computing the local VEM projectors as a function of the scaled monomial basis reset on more well-shaped polytopes. It allows to limit the condition number of local projection matrices and of the global system matrix in presence of badly-shaped elements with an overall cost which depends only on the geometric dimension of the problem.

Throughout different numerical experiments of increasing complexity in 2D and 3D, we show that the proposed approach can reach reasonable and comparable results with respect to the use of orthonormal polynomial bases, while being less expensive from a computational point of view.

Keywords: Ill-conditioning, Virtual Element Method, Polygonal mesh, Polyhedral mesh, Polynomial basis

References

[1] S. Berrone, G. Teora, F. Vicini (2023). *Improving high-order VEM stability on badly-shaped elements.* https://arxiv.org/abs/2302.11284

[2] S. Berrone, A. Borio (2017). *Orthogonal polynomials in badly shaped polygonal elements for the Virtual Element Method.* Finite Elements in Analysis and Design. Vol. 128, 14–31.

[3] L. Mascotto (2018). *Ill-conditioning in the virtual element method: Stabilizations and bases.* Numerical Methods for Partial Differential Equations. Vol. 34, n. 4, 1258–1281.

Virtual Element Method for the Navier–Stokes Equation coupled with the Heat Equation

Marco Verani*[1], Paola F. Antonietti*[1], and Giuseppe Vacca[2]

[1]MOX-Department of Mathematics, Politecnico di Milano
[2]Department of Mathematics, Università di Bari
giuseppe.vacca@uniba.it; {paola.antonietti,marco.verani}@polimi.it

Abstract

We consider the Virtual Element discretization of the Navier–Stokes equations coupled with the heat equation where the viscosity depends on the temperature. We present the Virtual Element discretization of the coupled problem, show its well-posedness, and prove optimal error estimates. Numerical experiments which confirm the theoretical error bounds are also presented.

Keywords: Virtual Element Method, Navier-Stokes equations, Heat equation, polygonal meshes.

*PRIN2020 n. 20204LN5N5 "*Advanced polyhedral discretisations of heterogeneous PDEs for multiphysics problems*", funded by the Italian Ministry of Universities and Research (MUR).

A mass conservative scheme for the coupled Brinkman-Darcy flow and transport

Lina Zhao[1] and Shuyu Sun[2]

[1]Department of Mathematics, City University of Hong Kong
[2]Division of Physical Science and Engineering, King Abdullah University of Science and Technology
linazha@cityu.edu.hk; shuyu.sun@kaust.edu.sa

Abstract

In this talk, I will present a strongly mass conservative scheme for the coupled Brinkman-Darcy flow and transport. Staggered DG method and mixed finite element method are judiciously balanced to ensure the mass conservation. Moreover, the interface conditions are naturally incorporated into the formulation without resorting to Lagrange multipliers. In particular, the scheme is robust with respect to the values of the viscosity, which makes it highly flexible for a variety of applications. Using the velocity generated from the coupled Brinkman-Darcy flow, the upwinding staggered DG method is devised for the transport equation. A rigorous convergence error analysis is performed for the proposed scheme, showing the optimal convergence error estimates. Several numerical experiments will be presented to demonstrate the performance of the proposed scheme.

Keywords: Coupled Brinkman-Darcy flow, Mass conservation, Staggered DG

References

[1] Lina Zhao, E. Chung, M. Lam (2020). *A new staggered DG method for the Brinkman problem robust in the Darcy and Stokes limits*. Comput. Methods Appl. Mech. Engrg., 364.

[2] Lina Zhao, Shuyu Sun (2023). *A strongly mass conservative method for the coupled Brinkman-Darcy flow and transport*. SIAM J. Sci. Comput., 45, B166–B199.

MS32 - Numerical methods for perturbed saddle-point formulations arising in coupled problems and applications to poromechanics

Stabilization free virtual element method and discrete compactness property: the acoustic problem

Linda Alzaben[1], Daniele Boffi[1,2], Andreas Dedner[3], and Lucia Gastaldi[4]

[1]Applied mathematics and computational sciences, King Abdullah University of Science and Technology
[2]Mathematics department, Università degli Studi di Pavia
[3]Mathematics institute, University of Warwick
[4]Dipartimento di Ingegneria Civile, Architettura, Territorio, Ambiente e di Matematica, Università degli Studi di Brescia
{linda.alzaben, daniele.boffi}@kaust.edu.sa; A.S.Dedner@warwick.ac.uk; lucia.gastaldi@unibs.it

Abstract

The Virtual Element Method (VEM) was introduced as a generalization of the Finite Element Method to polygonal meshes. We focus on the use of VEM to discretize the acoustic vibration problem. The original research presented in [1] proposes a VEM-based system that stabilizes the stiffness and mass matrix, which are also dependent on scalar parameters. The stabilization term has been extensively studied and remains somehow arbitrarily chosen. We explore the use of a non-stabilized discrete bilinear form and demonstrate its equivalence to the L^2 norm. A good approximation of eigenvalues depends on the convergence of the discrete solution operator. The convergence of the discrete solution operator relies on two main ingredients: the equivalence of a mixed variational formulation [2] and the discrete compactness property [3]. We conduct several numerical tests using the Dune library [4] to evaluate the method's performance. These experiments validate the theoretical findings and provide insight into the practical effectiveness of the VEM-based approach to solve the acoustic vibration problem.

Keywords: Eigenvalue problem, Virtual element method, Acoustic problem, Discrete compactness property.

References

[1] L. Beirão da Veiga, D. Mora, G. Rivera, R. Rodríguez (2017). *A virtual element method for the acoustic vibration problem*. Numerische Mathematik, 136(3), 725–763.

[2] D. Boffi, F. Brezzi, L. Gastaldi (1997). *On the convergence of eigenvalues for mixed formulations*. Annali della Scuola Normale Superiore di Pisa-Classe di Scienze, 25(1-2), 131–154.

[3] D. Boffi (2007). *Approximation of eigenvalues in mixed form, discrete compactness property, and application to hp mixed finite elements*. Computer methods in applied mechanics and engineering, 196(37-40), 3672–3681.

[4] A. Dedner, R. Kloefkorn, M. Nolte (2020). *Python bindings for the DUNE-FEM module*. Zenodo. doi, 10.

Contact problems in porous media

Lothar Banz[1] and Fleurianne Bertrand[2]

[1]Department of Mathematics, University of Salzburg, Salzburg, Austria
[2]Faculty of Electrical Engineering, Mathematics and Computer Science, University of Twente, Enschede, Netherlands
lothar.banz@plus.ac.at; f.bertrand@utwente.nl

Abstract

Biot's poroelasticity describes the deformation of a fluid saturated elastic porous medium due to fluid flow, and the other way around, fluid flow due to deformation of the medium. In this talk we extend the Biot problem by Signorini contact conditions leading to a two field variational inequality of a perturbed saddle point structure. We prove well posedness of the continuous as well as of the hp-finite element discretized problem. By combing the Strang-Lemma with the Falk-Theorem we can prove an a priori error estimate and guaranteed convergence (rates). Moreover, we derive a residual based a posteriori error estimate which is both efficient and reliable. We present several numerical experiments regarding an active set solver and realizable convergence rates of different uniform and adaptive schemes.

Keywords: porous media, Biot, contact problem, a priori error estimate, a posteriori error estimate, *hp*-FEM

A projection scheme for a nearly incompressible soft material poromechanics model

Mathieu Barré[1], Céline Grandmont[2], and Philippe Moireau[1]

[1]Inria – LMS, École Polytechnique, CNRS, Institut Polytechnique de Paris
[2]Inria – LJLL, Sorbonne Université, CNRS – Université Libre de Bruxelles
mathieu.a.barre@inria.fr

Abstract

We consider the linearized version of a poromechanics model developed to simulate biological tissues perfusion [1, 2]. This is a fully dynamical model in which the fluid and solid equations are strongly coupled through the interstitial pressure. As such, it generalizes Darcy, Brinkman and Biot equations of poroelasticity. The numerical analysis of this model was performed for a monolithic implicit time scheme both in compressible [3, 4] and incompressible [5] regimes. More recently, an alternating minimization splitting scheme was proposed, leading to a solver closely related to the undrained and fixed-stress splits for Biot equations [6].

In this work, we present a projection scheme that enables to decouple the solid, fluid and pressure equations at each time step. Our approach is close to Chorin-Temam projection method but takes into account the specific saddle-point structure of the problem. Moreover, it includes the case of total stress boundary conditions thanks to a Robin-Robin coupling technique inspired by fluid-structure interaction [7]. We provide an error estimate that is robust with respect to the bulk modulus. Finally, the efficiency of the resulting solver is compared to a monolithic approach.

Keywords: Mixture theory, fractional-step method, error analysis, incompressible limit, Robin-Robin coupling

References

[1] D. Chapelle, P. Moireau (2014). *General coupling of porous flows and hyperelastic formulations—from thermodynamics principles to energy balance and compatible time schemes.* European Journal Of Mechanics-B/Fluids, 46, 82–96.

[2] M. Barré, C. Grandmont, P. Moireau (2022). *Analysis of a linearized poromechanics model for incompressible and nearly incompressible materials.* Evolution Equations And Control Theory.

[3] B. Burtschell, P. Moireau, D. Chapelle (2019). *Numerical analysis(..)poromechanics model with inf-sup stability.* Acta Mathematicae Applicatae Sinica, English Series, 35, 28–53.

[4] N. Barnafi, P. Zunino, L. Dedè, A. Quarteroni (2021). *Mathematical analysis and numerical approximation of a general linearized poro-hyperelastic model.* CAMWA, 91, 202–228.

[5] M. Barré, C. Grandmont, P. Moireau (2023). *Numerical analysis of an incompressible soft material poromechanics model using T-coercivity.* Comptes Rendus. Mécanique.

[6] J. Both, N. Barnafi, F. Radu, P. Zunino, A. Quarteroni (2022). *Iterative splitting schemes for a soft material poromechanics model.* CMAME, 388, 114183.

[7] E. Burman, R. Durst, M. Fernández, J. Guzmán (2022). *Fully discrete loosely coupled Robin-Robin scheme for incompressible fluid–structure interaction: stability and error analysis.* Numerische Mathematik, 151, 807–840.

How to deal with the coupling term in the approximation of fluid structure interactions with Lagrange multiplier

Daniele Boffi[1], Fabio Credali[2], and Lucia Gastaldi[3]

[1]CEMSE Division, King Abdullah University of Science and Technology, Saudi Arabia
[2]Dipartimento di Matematica "F. Casorati", University of Pavia, Italy
[3]DICATAM, University of Brescia, Italy
daniele.boffi@kaust.edu.sa; fabio.credali01@universitadipavia.it; lucia.gastaldi@unibs.it

Abstract

In this talk we discuss some implementation aspects related to the use of a Lagrange multiplier approach in the numerical simulation of fluid-structure problems.

We base our analysis on a fictitious domain approach introduced in [3] as a followup of [1].

One of the crucial aspects of our simulations is that the coupling term related to the multiplier and responsible for the transfer information from the fluid and the solid, involves shape functions defined on two different meshes.

In this study we describe how to deal with this term, with particular emphasis on the intersection of the meshes and on the required quadrature rules [2]. A rigorous analysis shows how get optimal error estimates.

Keywords: Fluid-structure interaction problems, Fictitious domain, Finite elements, Coupling

References

[1] D. Boffi, N. Cavallini, L. Gastaldi (2015). *The finite element immersed boundary method with distributed Lagrange multiplier*. SIAM J. Numer. Anal., 53, 2584–2604.

[2] D. Boffi, F. Credali, L. Gastaldi (2022). *On the interface matrix for fluid-structure interaction problems with fictitious domain approach*. Comput. Methods Appl. Mech. Engrg., 401.

[3] D. Boffi, L. Gastaldi (2017). *A fictitious domain approach with Lagrange multiplier for fluid-structure interactions*. Numer. Math., 135, 711–732.

Robust solvers for multiphase poroelasticity

Jakub Wiktor Both[1], Konstantin Brenner[2], Clément Cancès[3], and Omar Duran[1]

[1]Department of Mathematics, University of Bergen, Norway
[2]Laboratoire J.A. Dieudonné, UMR CNRS, Université de Nice Sophia-Antipolis, France
[3]Inria Lille, Laboratoire Paul Painlevé, UMR CNRS, Université de Lille, France
{jakub.both, omar.duran}@uib.no; konstantin.brenner@unice.fr;
clement.cances@inria.fr

Abstract

Multiphase poromechanics constitutes the coupled multiphase flow and geomechanics in deformable porous media. Strongly coupled processes governed by multiphase poromechanics are relevant in applications such as CO2 sequestration, geothermal energy, and many more. The resulting model is highly nonlinear, possibly degenerate and strongly coupled. Thus, robust and efficient numerical solution strategies are required for effective numerical simulations.

Numerical solvers have been well understood for linear poromechanics, being often based on stabilized iterative schemes (often also formulated as preconditioners). Such have been shown to be directly linked to the gradient flows nature of linear poromechanics [1]. E.g., the widly-used fixed-stress split [2] has been identified as alternating minimization [3] for the respective Biot equations, written in dual form.

A sound, comprehensive mathematical understanding in the presence of multiphase flow has been lacking. In this talk, we investigate gradient flow structures of the coupled mathematical model for multiphase poromechanics, extending [4], and discuss iterative solvers utilizing this structure, i.e., aiming at decreasing a suitable energy functional in order to converge robustly.

Keywords: Porous media, multiphase, poroelasticity, saddle-point problem, gradient flow, numerical solver

References

[1] J. W. Both, K. Kumar, J. M. Nordbotten, F. A. Radu (2019). *The gradient flow structures of thermo-poro-visco-elastic processes in porous media.* arXiv preprint arXiv:1907.03134.

[2] J. W. Both, M. Borregales, J. M. Nordbotten, K. Kumar, F. A. Radu (2017). *Robust fixed stress splitting for Biot's equations in heterogeneous media.* Applied Mathematics Letters, 68, 101–108.

[3] J. W. Both (2022). *On the rate of convergence of alternating minimization for non-smooth non-strongly convex optimization in Banach spaces.* Optimization Letters, 16(2), 729–743.

[4] C. Cancès, O. G. Thomas, L. Monsaingeon (2015). *The gradient flow structure for incompressible immiscible two-phase flows in porous media.* Comptes Rendus Mathematique 353.11, 985–989.

A parallel solver for fluid-structure interaction problems with Lagrange multiplier

Fabio Credali[1], Daniele Boffi[2], Lucia Gastaldi[3], and Simone Scacchi[4]

[1]Dipartimento di Matematica "F. Casorati", University of Pavia, Italy
[2]CEMSE Division, King Abdullah University of Science and Technology, Saudi Arabia
[3]DICATAM, University of Brescia, Italy
[4]Dipartimento di Matematica "F. Enriques", University of Milano, Italy
fabio.credali01@universitadipavia.it; daniele.boffi@kaust.edu.sa;
lucia.gastaldi@unibs.it; simone.scacchi@unimi.it

Abstract

We consider a fictitious domain formulation with distributed Lagrange multiplier for fluid-structure interaction problems [1]. The evolution of the structure is modeled by Lagrangian description on a reference domain, which is mapped, at each time step, to the actual position of the solid body. The fluid is described by an Eulerian model and its mesh is extended also in the region occupied by the structure: the coupling is weakly enforced making use of a Lagrange multiplier.

We focus on the analysis of parallel block preconditioners for the linear system arising from the finite element discretization of this family of problems [2, 3].

The fluid is governed by the time dependent Stokes equations with velocity and pressure discretized by the popular $\mathcal{Q}_2 - \mathcal{P}_1$ element, while the solid variables are approximated by $\mathcal{Q}_1$ finite elements. For the structure material both linear and nonlinear constitutive laws are considered.

A first order semi-implicit finite difference scheme is considered for the time discretization. At each time step, the linear system is solved by parallel GMRES accelerated by coupled block diagonal or triangular preconditioners; the diagonal blocks are inverted exactly by parallel direct methods. The implementation is based on the PETSc [4] library and several numerical tests have been performed on Linux clusters to investigate optimality and scalability of the proposed solver.

Keywords: fluid-structure interactions, fictitious domain, preconditioners, parallel solver

References

[1] D. Boffi, N. Cavallini, L. Gastaldi (2015). *The finite element immersed boundary method with distributed Lagrange multiplier*. SIAM J. Numer. Anal. 53 (2015), no. 6, 2584–2604.

[2] D. Boffi, F. Credali, L. Gastaldi, S. Scacchi (2022). *A parallel solver for fluid structure interaction problems with Lagrange multiplier*. arXiv preprint arXiv:2212.13410.

[3] D. Boffi, F. Credali, L. Gastaldi, S. Scacchi (2023). *A parallel solver for FSI problems with fictitious domain approach*. Math. Comput. Appl. 2023, 28, 59.

[4] S. Balay, S. Abhyankar, M. F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, D. A. May, L. C. McInnes, R. T. Mills, T. Munson, K. Rupp, P. Sanan, B. F. Smith, S. Zampini, H. Zhang, and H. Zhang (2018). *PETSc users manual*. Technical Report ANL-95/11 - Revision 3.9, Argonne National Laboratory.

A comparison of unfitted techniques for coupled problems across non-matching interfaces

Daniele Boffi[1,2], Andrea Cangiani[3], Marco Feder[3], Lucia Gastaldi[4,5], and Luca Heltai[3]

[1]CEMSE division, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia
[2] Dipartimento di Matematica F. Casorati, Università degli Studi di Pavia, Pavia, Italy
[3]Mathematics Area, SISSA, Trieste, Italy
[4]DICATAM Sez. di Matematica, Università degli Studi di Brescia, Brescia, Italy
[5]Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI-CNR), Pavia, Italy
daniele.boffi@kaust.edu.sa, {andrea.cangiani, marco.feder, luca.heltai}@sissa.it, lucia.gastaldi@unibs.it

Abstract

We perform a systematic comparison between three different unfitted approaches for coupled problems across non-matching grids, where no a priori information on the relation between the different meshes is required, and we analyze them in terms of accuracy, computational cost, and implementation effort. In particular, we consider the Lagrange multiplier method, Nitsche's penalization method, and cut-FEM for different test cases, varying the complexity of the interface and the smoothness of the exact solution in both two and three dimensions. Special attention is given to implementation considerations such as computing accurate quadrature rules on mesh intersections and to the costs associated with the various simulation phases. The results presented here and in [1] have been obtained after the integration of some facilities of the C++ library CGAL [4] into the finite element library deal.II [3], in order to perform most of the computational geometry related tasks, providing at the same time robust routines to compute coupling terms within a finite element framework.

Keywords: Interface problems, Unfitted methods, Non-matching grids, Scientific software.

References

[1] D. Boffi, A. Cangiani, M. Feder, L. Gastaldi, L. Heltai (2023). *A comparison of non-matching techniques for the finite element approximation of interface problems.* Submitted.

[2] E. Burman, S. Claus, P. Hansbo, M. G. Larson, and A. Massing (2023). *Cutfem: Discretizing geometry and partial differential equations.* International Journal for Numerical Methods in Engineering, 104(7):472–501.

[3] D. Arndt, W. Bangerth, M. Feder, M. Fehling, R. Gassmöller, T. Heister, L. Heltai, M. Kronbichler, M. Maier, P. Munch, J.P. Pelteret, S. Sticko, B. Turcksin and David Wells (2022). *The `deal.II` Library, Version 9.4.* Journal of Numerical Mathematics, 30(3), 231–246.

[4] The CGAL Project. *CGAL User and Reference Manual.* CGAL Editorial Board, 5.5 edition, 2022.

Least-Squares Finite Element Methode for a non-linear Sea-Ice problem

Henrik Schneider*[1] and Fleurianne Bertrand[2]

[1]Fakultät für Mathematik, Universität Duisburg-Essen
[2]Fakultät für Mathematik, TU Chemnitz
henrik.schneider@uni-due.de; fleurianne.bertrand@mathematik.tu-chemnitz.de

Abstract

A nonlinear sea-ice problem is considered in a least-squares finite element setting. The corresponding variational formulation approximating simultaneously the stress tensor and the velocity is analysed. In particular, the least-squares functional is coercive and continuous in an appropriate solution space. As the method does not require a compatibility condition between the finite element space, the formulation allows the use of piecewise polynomials spaces of the same approximation order for both the stress and the velocity approximations. A Newton-type iterative method is used to linearize the problem and numerical tests are provided to illustrate the theory.

Keywords: Sea-Ice problem, Least-Squares FEM

References

[1] F. Bertrand, H. Schneider. *Least-Squares Finite Element methode for non-linear sea-ice dynamics.* In prepration.

[2] F. Bertrand (2018). *Stress-based Finite Element Methods for Sea Ice Dynamics* PAMMM.

*H.S. gratefully acknowledges support by DFG in the Priority Programme SPP 1962 Non-smooth and Complementarity-based Distributed Parameter Systems under grant number STA 402/13-2.

MS34 - Efficient Solvers for Coupled Problems in Porous Media

Simulation of phreatic surface movement in unsaturated density driven flow

Niklas Conen*[1]

[1]Institute of Computer Science, Goethe University Frankfurt
niklas.conen@student.kit.edu

Abstract

A system of coupled partial differential equations for modelling unsaturated density driven flow in porous media is presented. Liquid phase flow is modelled with a generalized Richards equation, transport of a pollutant is modelled with a convection diffusion equation, resulting in a system of coupled PDEs. Constitutive relations for the unsaturated flow are modelled with the van Genuchten model. Options for modelling of biochemical processes are introduced. Strategies for solving the resulting PDE System are discussed and evaluated using the UG4 framework. Results of several simulations of selected test cases are presented. The movement of the phreatic surface, the interface between saturated and unsaturated zones, is studied and the stability of the numerical methods is discussed.

Keywords: Richards equation, water retention curves, phreatic surface

References

[1] J. Bear, A. H.-D. Cheng (2010). *Modeling Groundwater Flow and Contaminant Transport*. Theory and Applications of Transport in Porous Media. Springer Science+Business Media B.V.

[2] M. V. Genuchten (1980). *A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils*. Soil Science Society of America Journal, 44, 09.

[3] A. Vogel, S. Reiter, M. Rupp, A. Nägel, G. Wittum (2013). *UG 4: A novel flexible software system for simulating PDE based models on high performance computers*. Computing and Visualization in Science, 16(4), 165—179.

*The authors thanks Arne Nägel, Dmitry Logashenko and Gabriel Wittum

Fractures as Wentzell Interface Conditions for Darcy flow and Biot's equations

Marco Favino[1,2,3] and Rolf Krause[1,3]

[1]Euler Institute, Università della Svizzera italiana
[2]Institute of Earth Sciences, University of Lausanne
[3]FernUNI Schweiz
favinom@usi.ch

Abstract

Fractures are thin heterogeneities that are embedded in a background domain and are characterized by hydraulic and mechanical material properties that differ significantly from those of the surrounding medium. The complex geometries of fractures make mesh generation for fractured media particularly challenging. One common approach to modeling fractures involves using hybrid-dimensional models, where fractures are downscaled to objects of a lower dimension and separate problems are solved in the background and fracture domains with suitable coupling conditions [1, 2].

A novel formulation for modeling fractures is proposed, which considers fractures as cuts in the domain and models their effects using Wentzell interface conditions [3]. This new approach is applied to the primal formulation of the Darcy flow problem, where the only unknown is the pressure, and a hydro-mechanical problem described by Biot's equations, where the unknowns are displacement and pressure.

The model for the Darcy flow problem is elegant and straightforward, resulting in a primal formulation where the only unknown is the pressure in the background domain. The model can naturally handle fractures that cross each other, including those with variable apertures, and does not rely on a "quadrature parameter". Although the formulation is suitable for use with XFEM or CutFEM, we focus on a standard finite element discretization, where cuts are resolved by mesh element boundaries.

For the flow problem, we analyze the discretization error for different orders of finite element and material properties, and we use such observations to gain insight into the regularity of the solution. For Biot's equations, we compare the arising conditions with standard analytical models used for fractured poroelastic media [4]. Overall, the proposed approach provides a clear and concise strategy to modeling fractured porous media that can be applied to a range of related problems.

Keywords: Fractured porous media, lower-dimensional models, Wentzell boundary conditions

References

[1] B. Flemisch et al. (2018). *Benchmarks for single-phase flow in fractured porous media.* Advances in Water Resources, 111, 239–258.

[2] I. Berre, et al. (2021). *Verification benchmarks for single-phase flow in three-dimensional fractured porous media.* Advances in Water Resources 147, 103759.

[3] Kashiwabara, T., Colciago, C. M., Dedè, L., Quarteroni, A. (2015). *Well-posedness, regularity, and convergence analysis of the finite element approximation of a generalized Robin boundary value problem.* SIAM Journal on Numerical Analysis, 53(1), 105–126.

[4] Seiji Nakagawa, M. A. Schoenberg (2007). *Poroelastic modeling of seismic boundary conditions across a fracture.* The Journal of the Acoustical Society of America 122.2, 831–847.

Application of fully implicit Nested Newton solvers to multicomponent multiphase flow in porous media and to elastoplastic deformations of biological tissue

Markus M. Knodel[1]

[1]Simulation in Technology, TechSim, Ölbronn-Dürrn, Germany
markus.knodel@techsim.org

August 22, 2023

Abstract

Advanced models of complicated physical and biological processes incorporate huge equation systems which combine partial differential equations (PDEs), ordinary differential equations (ODEs), and algebraic equations (AEs). The monolithic solution of such extended equation systems all together using standard techniques sometimes is very time consuming. The application of nested Newton solvers allows to shift a substantial part of the nonlinear computations to the so-called local system containing only non-spatially coupling equations (ODEs, AEs). The global equations contain all PDEs. The local variables are coupled with the global variables by means of a so-called resolution function. The solution technique remains monolithic and fully implicit. The number of the local Newton steps (which can be performed with perfectly parallel scalability) displays an upper bound for the global Newton steps.

We present two examples of applications of a nested Newton algorithms which allow the efficient evaluation of the corresponding models:

We simulate elastoplastic deformation of biological tissue with anisotropic structure in case of a highly nonlinear material model [1]. Applying the BilbyKrönerLee (BKL) multiplicative decomposition of the deformation gradient into an elastic and a plastic part, a natural split into local and global system is achieved. Performing different numerical experiments of a monophasic model of fiber-reinforced tissues and comparing to another plasticity algorithm, we observe a strong improvement of the performance.

Further, we apply the globally fully implicit PDE reduction method developed 2007 by Kräutle and Knabner for one-phase flow extending the method to the case of an arbitrary number of gases in gaseous phase in order to study the efficacy of mineral trapping scenarios for CO_2 storage behavior in deep layers [2]. The chemistry of the multiphase multicomponent flow in porous media model includes both general kinetic and equilibrium reactions.

Our applications demonstrate the potential of nested Newton procedures for efficient solution techniques in case of highly nonlinear models of complicated scenarios.

Keywords: Nested Newton, elastoplastic deformations, anisotropic tissue, reactive flow, porous media

References

[1] M.M. Knodel, S. Di Stefano, A. Nägel, A. Grillo (2022). *An efficient algorithm for biomechanical problems based on a fully implicit nested Newton solver*. Theoretical and Applied Mechanics (TAM) 49, 2, 183–221. doi: 10.2298/TAM221115012K

[2] M.M. Knodel, S. Kräutle, P. Knabner (2022). *Global implicit solver for multiphase multicomponent flow in porous media with multiple gas components and general reactions*. Comput. Geosci. 26, 697–724 doi.org/10.1007/s10596-022-10140-y

On multipreconditioning Conjugate Gradient method with the additive multigrid for solving highly anisotropic problems

Hardik Kothari[1] and Rolf Krause[1,2]

[1]Euler Institute, Università della Svizzera italiana, Switzerland
[2]UniDistance, Switzerland
{hardik.kothari, rolf.krause}@usi.ch

Abstract

The multigrid (MG) methods are one of the most robust solution methods in the field of numerics due to their optimal complexity. However, for large-scale problems, the standard multigrid method, which we will refer to as a multiplicative multigrid method, suffer from increasing communication complexity [3]. In such cases, the additive variant of the multigrid method provides a good alternative due to its parallel nature, but also it exhibits slower convergence than its multiplicative counterpart [1].

In this work, we propose to employ a multi-preconditioned conjugate gradient (CG) method [2] that employs the additive multigrid method as a preconditioner. By employing the multi-preconditioning approach, we allow the multi-preconditioned CG method to update the iterate by automatically choosing the optimal parameters for a linear combination of the corrections from the different levels of the multilevel hierarchy. Using this approach, we exploit the energy norm minimization property of the CG method, that combines A-conjugacy of the Krylov subspaces and optimally weighted H_1-orthogonal corrections from the multigrid method. In the numerical section, we will show the performance of the proposed additive-MG multi-preconditioned CG method in comparison with the standard additive-MG preconditioned CG method and the multiplicative-MG preconditioned CG method, for solving highly anisotropic problems. We will show that for the highly anisotropic problems, the additive-MG multi-preconditioned CG method demonstrates similar convergence behavior as the multiplicative-MG preconditioned CG method.

Keywords: highly anisotropic problems, additive multigrid, multi-preconditioning

References

[1] P. Bastian, G. Wittum, W. Hackbusch (1998). *Additive and multiplicative multi-grid – a comparison.* Computing, 60, 345–364.

[2] R. Bridson, C. Greif (2006). *A Multipreconditioned Conjugate Gradient Algorithm.* SIAM Journal on Matrix Analysis and Applications, 27(4), 1056–1068.

[3] P. S. Vassilevski and U. M. Yang (2014) *Reducing communication in algebraic multigrid using additive variants.* Numerical Linear Algebra with Applications, 21, 275–29, 21, 275–296.

Numerical Simulation of Propagation of Uncertainties in Coastal Aquifers

Dmitry Logashenko[1], Alexander Litvinenko[2], Raul Tempone[1,2], Ekaterina Vasilyeva[1], and Gabriel Wittum[1]

[1]King Abdullah University of Science and Technology, Saudi Arabia
[2]RWTH Aachen, Germany
dmitry.logashenko@kaust.edu.sa

Abstract

Simulation of salinization of coastal aquifers plays an important role in prediction of availability of pure water resources. However uncertain variations in hydrogeological parameters may affect the groundwater flow and therefore significantly reduce accuracy of the prediction of the transport phenomena. In this talk, we present numerical approaches for estimation of propagation of the uncertainty from the parameters to the solution in the subsurface density-driven flow models represented by a system of nonlinear PDEs. We test them on model problems with random fields for porosity that represent the limited knowledge of the data. We construct a low-cost generalized polynomial chaos (gPC) expansion surrogate model. Computation of the gPC coefficients is performed by projection on sparse and full tensor grids. Furthermore, we consider a multilevel Monte-Carlo technique (MLMC). Parallelization is applied to both the numerical solution of the deterministic problems (scenarios) and the high-dimensional quadrature over the parametric space. We present results of numerical experiments in 2d and 3d.

Keywords: Uncertainty quantification, Groundwater flow, Numerical simulation, Multilevel Monte-Carlo, High-Performance Computing

Scalable and Adaptive Multigrid Methods for Problems Coupling Flow, Geomechanics and Transport

Arne Nägel and Martin Parnet

Modular Supercomputing and Quantum Computing,
Goethe Universität Frankfurt am Main, Germany
naegel@uni-frankfurt.de

Abstract

Developing efficient and scalable solvers for coupled PDE systems is a non-trivial task, since suitable schemes for discretization, time integration and linear solvers, must be combined. In this study, we suggest a combination of methods suitable for poroelastic media.

The fixed stress iteration, e.g. [2], can be interpreted as a special block-LU decomposition, which separates degrees of freedom for deformations and pressures. When the Schur complement is formed with respect to the pressure, it can be approximated by a properly scaled identity. The method can be generalized to heterogeneous media with jumping coefficients [3]. In this work, we avoid the aforementioned splitting and employ a multigrid solver for the fully-coupled system. The method is based on the fixed-stress smoothers suggested in [4]. The derived method turns out to be highly scalable.

However, as soon as the spatial coarse grid solver becomes a bottleneck, the parallel scalability may be limited. To that end, the temporal direction is included in the analysis. On the one hand, acceleration is achieved by linearly-implicit extrapolation schemes and adaptive time-stepping, which is also applicable to non-linear transport [5]. Moreover multigrid-reduction in time (MGRIT) provides an additional tool to improve the strong scalability [6].

For all methods, we investigate robustness and provide a scaling study in a HPC environment. This is complemented by a theoretical analysis, that is based on a Fourier decomposition and uses suitable problem dependent norms.

Keywords: Quasi-static Biot equations, Parallel algorithms, Multilevel methods in space and time

References

[1] J. Kim et al. (2011). *Stability and convergence of sequential methods for coupled flow and geomechanics: Fixed-stress and fixed-strain splits.* CMAME, 200, 1591–1606.

[2] A. Mikelić, M. F. Wheeler (2013). *Convergence of iterative coupling for coupled flow and geomechanics.* Computational Geosciences, 17, 455–461

[3] J. W. Both et al. (2017). *Robust fixed stress splitting for Biot's equations in heterogeneous media.* Applied Mathematics Letters, 68, 101–108.

[4] F. J. Gaspar, C. Rodrigo (2017). *On the fixed-stress split scheme as smoother in multigrid methods for coupling flow and geomechanics.* CMAME, 326, 526–540.

[5] A. Nägel, P. Deuflhard, G. Wittum (2018). *Efficient Stiff Integration of Density Driven Flow Problems.* ZIB-Report 18–54.

[6] R. Buijse et al. (2023). *Large scale simulations of partial differential equation models on the Hawk supercomputer.* High Performance Computing in Science and Engineering '21, Springer, 453–466.

MS35 - Solving Multiphysics/Multiscale Problems: A Challenge between (Reduced) Model-Driven and Data-Driven approaches

Samplets-Kernel Method in Computational Learning

Davide Baroli*[1] and Micheal Multerer†[1]

[1]Euler Insitute, Universita' della Svizzera Italiana,
davide.baroli@usi.ch; micheal.multerer@usi.ch

Abstract

In this talk, we consider the uncertain input parameter on quantities of interest of computational model or of data-driven challenge.
To this end, we develop a surrogate models based on low-rank multiresolution approximation and Gaussian process learning [1, 2, 3].
The framework integrates the multiresolution of the input data, which allows treating multiscale signal and account for irregular and discrete observations. Additionally, we have developed different optimization methods for regularized Gaussian process learning in multiresolution analysis [4].
Finally, we integrate different surrogate model defined based on hierarchical fidelity of the computational model or data granularity into a fusion multi-fidelity model. As numerical experiments, we show the results obtained in different pilot case: industrial pilot of decarbonised maritime, global climate and weather prediction (ECMWF reanalysis) [5], computer vision and computational energy.

Keywords: Computational Learning, industrial pilot, fluid dynamics, climate, energy, resilience, uncertainty

References

[1] H. Harbrecht, M. Multerer (2021). *A fast direct solver for nonlocal operators in wavelet coordinates.* Journal of computational physics 428, 110056.

[2] H. Harbrecht, M. Multerer (2022). *Samplets: Construction and scattered data compression.* Journal of Computational Physics, 471, 111616.

[3] H. Harbrecht, M. Multerer, O. Schenk, C. Schwab (2023). *Multiresolution kernel matrix algebra.* arXiv preprint arXiv:2211.11681.

[4] D. Baroli, H. Harbrecht, M. Multerer. *Samplets Basis Pursuit.* manuscript.

[5] H. Hersbach et al (2020). *The ERA5 global reanalysis.* Quarterly Journal of the Royal Meteorological Society, 146(730), 1999-2049. https://doi.org/10.1002/qj.3803

*The research results was carried out with the support of the Swiss Federal Office of Energy SFOE as part of the SWEET project SURE and simOCean (H2020 EuroHP).
†The research results was carried out with the support of the Swiss Federal Office of Energy SFOE as part of the SWEET project SURE and SNSF ERC StG

State estimation for brain poro-elastography data

Felipe Galarce Marin[1], Alfonso Caiazzo[2], and Cristian Carcamo[2]

[1]Escuela de Ingeniería Civil, Pontificia Universidad Católica de Valparaíso. Chile.
[2]Weierstrass-Institut für Angewandte Analysis und Stochastik. Leibniz-Institut im Forschungsverbund Berlin e. V.
felipe.galarce@pucv.cl

Abstract

Noisy curves are common when assimilating signals from several fields. Poro-elasticity is one such field, and this work takes inspiration from inverse problems for Magnetic Resonance Elastography (MRE) data [1]. Non-invasive methods are desired by the medical community to assess certain pathologies, such as hydrocephalus or neurological disorders (see, e.g., [2]). In this context, radiologists can provide information about the brain's sensitivity to a harmonic mechanical stimulus. The task is both to compute a fully resolved displacement field in a 3D domain and to compute pressure-related quantities.

Recently, a variational state estimation numerical pipeline was proposed in [3], where the brain tissue is understood at a macroscopic level as biphasic media, and an inverse problem is solved for synthetic MRE data over a real brain model. To bridge the gap between the applied mathematics community and the medical one, it is essential to extend the approach to account for real MRE data, which involves a noise structure and artifacts intrinsic to the observation process.

This work builds upon [3] to propose, analyze, and test a modification of the currently used variational approach [4]. An operator is added to the optimization problem to invert the data, which is specially designed to counter the measurement noise given either an experimental or analytical model for the observation process, while still keeping some relevant and desirable properties of the initially linear inverse problem. The convergence is demonstrated with numerical experiments and mathematically worked out from the original error bound derived in [4].

Keywords: Poro-elasticity, data-assimilation, state estimation, elastography, inverse problems

References

[1] S. Hirsch, J. Braun, I. Sack (2017). *Magnetic Resonance Elastography: Physical Background and Medical Applications*. Wiley, 2017.

[2] L.M. Solamen, M. McGarry, J. Fried, J.B. Weaver, S.S. Lollis, K.D. Paulsen (2021). *Poroelastic mechanical properties of the brain tissue of normal pressure hydrocephalus patients during lumbar drain treatment using intrinsic actuation mr elastography*. Academic Radiology, 28(4), 457–466.

[3] F. Galarce, K. Tabelow, J. Polzehl, C.P. Panagiotis, V. Vavourakis, L. Lilaj, I. Sack, A. Caiazzo (2023). *Displacement and pressure reconstruction from magnetic resonance elastography images: Application to an in silico brain model*. SIAM Journal on Imaging Science.

[4] Y. Maday, A. T. Patera, J. D. Penn, M. Yano (2015). *A parameterized-background data-weak approach to variational data assimilation: formulation, analysis, and application to acoustics*. International Journal for Numerical Methods in Engineering, 102(5), 933–965.

Error bounds for PDE-regularized learning

Carsten Gräser[1] and Prem Anand Alathur Srinivasan[2]

[1]Department of Mathematics, FAU Erlangen-Nürnberg
[2]Institut für Mathematik, FU Berlin
graeser@math.fau.de

Abstract

In the talk we consider the regularization of a supervised learning problem by partial differential equations (PDEs) and present error bounds for the obtained approximation in terms of a PDE error term and a data error term. Assuming that the solution solves an unknown PDE, the PDE error term quantifies how well this PDE is approximated by the auxiliary PDE used for regularization, while the data error term quantifies the coverage by the given data. Furthermore, the PDE-regularized learning problem is discretized by generalized Galerkin discretizations using finite elements and neural networks. For such discretizations an error bound in terms of the PDE error, the data error, and a best approximation error is derived using a nonlinear version of Céa's lemma.

Keywords: Machine learning, regularization, generalization error, physics informed neural networks, Ceá's lemma

References

[1] C. Gräser, P. A. Alathur Srinivasan (2020). *Error bounds for PDE-regularized learning*. Preprint. arxiv:2003.06524.

Physics-informed deep learning for viscoelastic flows

Birane Kane[1]

[1]NORCE
birane.kane@norceresearch.no

Abstract

We present Physics-Informed Neural Network simulations of viscoelastic fluid flow problems. Viscoelastic fluid flow modeling is important in many industrial and medical applications from enhanced oil recovery to blood flow in arteries and polymer processing. The behaviour of those non-newtonian flows is complex and requires a careful treatment of the physical processes involved as well as accurate and efficient numerical techniques.

There are many models aiming at describing viscoelastic flow, however we will mainly focus on two namely the Olroyd-B type [1] and the FENE-P(Finitely Extensible Nonlinear Elastic) model. As opposed to Newtonian (resp. quasi-newtonian) fluids where the stress tensor is a linear (resp. non-linear) functional of the velocity and pressure field, the viscoelastic flows require to take into account another constitutive equation where the stress tensor is another unknown. Simulation of such problem class becomes quite challenging when the amount of fluid elasticity is highly increased. This phenomenon is known as the High Weissenberg Number problem (HWNP). Another challenges comes from the hyperbolic constitutive equation when the advection term becomes dominant. Traditional numerical methods for solving PDEs, such as finite difference, finite elements and Galerkin methods have mostly failed to fully and efficiently address the aforementioned shortcomings. Recently, Raissi et al. [2], demonstrated that it is possible to combine Machine Learning approaches with more traditional physics approaches. These so-called physics informed machine learning (PINN) approaches are designed to obtain solutions of general nonlinear PDEs, and they may be a promising alternative to traditional numerical methods for solving PDEs, such as finite difference and finite elements methods. The core idea of PINN is to explicitly embed the physical laws (e.g., the governing partial differential equations ,initial/boundary conditions, etc.) into a deep neural network, constraining the network's trainable parameters within a feasible solution space.

Thus, following this approach we introduce here a framework where we explicitly embed physical laws aiming at describing viscoelastic fluid flow (e.g., Oldroyd/FENEP equations) to constrain neural networks for training a reliable model. The effectiveness of the proposed framework is demonstrated through some benchmarks tests. The implementation of our model is based on a suitable open source numerical modeling platform using the TensorFlow library.

Keywords: Navier-Stokes equations, Free boundary problems, Capillarity

References

[1] J. Oldroyd (1950). *On the formulation of rheological equations of state.* Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences 200 (1063), 523–541.

[2] M. Raissi, P. Perdikaris, G. E. Karniadakis (2019). *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations.* Journal of Computational Physics 378, 686–707.

Analysis of Endovascular and Open Surgery Repair for Descending Thoracic Aortic Aneurysms using Multiscale 0D-1D Fluid-Structure Interaction

Leonardo Molinari[1], Alessandro Veneziani[1], Hannah Cebull[2], Marina Piccinelli[2], and Bradley G Leshnower[3]

[1]Department of Mathematics and Computer Science, Emory University
[2]Department of Radiology and Imaging Sciences, Emory University
[3]Division of Cardiothoracic Surgery, Emory University School of Medicine

Abstract

The treatment of descending thoracic aortic aneurysms (DTAA) using open surgical and endovascular (TEVAR) methods is widely accepted in medicine. However, these procedures modify the aorta's anatomy and biomechanics, triggering anomalous wave reflections and cardiac remodeling. The complex interplay among these factors is largely unexplored, hampering procedural efficacy and long-term predictability. Multiscale fluid-structure interaction (FSI) is a powerful tool for exploring these dynamics, but the computational complexity of simulating 3D scenarios often poses practical challenges.

To address this, we employ cost-effective multiscale 0D-1D FSI models. Integrating a simplified lumped parameter model of the left heart [4] and an extended 1D systemic circulation model (covering 55 arteries) [3], implemented in the Multiscale module in the C++ LifeV finite element library [1, 2]. Patient-specific pre- and post-operative 1D-FSI models were derived from CT angiography data of 12 patients (6 open surgery, 6 TEVAR), with implant stiffness adhering to established literature values (1.2 MPa Dacron grafts, 51.7 MPa metallic stents). Physiological inflow conditions are imposed at the ascending aorta, while three-element Windkessel models accounts for peripheral circulation. We simulated a total of 24 cases (spanning 3 heartbeats each), and compared peak systolic pressure, pressure-volume (PV) loops, and Pulse Wave Velocity (PWV) across vessels.

Our findings demonstrate that implant presence increases ascending aorta pressure due to pressure wave back-propagation, particularly notable in stiffer implants. Postoperative pressure decreases in two cases due to increased patient geometry length. TEVAR cases exhibit higher PWV, indicative of larger stiffness of the implant. Complex geometric cases, like aortic dissections, exhibit smoother pressure-flow profiles post-surgery.

Extending these insights to larger patient cohorts holds the potential to unveil mechanisms shaping the long-term effects of DTAA repair, including the impact of stiffening resulting from endovascular and open surgery interventions.

References

[1] Malossi, A. C. I., Blanco, P. J., & Deparis, S. (2012). *A two-level (...) of one-dimensional arterial networks.* Computer Methods in Applied Mechanics and Engineering, 237, 212-226.

[2] Malossi, A. C. I., Deparis, S., & Blanco, P. J. (2011). Algorithms for the coupling (...) with three-dimensional FSI problems. In Proceedings of the ECCOMAS SIMBIO 2011.

[3] Formaggia, L., Lamponi, D., Tuveri, M., & Veneziani, A. (2006). Computer methods in biomechanics and biomedical engineering, 9(5), 273-288.

[4] Kim, H. J., Vignon-Clementel, I. E., Figueroa, C. A., LaDisa, J. F., Jansen, K. E., Feinstein, J. A., & Taylor, C. A. (2009). Annals of biomedical engineering, 37, 2153-2169.

Data-driven modelling of turbulent reacting flows: from physics-based models to digital twins

Alessandro Parente[1], Alberto Procacci[1], Laura Donato[1], and Aysu Özden[1]

[1]Aero-Thermo-Mechanics Department, Université libre de Bruxelles
alessandro.parente@ulb.be; alberto.procacci@ulb.be, laura.donato@ulb.be;
aysu.ozden@ulb.be

Abstract

The simulation of turbulent combustion is challenging for several aspects beyond turbulence. Indeed, combustion is intrinsically multi-scale and multi-physics. It is characterised by various scales inherently coupled, in space and time, through thermo-chemical and fluid dynamic interactions [1]. Typical chemical mechanisms describing the evolution of fuels consist of hundreds of species involved in thousands of reactions, spanning twelve decades of temporal scales [2]. The interaction of these scales with the fluid dynamic ones defines the nature of the combustion regime and the limiting process in determining the overall fuel oxidation rate [3]. The challenges associated with turbulent combustion modelling make the use of machine learning very attractive. This paper reviews the current state-of-the-art in developing reduced-order models to accelerate high-fidelity simulations of turbulent reacting flows and develop surrogate models and digital twins of complex combustion systems. The methods are demonstrated in the context of developing the digital twins for a combustion furnace operating with hydrogen as a fuel. Strategies are discussed to bring together data of different fidelity and to assimilate experimental data into cyber-physcial infrastructures.

Keywords: Combustion, Data-driven modelling, Digital twins, Reduced-order models, Turbulent reacting flows.

References

[1] Stephen B. Pope (2015) *Small scales, many species and the manifold challenges of turbulent combustion.* Proc. Combust. Inst., 34, 1-31.

[2] A. Frassoldati and T. Faravelli and E. Ranzi (2015) *Kinetic modeling of the interactions between NO and hydrocarbons at high temperature.* Combust. Flame, 135, 97-112.

[3] Kuo, K.K. and Acharya, R. (2012) *Fundamentals of Turbulent and Multi-Phase Combustion.* Wiley.

Physics-based reduced order modelling for efficient urban air pollution prediction

G. Rozza[1], M. Khamlich[1], and G. Stabile[2]

[1]SISSA, International School for Advanced Studies, Trieste, Italy.
[2]University of Urbino Carlo Bo , Urbino, Italy
{grozza, mkhamlic}@sissa.it; giovanni.stabile@uniurb.it

Abstract

Air pollution is a significant global issue that harms health, climate, and ecosystems, with widespread pollution causing over 3 million deaths and a $5 trillion economic cost annually.

Since at the urban level, pollutant dispersion depends on daily weather conditions, CFD models with low time scales, repeated evaluation, and fine mesh discretization must be used. The former requirements translate into huge memory requirements, making it essential to use HPC facilities to get results in reasonable time frames.

In our study, we aimed to address the challenge of computational cost by using a Reduced Order Model (ROM) to obtain fast and accurate solutions. We chose to simplify our model by describing the pollutant's evolution through the transport equation, with the convective field determined by solving the Navier-Stokes equation and the source term represented by an empirical time series. We studied two different options for the reduced order model, namely extracting a proper orthogonal decomposition (POD) basis onto which the full order empirical source field is projected or using the Discrete Empirical Interpolation Method (DEIM) as a hyper-reduction strategy [2]. Both these approaches are proven effective, even when the basis for the source term is extracted on a subset of the time series and then used for future state prediction. To address the parametrized convective field case, we changed boundary velocity's direction and intensity. We also proposed a novel data-driven approach based on a POD-NN [1] reconstruction of the flux field to non-intrusively recover reduced-order operators needed for online evaluation.

We validated our framework on a computational domain modeling the University of Bologna's main campus, using a mesh with approximately 40k cells. We employed real inlet conditions for wind flow around buildings based on one-year-long measurement station data with hourly resolution. The source term was obtained synthetically through realistic traffic flow modeling and used to calculate NOx emission.

Keywords: reduced order modelling; proper orthogonal decomposition; air pollution; DEIM; large-scale simulations; air pollution, CFD, environment modelling

References

[1] J. S. Hesthaven and S. Ubbiali. Non-intrusive reduced order modeling of nonlinear problems using neural networks. *J. Comput. Phys.*, 363:55–78, 2018.

[2] G. Stabile, M. Zancanaro, and G. Rozza. Efficient geometrical parametrization for finite-volume-based reduced order methods. *International Journal for Numerical Methods in Engineering*, 121(12):2655–2682, 2020.

MS36 - Meshfree methods for direct and inverse problems in partial differential equations. In memoriam of Prof. Carlos J.S. Alves

Elasticity Imaging–In memory of Carlos Alves

Habib Ammari

Department of Mathematics, ETH Zürich, Rämistrasse 101, CH-8092 Zürich, Switzerland
habib.ammari@math.ethz.ch

Abstract

Carlos Alves made significant contributions to the field of wave propagation and scattering in elastic media. I will describe some of his ideas and results.

Keywords: Carlos Alves' work, Method of fundamental solutions, Integral equations, Inverse problems, Scattering resonances

References

[1] Carlos J.S. Alves. On the choice of source points in the method of fundamental solutions. Eng. Anal. Bound. Elem. 33 (2009), no. 12, 1348–1361.

[2] Carlos Alves, Habib Ammari. Boundary integral formulae for the reconstruction of imperfections of small diameter in an elastic medium. SIAM J. Appl. Math. 62 (2001), no. 1, 94–106.

[3] Habib Ammari, Elie Bretin, Josselin Garnier, Hyeonbae Kang, Hyundae Lee, Abdul Wahab. *Mathematical Methods in Elasticity Imaging*. Princeton Ser. Appl. Math., Princeton University Press, Princeton, NJ, 2015.

A well-conditioned Method of Fundamental Solutions for Laplace equation

Pedro R. S. Antunes

Departamento de Matemática, Instituto Superior Técnico, Universidade de Lisboa

Grupo de Física Matemática, Universidade de Lisboa

prsantunes@tecnico.ulisboa.pt

Abstract

The method of fundamental solutions (MFS) is a numerical method for solving boundary value problems involving linear partial differential equations. It is well-known that it can be very effective assuming regularity of the domain and boundary conditions. The main drawback of the MFS is that the matrices involved are typically ill-conditioned and this may prevent the method from achieving high accuracy.

In this work, we propose a new algorithm to remove the ill-conditioning of the classical MFS in the context of the Laplace equation defined in planar domains. The main idea is to expand the MFS basis functions in terms of harmonic polynomials. Then, using the singular value decomposition and Arnoldi orthogonalization we define well conditioned basis functions spanning the same functional space as the MFS's. Several numerical examples show that when possible to be applied, this approach is much superior to previous approaches, such as the classical MFS or the MFS-QR.

Keywords: Method of fundamental solutions, Laplace equation, ill conditioning

References

[1] C. J. S. Alves (2009). *On the choice of source points in the method of fundamental solutions*, Eng. Anal. Bound. Elem. **33**, 1348–1361.

[2] P. R. S. Antunes (2022). *A well-conditioned Method of Fundamental Solutions for Laplace equation*, Numer. Algorithms **91**, 1381–1405.

[3] P. D. Brubeck, Y. Nakatsukasa and L. N. Trefethen (2021). *Vandermonde with Arnoldi*, SIAM Rev. **63**(2), 405–415.

[4] C. S. Chen, A. Karageorghis and Y. Li (2016). *On choosing the location of the sources in the MFS*, Numer. Algorithms **72**(1), 107–30.

A Localized Multi-Level Method of Fundamental Solutions for Inhomogeneous Problems

Csaba Gáspár[1]

[1]Department of Mathematics and Computational Sciences, Széchenyi István University, Győr, Hungary
gasparcs@math.sze.hu

Abstract

The Method of Fundamental Solutions (MFS) is a popular, truly meshless and boundary-only method. It requires neither domain nor boundary mesh structure, only a set of scattered points on the boundary and another set of external source points. The approximate solution is sought as a linear combination of the fundamental solution of the original differential equation shifted to the source points; the coefficients of this linear combination are computed by enforcing the original boundary conditions at some predefined boundary collocation points. This results in a linear system of equations with a fully populated (and often ill-conditioned) matrix.

Originally, the method was defined for solving homogeneous problems. It has been generalized to inhomogeneous problems by applying the Method of Particular Solutions (MPS), where the particular solution can be constructed via various methods, e.g. a scattered data interpolation. However, this approach leads to a much larger linear system. To make the computations more economic, localization techniques have been introduced which make the resulting linear system sparse, see e.g. [1], [2].

In this talk, a special localization is presented for the Poisson equation, which mimics the classical Schwarz alternating method [3]. The domain is covered by a finite number of small overlapping subdomains, and the original problem is converted to the solutions of local – much less – subproblems, which are solved by the MFS and the MPS based on the use of radial basis functions, and this process is repeated iteratively. See also [4] for homogeneous problems. The speed of convergence of the overall iteration is moderate, but the iteration significantly damps the high-frequency error components, therefore it can be used as a smoothing procedure in a natural multi-level context.

Keywords: Method of Fundamental Solutions, Localization, Inhomogeneous problems

References

[1] V.M.A. Leitão (2010). *Generalized finite differences using fundamental solutions.* Int. J. Numer. Meth. Engng 81, 564–583.

[2] J. Zhang, C. Yang, H. Zheng, C.M. Fan, M.F. Fu (2022). *The localized method of fundamental solutions for 2D and 3D inhomogeneous problems.* Mathematics and Computers in Simulation 200, 504–524.

[3] P.L. Lions (1988). *On the Schwarz alternating method I.* In *First International Symposium on Domain Decomposition Methods for Partial Differential Equations*, eds.: R. Glowinski, G. H. Golub, G. A. Meurant, and J. Périaux. SIAM, Philadelphia, PA, 1–42.

[4] C. Gáspár (2023). *A Localized Version of the Method of Fundamental Solutions in a Multi-level Context*, Periodica Polytechnica Civil Engineering, https://doi.org/10.3311/PPci.21535

Applications and numerical solution of vibrations of the elastic membrane by using a meshless method of lines

Arshad Hussain[1], Sirajul Haq[2], and Rohul Amin[3]

[1]Department of Mathematics, Karakoram International University, Hunza Campus, Gilgit-Baltistan, Pakistan
[2]FES, GIK Institute of Engineering Sciences and Technology, Topi, Khyber Pakhtunkhwa, Pakistan
[3]Department of Mathematics, University of Peshawar, Khyber Pakhtunkhwa, Pakistan
math_pal@hotmail.com; siraj_jcs@yahoo.co.in; raminmath@uop.edu.pk

Abstract

This study investigates the applications of the wave equation in many real-world problems arising in science and engineering. A radially symmetric circular membrane of unit radius is considered, and a meshless method of lines approach using a multiquadric radial basis function collocation method is proposed for solving the circular membrane model in polar coordinates. The method can be applied to a wide range of problems with arbitrary domains. The multiquadric radial basis function is used for space discretization. The meshless characteristic gives it an edge over mesh-based methods by reducing the computational time considerably. Stability is discussed in the light of eigenvalues. The numerical method is validated by comparing the results with the exact solution, and MATLAB software is used for numerical simulations. Overall, this study presents a useful approach for solving circular membrane problems in a wide range of applications.

Keywords: Vibrations, circular membrane, meshless methods, method of lines, radial basis functions

Accelerated iterative MFS algorithms for the Cauchy problem in steady-state anisotropic heat conduction

Liviu Marin[1,2]

[1]Department of Mathematics, Faculty of Mathematics and Computer Science, University of Bucharest, 14 Academiei, 010014 Bucharest, Romania
[2]"Caius Iacob - Gheorghe Mihoc" Institute of Mathematical Statistics and Applied Mathematics of the Romanian Academy, 13 Calea 13 Septembrie, 050711 Bucharest, Romania
liviu.marin@fmi.unibuc.ro

Abstract

We investigate, from both the theoretical and the numerical viewpoints, the acceleration of the iterative algorithms of Kozlov *et al.* [1] for the accurate, convergent and stable reconstruction of the missing temperature and normal heat flux on an inaccessible boundary of the domain occupied by a solid from the knowledge of Cauchy data on the remaining and accessible boundary in the framework of stationary anisotropic heat conduction without heat sources [2]. For each of the two algorithms with relaxation considered, the inverse Cauchy problem in anisotropic heat conduction with exact data is transformed into an equivalent fixed point problem for an associated operator that is defined on and takes values in a suitable function space and, at the same time, takes into account the relaxation parameter. Hence the convergence of each relaxation algorithm reduces to investigating the properties of the corresponding operator. This enables one to determine, for each iterative algorithm and exact Cauchy data, the admissible range for the relaxation parameter along with a criterion for selecting its optimal value at each iteration. The numerical implementation is realised for homogeneous anisotropic solids via the method of fundamental solutions (MFS) and confirms a significant reduction in the number of iterations and hence the CPU time required for the two relaxation algorithms proposed to achieve convergence, provided that the dynamical selection of the optimal value for the relaxation parameter is employed.

Keywords: Inverse Cauchy problem, anisotropic heat conduction, accelerated iterative algorithms, method of fundamental solutions (MFS)

References

[1] V.A. Kozlov, V.G. Mazya, A.V. Fomin (1991). *An iterative method for solving the Cauchy problem for elliptic equations*. U.S.S.R. Comput. Math. Math. Phys., 31, 45–52.

[2] M.N. Özişik (1993). *Heat Conduction*. John Wiley & Sons, New York.

Meshfree methods with particular solutions for nonhomogeneous Stokes and Brinkman systems

Nuno F. M. Martins[1]

[1]Department of Mathematics, FCT-Nova, Portugal
nfm@fct.unl.pt

Abstract

In this presentation we will discuss some meshfree methods for nonhomogeneous Stokes and Brinkman systems. The aim is to solve a problem containing a non null body force, starting from the well known decomposition in terms of a particular solution and the solution of a homogeneous force problem. We present two methods for the numerical construction of a particular solution. One method is based on the Neuber-Papkovich potentials, which, in [1], we extend to nonhomogeneous Brinkman problems. A second method relies on a Helmholtz-type decomposition for the body force and enables the construction of divergence-free basis functions. Such basis functions can be obtained, from instance, from Hänkel functions (cf. [1]). We will also present a method based on a combination of shear and pressure waves for the approximation of the body force (cf. [2]). Several 2D numerical experiments will be presented.

Keywords: Stokes systems, Brinkman systems, meshfree methods.

References

[1] Carlos J.S. Alves, Nuno F.M. Martins, Ana L. Silvestre (2022). *Numerical methods with particular solutions for nonhomogeneous Stokes and Brinkman systems.* Advances in Computational Mathematics, 48, 44.

[2] Nuno F. M. Martins, Magda Rebelo (2014) . *Meshfree methods for nonhomogeneous Brinkman flows.* Computers & Mathematics with Applications Vol 68 (4).872–886.

A meshfree alternating Schwarz method for elliptic BVP

Svilen S. Valtchev*

CEMAT, Instituto Superior Técnico, Universidade de Lisboa, Portugal and
School of Technology and Management, Polytechnic of Leiria, Portugal
ssv@math.ist.utl.pt

Abstract

The method of fundamental solutions (MFS) is a meshfree and integration-free boundary collocation method that, in its classical formulation [1], can be used for the approximate solution of BVP for certain homogeneous PDE. Due to its simple algorithm and remarkable accuracy, MFS has received significant attention from the scientific community in the last decades, resulting in the development of a large number of variants with application to complex physical and engineering problems, e.g. [2].

One of the difficulties that arise in the application of the MFS is related to the necessary solution of a large and ill-conditioned collocation linear system. The conditioning of this system deteriorates even further when large scale problems, posed in domains with complex geometry, are considered. A possible approach to alleviate this conditioning problem consists in splitting the original BVP into a set of smaller scale sub-problems using a domain decomposition technique.

In this talk, we develop an iterative numerical scheme by coupling the MFS with the alternating Schwarz method, see [3]. Special attention is required for the points where the boundaries of the sub-domains intersect. Numerical tests show that spurious oscillations of the MFS solution, due to the Gibbs phenomenon, occur in the neighborhood of those points and prevent the global convergence of the scheme. We solve this issue and recover the convergence of the Schwarz iterations by enriching the MFS approximation space with a set of appropriate singular particular solutions of the PDE. These particular solutions are developed in polar coordinates, using an idea from [4]. The convergence of the proposed method is illustrated for BVP for Helmholtz-type PDE in 2d domains.

Keywords: Method of fundamental solutions, Alternating Schwarz method, Singular basis functions

References

[1] V. D. Kupradze and M. A. Aleksidze (1964), *The method of fundamental equations for an approximate solution of certain boundary value problems*, Comput. Math. Math. Phys., 4, 82–126.

[2] C. Alves, A. Karageorghis, V. Leitão, and S. Valtchev, Eds. (2020), Advances in Trefftz Methods and Their Applications, ser. SEMA SIMAI Springer Series 23, Springer.

[3] A. Quarteroni and A. Valli (1999), Domain Decomposition Methods for Partial Differential Equations, ser. Numerical mathematics and scientific computing. Clarendon Press, Oxford.

[4] P. R. S. Antunes and S. S. Valtchev (2010), *A meshfree numerical method for acoustic wave propagation problems in planar domains with corners and cracks*, J. Comput. Appl. Math., 234, 2646-–2662.

*The financial support of the Portuguese Fundação para a Ciência e a Tecnologia (FCT), through the projects UIDB/04621/2020 and UIDP/04621/2020 of CEMAT/IST-ID (Center for Computational and Stochastic Mathematics) is gratefully acknowledged.

MS37 - Diseases, Diagnosis, Treatment: Mathematical Modeling and Numerical Analysis

Learning stable cross-diffusion with reaction systems for image restoration

Sílvia Barbeiro*[1] and Diogo Lobo†[1]

[1]CMUC, Department of Mathematics, University of Coimbra
{silvia, diogo.lobo}@mat.uc.pt

Abstract

Despeckling optical coherence tomograms from the human retina is a fundamental step to a better diagnosis or as a preprocessing stage for retinal layer segmentation. In this talk we will focus on nonlinear cross-diffusion systems for image filtering. We will start with a concise introduction about complex diffusion and cross-diffusion models for image restoration and report about their speckle filtering capabilities and potential to recover the original (uncorrupted) signal. Then, we will discuss a flexible learning framework in order to optimize the parameters of the models improving the quality of the denoising process. In particular, we use a back propagation technique in order to minimize a cost function related to the quality of the denoising process while we ensure stability during the learning procedure.

Keywords: nonlinear cross-diffusion, image denoising, machine learning, back-propagation, optimal parameters, stability

References

[1] A. Araújo, S. Barbeiro, E. Cuesta, A. Durán (2017). *Cross-diffusion systems for image processing: II. The nonlinear case*, Journal of Mathematical Imaging and Vision, 58 (3), 447–467.

[2] S. Barbeiro, D. Lobo (2020). *Learning Stable Nonlinear Cross-Diffusion Models for Image Restoration*. Journal of Mathematical Imaging and Vision 62, 223–237.

[3] R. Bernardes, C. Maduro, P. Serranho, A. Araújo, S. Barbeiro, J. Cunha-Vaz (2010). *Improved adaptive complex diffusion despeckling filter*. Optics Express, 18 (23), 24048–24059.

*Partially supported by the Centre for Mathematics of the University of Coimbra - UIDB/00324/2020, funded by the Portuguese Government through FCT/MCTES.

†DL is supported by FCT, Portugal grant PD/BD/142956/2018.

Numerical Analysis of Drug Release from Viscoelastic Polymers

Geovan C.M. Campos[1], Júlia S. Borges[2], Giuseppe Romanazzi[1], and José A. Ferreira[3]

[1]IMECC, State University of Campinas
[2]CCN, Federal University of São Carlos
[3]Department of Mathematics, University of Coimbra
geovan_carlos@hotmail.com; juliaborges@ufscar.br; roman@ime.unicamp.br;
ferreira@mat.uc.pt

Abstract

Viscoelastic polymer platforms are devices that has been used for active and passive target drug release due to their optimum control properties. We consider the drug release in a spherical polymer of radius R that is immersed in a solvent with concentration c_ℓ. The drug is then released from the platform with concentration c_s and dissolve. The dissolved drug with concentration c_d diffuses through the swelled polymer. Let $c_\ell(r,t)$, $c_d(r,t)$ and $c_s(r,t)$ be the solvent, dissolved drug and solid drug concentrations in the polymer at distance r at time t, they are modeled by the non-linear boundary initial value problem

$$\begin{cases} \dfrac{\partial c_\ell}{\partial t} = \dfrac{\partial}{\partial r}\Big(D_\ell(c_\ell)\dfrac{\partial c_\ell}{\partial r}\Big) + \dfrac{\partial}{\partial r}\Big(\displaystyle\int_0^t q(t,s,c_\ell(s),c_\ell(t))\dfrac{\partial c_\ell}{\partial r}(s)ds\Big), \\ \dfrac{\partial c_d}{\partial t} = \dfrac{\partial}{\partial r}\Big(D_d(c_\ell)\dfrac{\partial c_d}{\partial r}\Big) + f(c_s,\, c_d,\, c_\ell), \\ \dfrac{\partial c_s}{\partial t} = -f(c_s,\, c_d,\, c_\ell) \end{cases} \tag{1}$$

defined in $(0,R)\times(0,T]$, with initial and boundary conditions

$$\begin{cases} c_\ell(0) = c_{l,0} \\ c_d(0) = 0 \\ c_s(0) = c_{s,0} \end{cases}, \begin{cases} \dfrac{\partial c_\ell}{\partial r}(0) = \dfrac{\partial c_d}{\partial r}(0) = 0 \\ c_\ell(R) = c_{ext} \\ c_d(R) = 0 \end{cases} \tag{2}$$

where f is a modified Noyes-Whitney dissolution term and q describes the viscoelastic polymer properties [1]. Our goal is to propose a finite difference method (that is simultaneously a semi-discrete Galerkin finite element method) to solve (1)-(2) in non-uniform grids. We show that this method is second order convergent in time and space requiring less regularity conditions with respect those required in previous works [1, 2]: $c_l(t)$, $c_d(t)$ and $c_s(t)$ are now only in $H^3(0,R)$.

Keywords: Drug release, Dissolution, Dissolved drug transport, Convergence

References

[1] J. S. Borges, J. A. Ferreira, G. Romanazzi, E. Abreu, (2021). *Drug release from viscoelastic polymeric matrices - a stable and supraconvergent FDM.* Comp Math Appl, 99, 257–-269.

[2] J. A. Ferreira, R. D. Grigorieff (2006). *Supraconvergence and supercloseness of a scheme for elliptic equations on nonuniform grids.* Numerical Functional Analysis and Optimization, 27, 5-6, 539–-564.

Drug delivery enhanced by external stimuli: modelling, simulation and numerical analysis

José A. Ferreira*[1]

[1]University of Coimbra, CMUC, Department of Mathematics
ferreira@mat.uc.pt

Abstract

Conventional cancer drug delivery faces a set of barriers: drug non-selectivity, tumour tissue's characteristics and loss of efficacy of the drug. To reduce adverse drug effects and to increase drug availability in the target, new drug delivery systems have been proposed. In these novel systems, the drug is entrapped in a carrier and transported to the tissue. Combining the carrier material properties, the drug characteristics and the effects of an external stimulus, the drug is delivered on demand, meaning where, when and in the amount it is needed. Electric and magnetic fields, heat, ultrasound and light are used nowadays.

From the mathematical point of view, the description of the drug delivery driven by stimuli leads to several challenges: stimulus propagation and its influence in drug release from the system, and transport and uptake of the drug by the target tissue. From the numerical point of view, the development of stable and accurate numerical methods, that are able to simulate the entire drug delivery process, also leads to several challenges: the dependence of the drug release and drug transport on the stimulus effects requires the use of convenient numerical methods for the enhancer. These methods must not degrade the properties of the numerical approximations for the drug concentration.

This talk will be focused on the mathematical modelling, numerical simulation and numerical analysis of drug delivery driven by exterior stimuli in different scenarios. Mathematical models and numerical methods will be discussed. Numerical results illustrating the behaviour of the models and the obtained theoretical results will be presented.

Keywords: drug delivery systems, stimuli, mathematical modelling, numerical methods

References

[1] J. A. Ferreira, H. Gómez, L. Pinto (2022). *A mathematical model for NIR light protocol optimization in controlled transdermal drug delivery*. Applied Mathematical Modelling, 112, 1–17.

[2] J. A. Ferreira, D. Jordão, L. Pinto (2022). *Drug delivery enhanced by ultrasound: mathematical modelling and simulation*. Computers and Mathematics with Applications, 107, 57–69.

[3] J. A Ferreira, P. de Oliveira, G. Pena, S. Silveira (2021). *Coupling nonlinear electric fields and temperature to enhance drug transport: an accurate numerical tool*. Journal of Computational and Applied Mathematics, 384, 113127.

[4] D. Rosenblum, N. Joshi, W. Tao, J. Karp, D. Peer (2018). *Progress and challenges towards targeted delivery of cancer therapeutics*. Nature Communications 9, 1410.

*Partially supported by the Centre for Mathematics of the University of Coimbra - UIDB/00324/2020, funded by the Portuguese Government through FCT/MCTES.

Controlled drug delivery enhanced by temperature

Elías Gudiño[1], J. A. Ferreira[2], M. Grassi[3], and P. de Oliveira[2]

[1]Department of Mathematics, Universidade Federal do Paraná, Curitiba, Brazil
[2]Department of Mathematics, Universidade de Coimbra, Coimbra, Portugal
[3]Department of Chemical Engineering, University of Trieste, Italy
egudino@ufpr.br.com

Abstract

Over the past few years, the therapeutic effects from Controlled Drug Delivery Devices (CDD) have clearly outperform the effects from Conventional Drug delivery Devices (DD). Advances in material science and bionanotechnology have helped in the development of more efficient CDD, improving targeted release and decreasing undesirable side effects, largely attributable to the nonspecific bio-distribution and uncontrollable characteristic of DD.

Stimuli-responsive biomaterials (polymers, lipids and inorganic materials) have been used extensively as drug carriers nanoplatforms, preventing drug extravasation into healthy tissues, prolong blood circulation time, improve drug accumulation, and enhance bioavailability at the target site. In this talk, we propose a novel mathematical model for drug delivery enhanced by temperature taking into consideration the Non-Fickian behavior of the material.

Keywords: Thermosensitive polymers, drug delivery, non-Fickian diffusion

References

[1] J. A. Ferreira, M. Grassi, E. Gudiño, P. de Oliveira (2015). *A new look to non-Fickian diffusion.* Appl. Math. Model. 39 (1), 194–204.

[2] J. A. Ferreira, P. de Oliveira, E. Silveira (2020). *Drug release enhanced by temperature: An accurate discrete model for solutions in h3.* Comput. Math. with Appl. 79, 852–875.

Solvability and numerical solution of a cross-diffusion cancer invasion model

Mario Fuest[1], Shahin Heydari[2], Petr Knobloch*[2], Johannes Lankeit[1], and Thomas Wick[1]

[1]Institute of Applied Mathematics, Leibniz University Hannover, Germany
[2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic
{fuest, lankeit, thomas.wick}@ifam.uni-hannover.de;
{heydari, knobloch}@karlin.mff.cuni.cz

Abstract

We consider a model of a malignant cancer invasion proposed in [3] that describes the cancer cell density $u = u(x,t)$, connective tissue $c = c(x,t)$, and protease $p = p(x,t)$ and consists of the equations

$$\begin{aligned} u_t &= \mu u(1-u) - \chi \nabla \cdot (u \nabla c) && \text{in } \Omega \times (0,T], \\ c_t &= -pc && \text{in } \Omega \times (0,T], \\ p_t &= \epsilon^{-1}(uc - p) && \text{in } \Omega \times (0,T], \end{aligned}$$

equipped with initial conditions and an appropriate boundary condition of Neumann type. In addition, we consider a variant of this model containing a diffusion term in the first equation for which we proved the global existence of classical solutions in [1]. Both models are discretized using the θ-method in time and conforming P_1 or Q_1 finite elements in space. A stabilization based on the flux-corrected transport approach [2] is considered that introduces an additional nonlinearity in the discrete problem. The computation of the approximate solutions is based on fixed-point iterations. We present several results on the solvability and the positivity-preservation property for both the nonlinear discrete problems and and their linearizations. Numerical results illustrate the theoretical findings and the properties of the models and their discretizations.

Keywords: Haptotaxis, Tumour invasion, Global existence, Flux-corrected transport, Positivity preservation, Fixed-point scheme, Numerical simulations

References

[1] M. Fuest, Sh. Heydari, P. Knobloch, J. Lankeit, T. Wick (2022). *Global existence of classical solutions and numerical simulations of a cancer invasion model*. arXiv.2205.08168.

[2] D. Kuzmin (2012). *Algebraic flux correction I. Scalar conservation laws*. In *Flux-corrected transport. Principles, algorithms, and applications*, eds.: D. Kuzmin, R. Löhner, and S. Turek, Springer, Dordrecht, 145–192.

[3] A.J. Perumpanani, J.A. Sherratt, J.Norbury, H.M. Byrne (1999). *A two parameter family of travelling waves with a singular barrier arising from the modelling of extracellular matrix mediated cellular invasion*. Phys. D, 126, 145–159.

*The work of P. Knobloch has been supported through the grant No. 22-01591S of the Czech Science Foundation.

Controlled Transdermal Drug Delivery

J.A. Ferreira[1], H.P. Gómez[1], and L. Pinto[1]

[1]University of Coimbra, CMUC, Department of Mathematics, Coimbra, Portugal
ferreira@mat.uc.pt; hugopena@mat.uc.pt; luisp@mat.uc.pt

Abstract

Near-infrared light-controlled transdermal drug delivery (NIRTDD) has lower systemic and local toxicity than traditional drug delivery methods, such as intravenous or direct injection at the target site. The initial laboratory results with this game-changing technology are promising. In [2], e.g., the authors used a NIRTDD-based strategy to treat mice bearing superficial breast tumors. The NIRTDD-treated mice had complete tumor eradication after seven days without adverse side effects. There was no tumor recurrence after 50 days. Within 16 days, all of the untreated mice died.

One key feature of NIRTDD is the ability to keep the drug concentration within its optimal therapeutic window by employing a proper near-infrared light protocol. The problem is that this ideal protocol is usually unknown. In this talk, we will present a computational tool aiming to solve this problem. The computational tool relies on an optimization problem that involves the numerical simulation of a two-dimensional NIRTDD mathematical model. In addition, for a generalized version of this mathematical model, we investigate the convergence and stability of a finite difference spatial scheme [1].

Keywords: Controlled drug delivery, Transdermal, NIR light, Optimization, Numerical simulation, Convergence analysis.

References

[1] J. A. Ferreira, H. P. Gómez, L. Pinto (2022). *A Mathematical Model for NIR Light Protocol Optimization in Controlled Transdermal Drug Delivery.* Appl. Math. Model., 112, 1–17.

[2] C. Mei-Chin, L. Zhi-Wei, L. Ming-Hung (2016). *Near-infrared light-activatable microneedle system for treating superficial tumors by combination of chemotherapy and photothermal therapy.* ACS Nano, 10, 93–101.

Modeling and Numerical Analysis of Doxorubicin Transport and Uptake in Tumors

Giuseppe Romanazzi[1] and Daniela C. Ospina[1]

[1]Department of Applied Mathematics, State University of Campinas, Brazil
{romam, danielac}@ime.unicamp.br

Abstract

Transport and uptake of a anticancer drug (doxorubicin) in tumors is here modeled by a system of nonlinear partial differential equations that describes the dynamics of the free drug concentration C_f, bound drug concentration C_b, tumor intracellular drug concentration C_i and density of tumor cells D_c. This model includes cell degradation and proliferation, as well as doxorubicin binding to proteins in a similar way of that proposed in [1].We treat in particular a spherical tissue domain of radius R containing a spherical tumor of radius $R_i < R$, using a radial symmetric initial condition for the drug concentrations and tumor density. The drug transport and uptake is modeled by the following initial boundary value problem in $(0, R) \times (0, T]$

$$
\begin{cases}
\dfrac{\partial C_f}{\partial t}(r,t) + \nabla \cdot (C_f(r,t)v(r)) = D_f \Delta C_f(r,t) + F(r,t,C_f,C_i,D_c) \quad \text{in} \quad (0,R)\times(0,T], \\
\dfrac{\partial C_b}{\partial t}(r,t) + \nabla \cdot (C_b(r,t)v(r)) = D_b \Delta C_b(r,t) + k_a C_f(r,t) - k_d C_b(r,t) \quad \text{in} \quad (R_i,R)\times(0,T], \\
\dfrac{\partial C_i}{\partial t}(r,t) = V_{max}\left(\frac{C_f(r,t)}{C_f(r,t)+k_e\varphi} - \frac{C_i(r,t)}{C_i(r,t)+k_i}\right), \quad \text{in} \quad (0,R_i)\times(0,T], \\
\dfrac{\partial D_c}{\partial t}(r,t) = \left(k_p - \frac{f_{max}C_i(r,t)}{C_i(r,t)+EC_{50}}\right) D_c(r,t) - k_m D_c^2(r,t), \quad \text{in} \quad (0,R_i)\times(0,T] \\
v(R)C_f(R,t) - D_f \frac{\partial C_f}{\partial r}(R,t) = 0, \ \frac{\partial C_f}{\partial r}(0,t) = 0, \quad t \in (0,T], \\
v(\tilde{R})C_b(\tilde{R},t) - D_b \frac{\partial C_b}{\partial r}(\tilde{R},t) = 0, \quad \tilde{R} \in \{R_i, R\}, \quad t \in (0,T], \\
C_f(r,0) = C_{f0}, \ C_b(r,0) = C_{b0}, \ C_i(r,0) = 0, \ D_c(r,0) = D_{c_0}, r \in (R_a, R_b)
\end{cases}
$$

where F is a nonlinear doxorubicin source term, D_f, D_b are non homogeneous diffusion coefficients and $v(r)$ is the interstitial fluid velocity given by a Darcy's law. Remaining parameters are constants described in [1]. This nonlinear system is solved by a H^1 second-order finite difference method on non-uniform grids. Its stability analysis is here discussed. Numerical results are then illustrated to highlight the effects of different initial drug conditions in the tumor density during the simulated time periods.

Keywords: Drug Transport, Drug Uptake, Finite Difference Method, Numerical Stability.

References

[1] W. Zhan, W. Gedroyc, X. Yun Xu (2014). *Mathematical modelling of drug transport and uptake in a realistic model of solid tumour.* Protein and peptide letters 11, 1146–-1156.

Challenges in modelling light propagation in the human cornea

Milene Santos *[1], Adérito Araújo[1], and Sílvia Barbeiro[1]

[1]Department of Mathematics, University of Coimbra, Portugal
{milene, alma, silvia}@mat.uc.pt

Abstract

Mathematical modeling and simulations of the light scattering in the human cornea have been a subject of growing interest during the past decades amongst physicists, basic scientists and ophthalmologists [1]. An understanding of the physical basis of corneal transparency has motivated the development of several mathematical models [2] since diseases affecting the cornea are a major cause of visual morbidity worldwide. In this talk, we discuss the mathematical modeling, the numerical challenges that arise from considering the cornea as a curved boundary domain and the numerical simulation of light scattering in the human cornea in order to mimic the real OCT imaging system. We propose a numerical method based on nodal discontinuous Galerkin methods [3] combined with a strategy that is specially designed to deal with curved domains [4] which arise naturally in our domain of interest for the application. Numerical tests with boundary conditions prescribed on curved boundaries show that this method is promising on allowing to achieve the optimal convergence order without relying on curved meshes.

Keywords: Light propagation, Cornea, Arbitrary curved boundaries, Discontinuous Galerkin method, Reconstruction for off-site data method

References

[1] R. A. Farrell, D. E. Freund, R. L. McCaly (1990). *Research on corneal structure.* Johns Hopkins APL Technical Digest (Applied Physics Laboratory), 11(1–2), 191–199.

[2] A. Araújo, S. Barbeiro, R. Bernardes et al (2022). *A mathematical model for the corneal transparency problem.* J.Math.Industry 12, 10.

[3] J. S. Hesthaven, T. Warburton (2008). *Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Applications.* New York: Springer-Verlag.

[4] R. Costa, S. Clain, R. Loubère, G.J. Machado (2018). *Very high-order accurate finite volume scheme on curved boundaries for the two-dimensional steady-state convection-diffusion equation with Dirichlet condition.* Applied Mathematical Modelling, 54, 752–767.

*This work was partially supported by the Centre for Mathematics of the University of Coimbra - UIDB/00324/2020, funded by the Portuguese Government through FCT/MCTES. M. S. acknowledges FCT for the support under the Ph.D. scholarship UI/BD/153816/2022.

A porous-elastic model for convection enhanced drug delivery: stability and numerical approximation

R. F. Santos[1], J. A. Ferreira[2], and L. Pinto[2]

[1]CEMAT-IST and Department of Mathematics, University of Algarve, Portugal
[2]University of Coimbra, CMUC, Department of Mathematics, Portugal
rsantos@ualg.pt; {ferreira, luisp}@mat.uc.pt

Abstract

Convection enhanced drug delivery (CED) is a technique used to make therapeutic agents reach, through a catheter, sites of otherwise difficult access. With this technique, a convective flow is originated by a pressure gradient induced at the tip of the catheter.This flow enhances passive diffusion allowing for a more efficient spread of the agents through the target site. CED is particularly useful in the treatment of diseases that affect the central nervous system, where the blood-brain barrier prevents the diffusion of most therapeutic agents from the brain blood vessels to the brain interstitial space.

In this work we deal with the numerical analysis of a coupled system of partial differential equations that may be used to simulate CED in an elastic medium like brain tissue. The model variables are the fluid velocity, the pressure, the tissue deformation and the agents concentration. We prove the stability of the coupled problem and, from the numerical perspective, we propose a fully discrete piecewise linear finite element method. We do a convergence analysis proving that the method has second order rate of convergence for the pressure, displacement and concentration. Results of numerical experiments showing both their agreement with the theoretical rates of convergence and the qualitative behavior of the system are presented.

Suggestions to improve the model are also stated.

Keywords: Convection enhanced drug delivery, Passive diffusion, Finite element method

References

[1] J. A. Ferreira, L. Pinto, R. F. Santos (2022). *Numerical analysis of a porous-elastic model for convection enhanced drug delivery.* J. Comp. Appl. Math., 399, 113719.

Simulation of the trajectory of respiratory particles in violent events and ventilation of spaces.

P. M. da Silva*[1,2], J.A. Ferreira[2], and Paula de Oliveira[2]

[1]Department of Physics and Mathematics, Polytechnic of Coimbra, ISEC, DFM, Rua Pedro Nunes, Coimbra, Portugal
[2]Centre of Mathematics of the University of Coimbra, Coimbra, Portugal
pascals@isec.pt; ferreira@mat.uc.pt; poliveir@mat.uc.pt

Abstract

In the recent context of the pandemic, studies on contamination and propagation of respiratory particles have become more relevant. Mathematical modeling of this type of phenomenon is a tool that enables the simulation of particle expulsion mechanisms and the monitoring of particle trajectories - allowing the definition of health and prevention policies with regard to contamination between individuals. There are several factors to take into account and several models of high complexity can be found in the literature. In this lecture we present a model that combines two phases - the air and the particles - as a whole. An estimate will be presented that depends on the factors that characterize the phenomenon and simulation results will be presented to compare the difference between light particles and heavy particles in violent expulsion events - such as coughing or sneezing.

Keywords: Respiratory Particles, Evaporation, Settling, Partial Differential Equations, Drift model, Estimates, Numerical Simulation

*Author 1 thanks the Centre for Mathematics of the University of Coimbra- UIDB/00324/2020, funded by the Portuguese Government through FCT/MCTES and the organizers of the mini-symposium: Diseases, Diagnosis, Treatment: Mathematical Modeling and Numerical Analysis for the invitation to participate

Analysis and application of a kinetic framework modeling the immune system interactions

Ana Jacinta Soares*[1]

[1]CMAT – Centre of Mathematics of the University of Minho, Braga, Portugal
ajsoares@math.uminho.pt

Abstract

The dynamics of the immune system can be studied using the kinetic theory approach, which provides a system of nonlinear integro-differential equations for the evolution of the cellular populations, when the biological activity of the cells is taken into account [1, 2]. The integral terms appearing in the equations describe the cellular interactions, which could preserve the number of cells or may contribute to proliferation or destruction of cells. Since the cellular interactions modify, not only the cellular dynamics, but also the global behaviour of the cellular populations, the kinetic model can be completed with a sort of continuity equations derived from the kinetic system, by integrating over the biological activity. The resulting macroscopic equations constitute an autonomous system of ODEs whose equilibrium states and stability properties give important information about the solution.

In this talk, we present a kinetic model and its corresponding macroscopic system underlying typical features of autoimmune diseases. We study the mathematical properties of the model and discuss interesting problems related to the chronicity of the disease, equilibrium states of the kinetic equations in connection to those of the macroscopic system, impact of drug therapies and how the model could be extended in order to admit formation of spatial patterns [3, 4, 5].

Some numerical results are shown to illustrate the analytical results and the dynamics of the model.

Keywords: Kinetic equations, Multicellular systems, Equilibrium, Stability

References

[1] M. Lachowicz (2005). *Micro and meso scales of description corresponding to a model of tissue invasion by solid tumors.* Math. Models Methods Appl. Sci., 15, 1667–1683.

[2] N. Bellomo, A. Bellouquid, M. Delitala (2008). *From the mathematical kinetic theory of active particles to multiscale modelling of complex biological systems.* Math. Comput. Modelling, 47, 687–698.

[3] R. Della Marca, M.P. Machado Ramos, C. Ribeiro, A.J. Soares (2022). *Mathematical modelling of oscillating patterns for chronic autoimmune diseases.* Math. Meth. Appl. Sci., 45, 7144–7161.

[4] J. Oliveira, M.P. Machado Ramos, C. Ribeiro, A.J. Soares (2023). *Equilibrium of a kinetic model of oscillating patterns for chronic autoimmune diseases.* Submitted.

[5] J. Oliveira, A. J. Soares, R. Travaglini (2023). *Kinetic models leading to pattern formation in the response of the immune system.* Accepted for publication in Rivista di Matematica dell'Università di Parma.

*The author thanks the support of FCT Projects UIDB/00013/2020 and UIDP/00013/2020 of CMAT-UM and FCT Project CoSysM3–2022.03091.PTDC.

Computational hemodynamics in vascular disease

Jorge Tiago*[1]

[1]Department of Mathematics and CEMAT, Instituto Superior Tẽcnico
jorge.tiago@tecnico.ulisboa.pt

Abstract

Computational Fluid Dynamics and Fluid-Structure Interaction approaches have proven to play an important in the understanding of vascular disease. The use of patient-specific information with such approaches opens the way for other uses such as diagnosis and prognosis. We will present several results considering the integration of patient-specific data for the improvement of reliability in hemodynamics analysis.

Keywords: Navier-Stokes equations, fluid-strucutre interaction, patient-specific

References

[1] N. El Khatib, O. Kafi, D. Oliveira, A. Sequeira, J. Tiago (2023) *A Numerical 3D fluid-structure interaction model for blood flow in a MRI-based atherosclerotic artery.* Math. Model. Nat. Phenom. Accepted.

[2] D. Oliveira, S. Aguiar Rosa, J. Tiago, A. Sequeira (2019). *Bicuspid aortic valve aorthopaties: a patient-specific modelling approach.* Computer Methods in Biomechanics and Biomedical Engineering, 22(8), 815–826.

[3] I. Marín-Gayte, J. Tiago, T. Guerra, (2023). *An optimal boundary control problem related to the Navier-Stokes equations in dimension 2 and 3.* Submitted.

*Author acknowledges FCT for the research project PTDC/MAT-APL/7076/2020.

MS38 - Optimal control and parameter estimation problems with applications in biomedicine

Optimal design of an estuarine water health monitoring network by means of optimal control techniques

Lino J. Alvarez-Vázquez*[1], Aurea Martínez[1], Carmen Rodríguez[2], and Miguel E. Vázquez-Méndez[3]

[1]Departamento Matemática Aplicada II, EI Telecomunicación, Universidade de Vigo, 36310 Vigo, Spain
[2]Departamento Matemática Aplicada, Facultad Matemáticas, Universidade de Santiago de Compostela, 15782 Santiago, Spain
[3]CITMAGA, 15782 Santiago de Compostela, Spain; and Departamento Matemática Aplicada, EPS, Universidade de Santiago de Compostela, 27002 Lugo, Spain
{lino,aurea}@dma.uvigo.es; {carmen.rodriguez,miguelernesto.vazquez}@usc.es

Abstract

In this work we propose a methodology to optimize the location of the sampling points for a water health monitoring network in an estuary, so that any unknown pathogen pollution episode can be identified (both in intensity and location) from data given by those sampling points [1]. The main aim of our research is presenting a novel approach to the problem of the optimal sampling points allocation within a simulation-based optimization framework. So, we formulate the optimal control problem as a bilevel optimization problem, where the upper-level problem concerns the finding of the optimal sampling locations which best determine a large set of random point source pollution episodes, and the lower-level problems correspond to the optimal identification of the many random pollution sources employed in the process. In the first case the minimization process is developed through a controlled random search procedure for global optimization, and in the second one by a linked simulation-optimization option, combining the gradient-free Nelder-Mead algorithm for the minimization step with a convection-diffusion-reaction system for the simulation step. Thus, after a detailed mathematical formulation of the problem, we present the full algorithm for its numerical solution. Finally, we show and analyze the results when applying above proposed technique to study a real case in *Ría de Vigo* (NW Spain) [2].

Keywords: Optimal control, Sampling points, Mathematical modeling, Simulation-based optimization

References

[1] R.O. Strobl, P.D. Robillard (2008). *Network design for water quality monitoring of surface freshwaters: A review.* J. Environ. Manag., 87, 639–648.

[2] L. J. Alvarez-Vázquez, A. Martínez, C. Rodríguez, M. E. Vázquez-Méndez (2023). *Optimizing the design of an estuarine water quality monitoring network by optimal control techniques.* Environ. Model. Assess. In press.

*This research was funded by Ministerio de Ciencia e Innovación (Spain) grant number TED2021-129324B-I00.

Optimal boundary control problem related to the time-dependent Navier-Stokes equations

Irene Marín Gayte[1,4], Telma Guerra[1,2], and Jorge Tiago[1,3]

[1]CEMAT, Instituto Superior Técnico, Universidade de Lisboa, Portugal
[2]Instituto Politécnico de Setúbal, Escola Superior de Tecnologia do Barreiro, Portugal
[3]Departamento de Matemática, Instituto Superior Técnico, Universidade de Lisboa, Portugal
[4]Departamento de Ecuaciones Diferenciales y Análisis Numérico, Universidad de Sevilla, Spain
imgayte@us.es; telma.guerra@estbarreiro.ips.pt; jorge.tiago@tecnico.ulisboa.pt

Abstract

Fluid control presents great challenges. Specifically, in this case, we seek to control a fluid representing blood flow. This is particularly relevant to the understanding of some cardiovascular diseases such as an aneurysm, an arterial obstruction, [1]. We present some results for the case of the Navier-Stokes equations. In fact, we solve a boundary optimal control problem for the evolutionary Navier-Stokes equations with mixed Dirichlet - total stress boundary conditions. Following previous work,[2, 3], we provide additional details about the theoretical and numerical study of the solution of the boundary control problem associated with the Navier-Stokes equations under more realistic assumptions.We provide a comprehensive theoretical framework to address the analysis of the optimal control problem related to this system and the derivation of a system of first-order optimality conditions that characterizes the solution of the control problem.

Keywords: Optimal control, partial differential equations, fluid dynamics, Navier-Stokes equations, boundary control.

References

[1] T. Guerra, A. Sequeira, J. Tiago (2015). *Existence of optimal boundary control for the Navier-Stokes equations with mixed boundary conditions*. Port Math 72, 267—283.

[2] M. D. Gunzburger, S. Manservisi (2000). *The velocity tracking problem for Navier-Stokes flows with boundary control*. SIAM J. Control Optim. 39, 594-–634.

[3] M. Hinze, K. Kunisch, *Second order methods for boundary control of the instationary Navier-Stokes system*. ZAMM-Journal of Applied Mathematics and Mechanics, Applied Mathematics and Mechanics. Vol. 84 (3), 171–187.

Optimal control of the Navier-Stokes equations with regularized directional do-nothing open boundary conditions

Pedro Nogueira*[1] and Ana Silvestre*[1]

[1]Department of Mathematics and CEMAT, Instituto Superior Técnico, Universidade de Lisboa, Portugal
pedro.mendes.nogueira@tecnico.ulisboa.pt, ana.silvestre@math.tecnico.ulisboa.pt

Abstract

In many Engineering [1] and Biomedicine [5] research problems, it is necessary to carry out complex fluid dynamics numerical simulations. Typically, the fluid domain is very large or complex, and so, appropriate truncations are necessary in order to reduce the computational cost of the simulations. This gives rise to the question: which boundary conditions should be imposed at the open boundaries, in order to obtain a more stable and reliable numerical simulation?

Inspired by the mathematical models proposed in [2, 3], where open Directional-Do-Nothing (DDN) boundary conditions are proposed for the Navier-Stokes equations, we consider a mixed boundary problem with nonhomogeneous Dirichlet boundary conditions combined with Neumann DDN condition.

Our first approach to this problem replaces the DDN condition by a Regularised-Directional-Do-Nothing (RDDN) condition [4]. In an appropriate functional framework, associated with a saddle point approach, we begin by establishing the well-posedness of the direct steady problem. Then a comparative study of the DDN and RDDN conditions yields a convergence result.

Lastly, we analyse an optimal control problem of velocity tracking-type by means of a distributed force or boundary control. We prove the existence of optimal solutions, justify the Gâteaux derivative of the control-to-state map and deduce the first order necessary conditions for optimality.

Our results are illustrated by some two-dimensional numerical experiments.

Keywords: Navier-Stokes equations, Open boundaries, Regularized DDN boundary condition, Boundary and Distributed control

References

[1] C. Bertoglio, A. Caiazzo, Y. Bazilevs, M. Braack, M. Esmaily, V. Gravemeier, A.L. Marsden, O. Pironneau, I.E. Vignon-Clementel, W.A. Wall (2018). *Benchmark problems for numerical treatment of backflow at open boundaries*. Int. J. Numer. Meth. Biomed. Engng. 34:e2918.

[2] M. Braack, P.B. Mucha (2014). *Directional do-nothing condition for the Navier-Stokes equations*. J. Comp. Math., 32(5), 507–521.

[3] C.-H. Bruneau, P. Fabrie (1994). *Effective downstream boundary conditions for incompressible Navier-Stokes equations*. Int. J. Numer. Meth. Fluids, 19, 693–705.

[4] S. Dong (2015). *A convective-like energy-stable open boundary condition for simulations of incompressible flows*. J. Comput. Phys., 302, 300–328.

[5] A. Manzoni, A. Quarteroni, S. Salsa (2019). *A saddle point approach to an optimal boundary control problem for steady Navier-Stokes equations*. Mathematics in Engineering, 1(2), 252-280.

*The authors acknowledge the financial support of Fundação para a Ciência e a Tecnologia, through the projects UIDB/04621/2020 and UIDP/04621/2020 of CEMAT/IST-ID and project MAT-PTDC/MAT-APL/7076/2020.

Sensitivity analysis for incompressible Navier-Stokes equations

Nathalie Nouaime[1,2], Bruno Després[2], Maria Adela Puscas[1], and Camilla Fiorini[3]

[1]Université Paris-Saclay, CEA, Service de Thermo-hydraulique et de Mécanique des Fluides, F-91191, Gif-sur-Yvette, France
[2]LJLL, Sorbonne Université, Paris, France
[3]M2N, Conservatoire National des Arts et Métiers, Paris, France
nathalie.nouaime@cea.fr

Abstract

The Navier-Stokes equations are a system of PDEs which are nonlinear and involve second-order derivatives of the fluid velocity, making them difficult to solve analytically. Our present study focuses on sensitivity analysis for the Navier-Stokes equations [**?**], with an emphasis on the stability estimate of the discretised first-order sensitivity of the Navier-Stokes equations. Let Ω denote an open bounded subset of $\mathbb{R}^2$, the incompressible Navier-Stokes equations are

$$\begin{cases} \partial_t \mathbf{u}(\mathbf{x},t) - \nu\Delta\mathbf{u}(\mathbf{x},t) + (\mathbf{u}(\mathbf{x},t).\nabla)\mathbf{u}(\mathbf{x},t) + \nabla p(\mathbf{x},t) = \mathbf{f}(\mathbf{x},t) & \Omega,\ t>0, \\ \nabla.\mathbf{u}(\mathbf{x},t) = \mathbf{0} & \Omega,\ t>0, \\ \mathbf{u}(\mathbf{x},0) = \mathbf{0} & \Omega,\ t=0, \\ \mathbf{u}(\mathbf{x},t) = \mathbf{0} & \text{on} \quad \Gamma=\partial\Omega,\ t>0. \end{cases} \tag{1}$$

where $\mathbf{u} = (u^x, u^y)$ is the velocity, p the pressure, $\mathbf{f}$ the external force.
Sensitivity analysis studies how changes in the input of a model affect the output. This task can be performed in many different ways, depending on the nature of the model considered. The present study focuses on sensitivity analysis of incompressible Navier–Stokes equations (**??**) using the polynomial chaos method [**?**]. First, the first-order sensitivity of the Navier-Stokes equations is defined. A finite element-volume [**?**] numerical scheme for the Navier-Stokes equations is proposed. This discretisation is integrated into the open-source industrial code TrioCFD [**?**] promoted by the CEA. Second, the finite element-volume discretisation is extended to the first-order sensitivity Navier-Stokes equations; the most significant point is the discretisation of the non linear term. Finally, a stability estimate for the continuous and discrete Navier-Stokes equations is established.

Keywords: Sensitivity analysis, Navier-Stokes, polynomial chaos method, finite element-volume method

Reconstruction of flow domain boundaries from velocity data via multi-step optimization of distributed resistance

Ondřej Pártl[1], Ulrich Wilbrandt[1], Alfonso Caiazzo[1], and Joaquín Mura[2]

[1]Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany
[2]Departamento de Ingeniería Mecánica, Universidad Técnica Federico Santa María, Santiago, Chile
ondrej.partl@wias-berlin.de; ulrich.wilbrandt@wias-berlin.de;
alfonso.caiazzo@wias-berlin.de; joaquin.mura@usm.cl

Abstract

We will present an algorithm published in [1] for reconstructing the unknown shape of a flow domain using partially available internal velocity measurements.

This inverse problem is motivated by applications in cardiovascular imaging where motion-sensitive protocols, such as phase-contrast MRI, can be used to recover three-dimensional velocity fields inside blood vessels. In this context, the information about the domain shape serves to quantify the severity of pathological conditions, such as vessel obstructions.

We consider a flow modeled by a linear Brinkman problem with a fictitious resistance accounting for the presence of additional boundaries. To reconstruct these boundaries, we employ a multi-step gradient-based variational method to compute a resistance that minimizes the difference between the computed flow velocity and the available data. Afterward, we apply different post-processing steps to reconstruct the shape of the internal boundaries.

We will show how our algorithm performs when applied to three-dimensional examples based on synthetic velocity data and using realistic geometries obtained from cardiovascular imaging.

Keywords: Brinkmann equation, gradient-based optimization, stabilized finite elements, boundary reconstruction

References

[1] O. Pártl, U. Wilbrandt, J. Mura, A. Caiazzo (2023). *Reconstruction of flow domain boundaries from velocity data via multi-step optimization of distributed resistance*. Computers & Mathematics with Applications, 129, 11–33.

Opytimal - A Python/FEniCS framework to solve PDE-based optimal control problems considering multiple controls in 2D and 3D domains

Quintino, N.*[1] and Tiago, J.[2]

[1,2]Center for Computational and Stochastic Mathematics, IST/ULisboa
{natanaelquintino, jorge.tiago}@tecnico.ulisboa.pt

Abstract

Opytimal is a Python/FEniCS framework to solve PDE-based optimization problems considering multiple controls. That problems can consider mixed boundary conditions on n-dimensional domains, for $n \in \{1, 2, 3\}$, and be solved using distributed and boundary controls simultaneously with the possibility of the use H^1 norm in the cost functional. Those problems can be solved by the gradient descent method or in an all at once system. Will be shown examples considering the Poisson, Heat and Stokes equations.

Keywords: Optimal control, FEniCS, Partial differential equations, Mixed boundary, Multiple controls

References

[1] A. Logg and G. N. Wells (2010). *DOLFIN: Automated Finite Element Computing*, ACM Trans. on Math. Soft., 37.

[2] A. Manzoni, A. Quarteroni, S. Salsa(2021). *Optimal Control of Partial Differential Equations - Analysis, Approximation, and Applications*. Springer, Switzerland.

[3] M. D. Gunzburger (2003). *Perspective in flow control and optimization*. Siam, Philadelphia.

*This work was supported by the Fundação para a Ciência e a Tecnologia (FCT)

A continuum active structure model for the interaction of cilia with a viscous fluid

Astrid Decoene[1], Sébastien Martin[2], and Fabien Vergnet[3]

[1]Université de Bordeaux, France
[2]Université Paris Cité, France
[3]Sorbonne Université & Inria Paris, France
[3]astrid.decoene@math.u-bordeaux.fr; sebastien.martin@u-paris.fr;
fabien.vergnet@sorbonne-universite.fr

Abstract

Cilia and flagella are motile elongated structures, involved in swimming and/or transport mechanisms that arise in many living organisms. Flagella are used by micro-swimmers such as sperm-cells or bacteria for motility purpose at low Reynolds number, while cilia are involved in the transport of proteins, nutrients or dust inside bigger organisms. At the origin of all these mechanisms are two essential ingredients: the capacity for cilia and flagella to modify their shapes by generating internal stresses and the strong reciprocal interaction with the surrounding fluid.

Both aspects have been studied in several works, with very different strategies. Cilia can either be modeled as 1D elastic structures with self-oscillatory [1] and sliding regulation mechanisms [2] or as 3D structures with a discrete representation of their internal biological components [3]. In the first case, the coupling with the surrounding 3D fluid is often taken into account (numerically) with the slender body theory [4]. In the second case, the fluid-structure interaction is well resolved but the (discrete) model for cilia is not suitable for the mathematical analysis and introduces many parameters that may not be accessible in experiments.

Unlike all previous works on cilia and flagella, we propose a model that fits in the framework of continuum mechanics. In the context of 2D or 3D elasticity, the model is based upon the definition of a suitable Piola-Kirchoff tensor mimicking the action of the internal components that induce the motility of the structure. Moreover, the framework of continuum mechanics enables to fully consider the strong interaction with the surrounding fluid. During this presentation, we will show that the present model is suitable for both the mathematical study and the numerical simulation of fluid-structure interaction problems involving active structures and low Reynold number flows. We shall also discuss the question of the identification of the internal activity.

Keywords: Active structures, Fluid-structure interaction problems, Mucociliary transport, Optimal control

References

[1] C. J. Brokaw (2005). *Computer simulation of flagellar movement IX. Oscillation and symmetry breaking in a model for short flagella and nodal cilia.* Cell Motility and the Cytoskeleton, 60(1).

[2] D. Oriola, H. Gadeêlha, J. Casademunt (2017). *Nonlinear amplitude dynamics in flagellar beating.* Royal Society Open Science, 4(3).

[3] , S. Mitran (2007). *Metachronal wave formation in a model of pulmonary cilia.* Computers & Structures, 85(11).

[4] B. Chakrabarti, D. Saintillan (2019). *Spontaneous oscillations, beating patterns, and hydrodynamics of active microfilaments.* Physical Review Fluids, 4(4).

MS39 - Numerical methods for nonlinear and coupled processes (flow, reactive transport and deformation) in porous media

A high order, finite volume, multilevel WENO scheme for multidimensional problems

Todd Arbogast[*1], Chieh-Sen Huang[†2], and Chenyu Tian[1]

[1]Oden Institute for Computational Engineering and Sciences, Univ. of Texas at Austin
[2]Department of Applied Mathematics, National Sun Yat-sen University
arbogast@oden.utexas.edu; huangcs@math.nsysu.edu.tw; chenyu@ices.utexas.edu

Abstract

We develop a novel and general framework for solving partial differential equations (PDEs) using finite volume weighted essentially non oscillatory (WENO) techniques on general computational meshes. Such techniques are able to handle both advective and (degenerate) diffusive behavior, even when the solution develops shocks or steep fronts. We resolve three fundamental issues. First, polynomial approximations on general stencils of mesh elements can be of poor quality, even for what appear to be geometrically nice stencils. We present a robust and efficient procedure for producing accurate stencil polynomial approximations. Second, the classic smoothness indicator can be quite expensive to compute in multiple space dimensions. We define an efficient smoothness indicator based on the polynomial coefficients. Third, most current WENO reconstructions can combine only stencil polynomials of exactly two different degrees, which restricts the types of stencil polynomials that can be used and also effectively precludes using single element (constant polynomial) stencils. We develop a novel and efficient finite volume, multilevel WENO (ML-WENO) reconstruction that combines stencil polynomial approximations of various degrees. The nonlinear weighting biases the reconstruction away from both inaccurate oscillatory polynomials of high degree (i.e., those crossing a shock or steep front) and smooth polynomials of low degree, thereby selecting the smooth polynomial(s) of maximal degree of approximation. We apply these ideas to develop a finite volume scheme for solving two-phase flow in porous media.

Keywords: weighted essentially non-oscillatory, stencil polynomial, smoothness indicator, ML-WENO, hyperbolic, degenerate elliptic

References

[1] T. Arbogast, Ch.-S. Huang, Chenyu Tian. *A Finite Volume Multilevel WENO Scheme for Multidimensional Problems*. In preparation.

[2] T. Arbogast, Ch.-S. Huang, Xikai Zhao (2019). *Finite volume WENO schemes for nonlinear parabolic problems with degenerate diffusion on non-uniform meshes*. J. Comput. Phys., 399(108921). http://dx.doi.org/10.1016/j.jcp.2019.108921

[3] T. Arbogast, Ch.-S. Huang, Xikai Zhao (2018). *Accuracy of WENO and adaptive order WENO reconstructions for solving conservation laws*. SIAM J. Numer. Anal., 56(3), 1818–1847. http://dx.doi.org/10.1137/17M1154758

[*]This author was supported in part by the U.S. National Science Foundation grant DMS-1912735.
[†]This author was funded by the Taiwan Ministry of Science and Technology grant MOST 109-2115-M-110-003-MY3 and the National Center for Theoretical Sciences, Taiwan.

Structure preserving discontinuous Galerkin approximation of dynamic poroelasticity

Markus Bause[1], Mathias Anselmann[1], and Sebastian Franz[2]

[1]Faculty of Mechanical and Civil Engineering, Helmut Schmidt University Hamburg
[2]Institute of Scientific Computing, Technical University Dresden
{bause,anselmann}@hsu-hh.de; sebastian.franz@tu-dresden.de

Abstract

Discontinuous Galerkin (DG) space-time finite element methods (STFEMs) feature the natural construction of (higher order) discretization schemes for hyperbolic and parabolic partial differential equations and coupled systems of these equations. DG-STFEMs offer the potential to inherit most of the rich structure of the continuous problem [4], while maintaining stability, and achieve accurate results on computationally feasible grids. However, the efficient solution of the arising algebraic systems with complex block structure continues to remain a challenging task [1, 2].

We present and analyse a structure preserving family of DG-STFEMs for a four-field formulation of the dynamic Biot system, modeling poro- and thermoelasticity,

$$\rho\partial_t^2\boldsymbol{u} - \nabla\cdot(\boldsymbol{C}\boldsymbol{\varepsilon}(\boldsymbol{u})) + \alpha\boldsymbol{\nabla}p = \rho\boldsymbol{f}\,, \qquad c_0\partial_t p + \alpha\nabla\cdot\partial_t\boldsymbol{u} - \nabla\cdot(\boldsymbol{K}\nabla p) = g\,. \tag{1}$$

For this, equations (1) are rewritten as a first-order in space and time system such Picard's abstract solution theory [5] for evolutionary problems becomes applicable; cf. [3]. The construction of the DG approach and its error analysis are built on this first-order system formulation and its abstract solution theory. Optimal order error estimates and their proofs are presented. The efficient solution of the algebraic system with block structure of growing complexity for higher order polynomial degrees in time is addressed. An universally applicable geometric multigrid preconditioning technique [1, 2] based on a patchwise local Vanka smoother is proposed. For a three-field approximation of (1), the performance of the algebraic solver is illustrated by challenging 3d benchmark studies [2].

Keywords: Hyperbolic-parabolic, Picard's theorem, error estimates, discontinuous Galerkin method, multigrid

References

[1] M. Anselmann, M. Bause (2023). *A geometric multigrid method for space-time finite element discretizations of the Navier–Stokes equations and its application to 3d flow simulation.* ACM Trans. Math. Softw., 49(5), 1–25. https://doi.org/10.1145/3582492; arXiv:2107.10561.

[2] M. Anselmann, M. Bause, N. Margenberg, P. Shamko (2023). *An energy-efficient GMRES–Multigrid solver for space-time finite element computation of dynamic poro- and thermoelasticity.* Comput. Mech., pp. 1–30. Submitted. arXiv:2303.06742.

[3] M. Bause, S. Franz (2023). *Structure preserving discontinuous Galerkin approximation of coupled hyperbolic-parabolic systems.* In progress, pp. 1–22.

[4] S. Franz, S. Trostorff, M. Waurick (2019). *Numerical methods for changing type systems.* IMA J. Numer. Anal., 39, 1009–1038.

[5] R. Picard (2009). *A structural observation for linear material laws in classical mathematical physics.* Math. Methods Appl. Sci., 32, 1768–1803.

Numerical analysis of a mixed-dimensional poromechanical model with frictionless contact at matrix–fracture interfaces

Francesco Bonaldi[1], Jérôme Droniou[2], and Roland Masson[3]

[1]Laboratoire de Modélisation Pluridisciplinaire et Simulations, Université de Perpignan Via Domitia, France
[2]School of Mathematics, Monash University, Victoria 3800, Australia
[3]Université Côte d'Azur, Inria, CNRS, Laboratoire J.A. Dieudonné, team Coffee, Nice, France
francesco.bonaldi@univ-perp.fr; jerome.droniou@monash.edu; roland.masson@univ-cotedazur.fr

Abstract

We present a complete numerical analysis for a general discretization of a coupled flow–mechanics model in fractured porous media, considering single-phase flows and including frictionless contact at matrix–fracture interfaces, as well as nonlinear poromechanical coupling. Fractures are described as planar surfaces, yielding the so-called mixed- or hybrid-dimensional models. Small displacements and a linear elastic behavior are considered for the matrix. The model accounts for discontinuous fluid pressures at matrix–fracture interfaces in order to cover a wide range of normal fracture conductivities.

The numerical analysis is carried out in the Gradient Discretization framework, encompassing a large family of conforming and nonconforming discretizations. The convergence result also yields, as a by-product, the existence of a weak solution to the continuous model. A numerical experiment in 2D is presented to support the obtained result, employing a Hybrid Finite Volume scheme for the flow and second-order finite elements ($\mathbb{P}_2$) for the mechanical displacement coupled with face-wise constant ($\mathbb{P}_0$) Lagrange multipliers on fractures, representing normal stresses, to discretize the contact conditions.

Keywords: poromechanics, discrete fracture matrix models, contact mechanics, Darcy flow, discontinuous pressure model, Gradient Discretization Method, convergence analysis.

Efficient and robust computation of speciation in aqueous solution

Ibtihel Ben Gharbia[1], Clément Cancès[2], Thibault Faney[1], Maxime Jonval[2,1], and Quang-Huy Tran[1]

[1]IFP Energies nouvelles, France
[2]Inria, Univ. Lille, CNRS, UMR 8524 – Laboratoire Paul Painlevé
{ibtihel.ben-gharbia, thibault.faney, quang-huy.tran}@ifpen.fr;
{clement.cances, maxime.jonval}@inria.fr

Abstract

The computation of chemical equilibria in aqueous solution is a long-standing problem having many applications, among which reactive transport in porous media. Given prescribed quantities of several atoms and a list of possible chemical reactions, one aims at computing the minimiser of the Gibbs free energy under the constraint of the conservation of the atoms. The Euler Lagrange equations then reduce to some relations on the chemical potentials in addition to the constraint on the quantities of each species. Despite the problem is quite standard from a theoretical point of view [2], naive methods face severe robustness issues. We present two approaches to mitigate these difficulties. Building on ideas of [1], a first approach consists in finding a suitable parametrization of the monotone relation between the fluid composition and the chemical potentials. The second approach, referred to as cartesian representation, relaxes this monotone along the Newton iterations by introducing variables both for the fluid composition and the chemical potentials.

Keywords: Chemical speciation, Newton method, parametrization, cartesian representation

References

[1] K. Brenner, C. Cancès (2017). *Improving Newton's method performance by parametrization: the case of Richards equation*. SIAM J. Numer. Anal., 55, 1760–1785.

[2] W. R. Smith, R. W. Missen (1982). *Chemical Reaction Equilibrium Analysis: Theory and Algorithms*. Wiley series in chemical engineering. John Wiley and Sons.

A robust two-level overlapping preconditioner for Darcy flow in high-contrast porous media

Eric Chung[1], Changqing Ye[1], and Shubin Fu[2]

[1]Department of Mathematics, The Chinese University of Hong Kong, Hong Kong SAR
[2]Eastern Institute for Advanced Study, China
{tschung, cqye}@math.cuhk.edu.hk; shubinfu@eias.ac.cn

Abstract

In this talk, we present a two-level overlapping domain decomposition preconditioner for solving linear algebraic systems obtained from simulating Darcy flow in high-contrast media. Our preconditioner starts at a mixed finite element method for discretizing the partial differential equation by Darcy?s law with the no-flux boundary condition and is then followed by a velocity elimination technique to yield a linear algebraic system with only unknowns of pressure. Then, our main objective is to design a robust and efficient domain decomposition preconditioner for this system, which is accomplished by engineering a multiscale coarse space that is capable of characterizing high-contrast features of the permeability field. A generalized eigenvalue problem is solved in each non-overlapping coarse element in a communication-free manner to form the global solver, which are accompanied by local solvers originated from additive Schwarz methods but with a non-Galerkin discretization to derive the two-level preconditioner. We provide a rigorous analysis indicating that the condition number of the preconditioned system could be bounded above with several assumptions. Extensive numerical experiments with various types of three-dimensional high-contrast models are exhibited. In particular, we study the robustness against the contrast of the media as well as the influences of numbers of eigenfunctions, oversampling sizes, and subdomain partitions on the efficiency of the proposed preconditioner. Besides, strong and weak scalability performances are also examined. The work is partially supported by the Hong Kong RGC General Research Fund (Projects: 14305222 and 14304021).

Keywords: Porous media, multiscale method, preconditioner

$\mathbb{P}^1$-bubble VEM method for a mixed-dimensional poromechanical model with frictional contact at matrix-fracture interfaces

Jérôme Droniou[1], Guillaume Enchéry [2], Isabelle Faille[3], Ali Haidar [*] [†] [4], and Roland Masson[‡] [5]

[1]Monash University
[2,3]IFPEN
[4,5] Côte d'Azur University, CNRS, Inria, LFAD
jerome.droniou@monash.edu; {guillaume.enchery, isabelle.faille}@ifpen.fr; {ali.Haidar, roland.Masson}@univ-cotedazur.fr

Abstract

In this work, we design and study a polytopal discretization of a coupled flow–mechanics model in fractured porous media, considering single-phase flows and including frictional contact at matrix–fracture interfaces. Our discretization combines a Hybrid Finite Volume (HFV) scheme for the fluid with a Virtual Element Method (VEM) for the contact-mechanics. Precisely, we investigate a $\mathbb{P}^1$-bubble VEM approach in order to ensure the discrete version of the *inf-sup* stability property on matrix–fracture interfaces. The contact mechanics model accounts for the poromechanical equilibrium equation with a Biot linear elastic constitutive law and a frictional contact model at matrix–fracture interfaces which will be described as planar surfaces, yielding the so-called mixed-dimensional models. Virtual bubble functions will be added on these fractures, which results in a new modified discrete VEM scheme ($\mathbb{P}^1$-bubble VEM) without violating the consistency and stability properties for the numerical scheme. The numerical method is then validated by evaluating the rates of convergence of the numerical scheme on analytical solution for the mechanical model. Finally, the method is assessed by some poromechanical test cases simulating the injection of the CO2 in a faulted reservoir.

Keywords: Poromechanical coupling, Contact mechanics model, frictional contact at matrix–fracture interfaces, virtual element method, virtual bubble functions

References

[1] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, A. Russo (2013). *Basic principles of virtual element methods.* Mathematical Models and Methods in Applied Sciences.

[2] J. Coulet, I. Faille, Isabelle, V. Girault, N. Guy , F. Nataf (2020). *A fully coupled scheme using virtual element method and finite volume for poroelasticity.* Computational Geosciences.

[3] F. Bonaldi, J. Droniou, R. Masson (2022). *Numerical analysis of a mixed-dimensional poromechanical model with frictionless contact at matrix-fracture interfaces.* ArXiv preprint.

[*] Centre national de la recherche scientifique (CNRS)
[†] Institut national de recherche en informatique et en automatique (Inria).
[‡] Institut français du pétrole énergies nouvelles (IFPEN).

Guaranteed, efficient, and robust a posteriori estimates for nonlinear elliptic/parabolic problems with applications in porous media flow

Koondanibha Mitra*[1] and Martin Vohralík[2,3]

[1]Faculty of Sciences, Hasselt University, Belgium
[2]INRIA Paris, France
[3]CERMICS, ENPC, France
koondanibha.mitra@uhasselt.be; martin.vohralik@inria.fr

Abstract

We firstly consider strongly monotone and Lipschitz-continuous nonlinear elliptic problems. We apply a finite element discretization in conjunction with an iterative linearization such as the fixed-point scheme or the Newton scheme. In this setting, we derive a posteriori error estimates that are robust with respect to the ratio of the continuity over monotonicity constants in the dual energy norm invoked by the linearization iterations. This is linked to an orthogonal decomposition of the total error into a linearization error component and a discretization error component, which can be further used to adaptively stop the linearization iterations for efficient error balancing. The applications cover diverse physical phenomena such as flow through porous media, mean curvature flow, and biological processes. Numerical experiments for the time-discrete Richards equation illustrate the theoretical results.

The results are further generalized to the Richards equation which is a nonlinear advection-reaction-diffusion (parabolic) equation exhibiting both parabolic-hyperbolic and parabolic-elliptic kinds of degeneracies. Reliable, fully computable, and locally space-time efficient a posteriori error bounds for numerical approximations of the fully degenerate Richards equation are derived by introducing a novel degeneracy estimator, time-integrated norms, and using the maximum principle. The estimates are also valid in a setting where iterative linearization with inexact solvers is considered. Numerical tests are conducted for nondegenerate and degenerate cases having exact solutions, as well as for a realistic case. It is shown that the estimators correctly identify the errors up to a factor of the order of unity.

Keywords: Iterative linearization, a posteriori estimators, nonlinear elliptic/parabolic problems, Richards equation

References

[1] K. Mitra, M. Vohralík (2021). *A posteriori error estimates for the Richards equation.* arXiv preprint arXiv:2108.12507.

*K. Mitra thanks FWO postdoctoral fellowship

A Lattice Boltzmann Method for Darcy- and Biot-Type Models

Stephan B. Lunowa[1], Natalia Nebulishvili[1], and Barbara Wohlmuth[1]

[1]School of Computation, Information and Technology, Technical University of Munich,
85748 Garching bei München, Germany
{luno, nebulish, wohlmuth}@cit.tum.de

Abstract

Poroelastic materials are commonly found in our environment, including living tissues, soils, and manufactured materials. Understanding the interaction between solids and fluids in these complex systems is of significant interest both for modeling and numerical simulation, as it can provide insight into their behavior and enable applications across a wide range of scales, from cell mechanics to hydrogeology. While Darcy's law is a common model to describe the flow in porous media, we employ the generalized Navier-Stokes equations for this purpose [1], as it includes all fluid, and solid drag forces, with Darcy's flow identified as a limiting case. It also allows us to extend the model to the Biot-type systems to describe the flow in deformable porous media. Biot's quasi-static theory of poroelasticity is a common model to describe the coupled system of the porous media deformation and the fluid flow through it. Typically, this system consists of linear elasticity for the skeletal deformations and Darcy's law for the flow in porous media, which is substituted by the above-mentioned generalized Navier-Stoked equations. In contrast to the commonly used finite element methods (FEM), we employ a lattice Boltzmann method (LBM) for the Darcy-type model [2] mentioned above and then couple it with the one for the linear elastic solids [3], which results into a new LBM for Biot-type system. We utilize the multi-relaxation-time (MRT) LBM for the elastic part of the system and apply a single-relaxation-time (SRT) LBM for the flow in porous media. By employing MRT-LBM we can adjust material parameters of linear elasticity independently and directly retrieve the Cauchy stress components from the second-order moments. In order to perform the validation of the methods, we first compare the simulation results of the LBM for the flow in porous media to the one in the fully resolved structure, which shows good agreement with each other and accredits us for further experiments for coupled LBMs. We present the numerical comparisons to analytical solutions of the system and to the simulation results obtained using FEM. While the proposed lattice Boltzmann method is currently applied to 2D systems, we aim to extend the approach to 3D cases in future work.

Keywords: Biot system, Poroelasticity, Lattice Boltzmann method, Porous media, Coupled system

References

[1] P. Nithiarasu, K.N. Seetharamu, T. Sundararajan (1997). *Natural convective heat transfer in a fluid saturated variable porosity medium.* Int. J. Heat Mass Transf., 40, 3955-3967

[2] Z. Guo and T. S. Zhao (2002). *Lattice Boltzmann model for incompressible flows through porous media.* Phys. Rev. E 66, 036304.

[3] O. Boolakee, M. Geier, L. De Lorenzis (2023). *A new lattice Boltzmann scheme for linear elastic solids: periodic problems.* Comput. Methods Appl. Mech. Engrg., 404, 15756

Coupled flow and energy models in permafrost with ice wedges

M. Peszynska [1], Zachary Hilliard[1], and Naren Vohra[1]

[1]Department of Mathematics, Oregon State University
[1]mpesz@math.oregonstate.edu; {hilliarz, vohran}@oregonstate.edu

Abstract

Numerical analysis for coupled systems faces challenges adding to those for the individual components as in thermal-flow coupled model in [1] which we generalize to nonlinear heat conduction with convection coupled to water flow in permafrost soil containing ice wedges described by

$$\partial_t w - \nabla \cdot (k\nabla\theta) + \nabla \cdot (c\theta q_f) = 0, \quad (1)$$

$$\partial_t(\gamma\eta S) + \nabla \cdot q_f = 0,\ q_f = -\frac{\kappa}{\mu}\kappa_r(S)(\nabla P - \rho G \nabla D) \quad (2)$$

solved for temperature θ, enthalpy w, pressure P and water flux q_f, and water fraction S. In (1)–(2) η is the the nonnegative porosity coefficient, μ is the viscosity, κ is the symmetric uniformly positive definite permeability tensor; the coefficients c, γ are positive. The system is closed with nonlinear relationships: (i) monotone piecewise smooth $w = \alpha(\theta)$; $S = \chi(\theta)$, (ii) $k = k(S)$ which is positive and bounded, and (iii) $k_r = k_r(S)$ which is nonnegative but potentially degenerate as $S \downarrow 0$. The data $\alpha, \chi, \kappa, k, \kappa_r$ can be obtained by upscaling from heterogeneous Stefan problem at the pore-scale, or obtained empirically. Development of (1)–(2) with upscaling extends [4, 2].

The solutions θ, S are expected to have low regularity typical for free boundary problems. Following [4] we apply P0-RT$_{[0]}$ to (1) and implicit-explicit time stepping, and the standard mixed P0-RT$_{[0]}$ approach for (2). The presence of ice wedges features Darcy scale heterogeneity of the nonlinear properties $S = \chi(x;\theta)$; these add to the difficulties encountered for the linear heat conduction discussed in [1], e.g., the formal lack of control of convective term. We revisit these challenges in practical scenarios, and evaluate efficiency and accuracy of variants of algorithms with focus on the choice of primary unknowns, solver, and time-stepping for the coupling. We also propose a practical solution to the complexity of upscaling following the off-line probabilistic strategies we introduced in [3].

Keywords: Free boundary problems, Darcy flow with buoyancy, coupled system, pore-scale to Darcy scale modeling

References

[1] C. Bernardi, S. Dib, V. Girault, F. Hecht, F. Murat, T. Sayah. *Finite element methods for Darcy's problem coupled with the heat equation.* Numerische Mathematik 139, 315–348.

[2] T. Costa, K. Kennedy, M. Peszynska (2018). *Hybrid three-scale model for evolving pore-scale geometries.* Computational Geosciences 22, 925–950. https://doi.org/10.1007/s10596-018-9733-9 2018

[3] M. Peszynska, J. Umhoefer, C. Shin (2021). *Reduced Model for Properties of Multiscale Porous Media with Changing Geometry.* Computation, 9(3), 28, 1–44.

[4] L. Bigler, M. Peszynska, N. Vohra (2022). *Heterogeneous Stefan problem and permafrost models with P0-P0 finite elements and fully implicit monolithic solver.* Electronic Research Archive 30, 1477–1531. doi: 10.3934/era.2022078

Efficient splitting schemes for coupled problems

Florin Adrian Radu[1]

[1]Department of Mathematics, University of Bergen, Norway
florin.radu@uib.no

Abstract

In this work we consider solving coupled partial differential equations (PDEs) by splitting schemes. There are plenty of relevant applications behind, e.g. CO2 sequestration, enhanced geothermal energy extraction, nuclear waste management or water and soil pollution. We will start with linear, coupled PDEs and classical splitting schemes (fixed-stress type [5]) as appear e.g. in the Biot model for poromechanics. We will briefly discuss the most important questions concerning splitting: optimization, stabilization (convergence) and acceleration [3, 4, 7]. The acceleration will be based on Anderson accelleration [1]. Its additional stabilization effect will be discussed [4]. Further, non-linear extensions of coupled PDEs will be considered [2]. In this case splitting and linearization are combined. Finally, a new family of splitting schemes based on approximate Schur complement will be presented [6].

Keywords: Coupled problems, Biot equations, Splitting schemes, Anderson acceleration, Stabilization, Linearization

References

[1] D.G. Anderson (1965). *Iterative procedures for nonlinear integral equations*, JACM, 12(4), 547–560.

[2] J.W. Both, N. Barnafi, F.A. Radu, P. Zunino, A. Quarteroni (2022). *Iterative splitting schemes for a soft material poromechanics model*. CMAME, 388, 114183.

[3] J.W. Both, M. Borregales, J.M. Nordbotten, K. Kumar, F.A. Radu (2017). *Robust fixed stress splitting for Biot´s equation in heterogeneous media*. Applied Math. Letters 68, 101–108.

[4] J.W. Both, K. Kumar, J.M. Nordbotten, F.A. Radu (2019). *Anderson accelerated fixed-stress splitting schemes for consolidation of unsaturated porous media*, CAMwA 77, 1479–1502

[5] K. Kim, H. Tchelepi, R. Juanes (2011). *Stability and convergence of sequential methods for coupled flow and geomechanics: Fixed-stress and fixed-strain splits*. CMAME, 200, 1591–1606.

[6] R. Nuca, E. Storvik, F.A. Radu, M. Icardi (2023). *Splitting Schemes for Coupled Differential Equations: Block Schur-Based Approaches and Partial Jacobi Approximation*. Submitted (also ArHiv 2212.11111).

[7] E. Storvik, J. W. Both, K. Kumar, J.M. Nordbotten, F.A. Radu (2019). *On the optimization of the fixed-stress splitting for Biot's equations*. IJNME, 120, 179–194.

A posteriori error estimates for the STDGM for solving the Richards equation

Hyun-Geun Shin[1] and Vít Dolejší[1]

[1]Charles University Prague, Faculty of Mathematics and Physics
dolejsi@karlin.mff.cuni.cz

Abstract

We deal with the numerical solution of the Richards equation describing a variably saturated/unsaturated flow through porous media. The Richards equation is a nonlinear parabolic equation which can degenerate either to an elliptic equation or to a system of ordinary differential equations. In [1], we solved the Richards equation by the space-time discontinuous Galerkin method (STDGM) which provides high order approximation with respect to space and time. The presented numerical experiments demonstrated a potential of this approach in combination with adaptive mesh refinement. However, the used adaptive technique in [1] has not been based on a rigorous a posteriori error estimates.

In this contribution, we deal with a posteriori error analysis of the solution of the Richards equation by STDGM. We adopt the approach from [2] based on spatial and temporal flux reconstructions. The spatial flux reconstruction uses known techniques from [3, 4], see also [5, 6]. The temporal one is based on a reconstruction taken into account the jumps with respect to the time.

We present the upper and lower error bounds justifying the reliability and effectivity of the method. The theoretical results are demonstrated by numerical experiments. We also mention some open problems related to this topic.

Keywords: A posteriori error estimates, space-time discontinuous Galerkin method, Richards equation

References

[1] V. Dolejší, M. Kuráž, P. Solin (2019). *Adaptive Higher-Order Space-Time Discontinuous Galerkin Method for the Computer Simulation of Variably-Saturated Porous Media Flows.* Appl. Math. Model., 72, 276–305.

[2] V. Dolejší, F. Roskovec, M. Vlasák (2021). *A posteriori error estimates for higer order space-time Galerkin discretizations of nonlinear parabolic problems.* SIAM J. Numer. Anal., 59, 1486–1509.

[3] V. Dolejší, A. Ern, M. VohralíK (2013). *A framework for robust a posteriori error control in unsteady nonlinear advection-diffusion problems.* SIAM J. Numer. Anal., 51, 773–793.

[4] A. Ern, M. Vohralík (2015) *Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations.* SIAM J. Numer. Anal., 53, 1058–1081.

[5] R. Verfürth (2013). *A posteriori error estimation techniques for finite element methods.* Oxford University Press.

[6] R. Nochetto, A. Schmidt (2000). *A posteriori error estimation and adaptivity for degenerate parabolic problems.* Math. Comput., 69, 1–24.

Computational orders of convergence for Richards equation

Nicolae Suciu[1], Florin A. Radu[2], Jakob S. Stokke[2], Emil Cătinaş[1], and Andra Malina[1]

[1]Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy, Romania
[2]Center for Modeling of Coupled Subsurface Dynamics, University of Bergen, Norway
{nsuciu, ecatinas, andra.malina}@ictp.acad.ro; {jakob.stokke, florin.radu}@uib.no

Abstract

The convergence of an arbitrary sequence of real numbers $x_k \to x^* \in \mathbb{R}$ is characterized by the behavior of the successive absolute values of the errors $e_k = |x^* - x_k|$. A sequence converges with the (classical) C-order $p > 1$ if (see [2] and the references therein)

$$\lim_{k\to\infty} \frac{e_{k+1}}{(e_k)^p} = Q_p \in (0, \infty), \tag{1}$$

which implies the (weaker) Q-order p, attained when

$$\lim_{k\to\infty} \frac{\ln e_{k+1}}{\ln e_k} = p. \tag{2}$$

If the limit x^* of the sequence is not known, the replacing of the errors e_k by the corrections $s_k = |x_{k+1} - x_k|$ leads to the equivalent computational convergence orders in a straightforward manner when $p > 1$, but the analysis is more tricky when $p = 1$ (as the convergence orders of errors and corrections are not anymore equivalent, as one may not take $p = 1$ in Eq. (1), etc).

Nonlinear problems for Richards equation are solved with iterative schemes. Successive correction norms, e.g., $\|\psi^{k+1} - \psi^k\| = x_k$ for the pressure head, form a sequence $\{x_k\}$ of positive real numbers that can be analyzed with general methods for convergent sequences [2]. We analyzed in this way Newton-Picard- and L-schemes [3] used in implicit finite element approaches [5] and L-schemes used in explicit finite difference and random walk approaches [4], with or without Anderson acceleration [1].

Assuming the convergence of the linearization schemes, which also can be proved theoretically under certain conditions [5], the limit x^* of the sequence $\{x_k\}$ vanishes. Therefore, we used both errors e_k and correction s_k to verify the C-convergence with Eq. (1) and to compute convergence orders p with Eq. (2) and we found a good agreement of the two approaches. We also found that Anderson acceleration reduces the number of iterations needed to reach the desired tolerance and the estimate of Q_p in Eq. (1) for the linearly convergent Picard- and L-schemes, while it has little influence on the Newton scheme.

Keywords: Orders of convergence, Richards equation, Linearization

References

[1] D.G. Anderson (1965). *Iterative procedures for nonlinear integral equations.* JACM, 12(4), 547–560.

[2] E. Cătinaş (2021). *How many steps still left to x*?.* SIAM Rev., 63(3), 585–624.

[3] F. List, F. A. Radu (2016). *A study on iterative methods for solving Richards' equation.* Comput. Geosci. 20(2), 341–353.

[4] N. Suciu, D. Illiano, A. Prechtel, F. A. Radu (2021). *Global random walk solvers for fully coupled flow and transport in saturated/unsaturated porous media.* Adv. Water Resour. 152, 103935.

[5] J. S. Stokke, K. Mitra, E. Storvik, J. W. Both, F. A. Radu (2023). *An adaptive solution strategy for Richards' equation.* https://arxiv.org/abs/2301.02055.

MS40 - Multi-scale mathematical modeling of human diseases

Variable size player game theory and the evolution of eusociality

Fabio Chalub*[1,2] and Matheus Hansen[2]

[1]Department of Mathematics, NOVA SST
[2] Center for Mathematics and Applications (NOVA Math), NOVA SST.
facc@fct.unl.pt

Abstract

Traditional game theory considers a fixed number of players. In this talk, we will discuss games in which the number of players is not defined a priory. We show the existence of the best strategy in finite and infinite populations, study the fixation probability, metastable and stable equilibria and discuss some relevant examples.

Keywords: Game theory; Wright-Fisher process; Evolution

*This work is funded by national funds through the FCT - Fundação para a Ciência e a Tecnologia, I.P., under the scope of the projects UIDB/00297/2020 and UIDP/00297/2020 (Center for Mathematics and Applications).

Modelling Self–organization or Disorder

Miroslaw Lachowicz*[1]

[1]Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Poland
M.Lachowicz@mimuw.edu.pl

Abstract

I am going to show, that the blow–ups of solutions, that usually are treated as *something "very bad"*, can in fact describe some *self–organization* phenomena, "positive" (like healing) or "negative" (like society polarization) — [1, 2]. Mathematically it is the theory of integro–differential equations (*kinetic equations*) that is applied to processes in Social Sciences (opinion formation) — [6], Economics ("lemons and cherries" theory) — [7], Biology (DNA denaturation) — [4], Medicine (tendon healing process) — [5] and the redistribution in a lift — [3].

Keywords: Kinetic equations, Integro–differential equations, Self–organization, Disorder

References

[1] M. Lachowicz, H. Leszczyński, M. Parisot (2016). *A simple kinetic equation of swarm formation: Blow–up and global existence*, Appl. Math. Letters, 57, 104-107.

[2] M. Lachowicz, H. Leszczyński, M. Parisot (2017). *Blow–up and global existence for a kinetic equation of swarm formation*, Math. Models Methods Appl. Sci., 27, 1153-1175.

[3] M. Dolfin, M. Lachowicz, A. Schadschneider (2018). *A Microscopic Model of Redistribution of Individuals Inside an "Elevator"*. In *Modern Problems in Applied Analysis*, eds.: P. Dryga and S. Rogosin. Trends in Mathematics, Springer Nature 2018, 77–86.

[4] M. Dębowski, M. Lachowicz, Z. Szymańska (2019). *Microscopic description of DNA thermal denaturation*, Appl. Math. Computation, 361, 47–60.

[5] G. Dudziuk, M. Lachowicz, H. Leszczyński, Z. Szymańska (2019). *A simple model of collagen remodeling*, Discrete Contin. Dyn. Syst. Ser. B, 24, 2205–2217.

[6] M. Lachowicz, H. Leszczyński, E. Puźniakowska–Gałuch (2019). *Diffusive and anti–diffusive behavior for kinetic models of opinion dynamics*, Symmetry, 11, 1024.

[7] M. Lachowicz, H. Leszczyński (2020). *Modeling asymmetric interactions in economy*, Mathematics, 8, 523–537.

*ML is happy to acknowledge the support from the New Ideas Grant — "Kinetic Equations in Description of Self–organization Phenomena" funded by the Excellence Initiative Research University Programme, Poland.

Epidemiological data assimilation for the assessment of the COVID 19 vaccination campaign in Italy

Damiano Pasetto[1], Enrico Bertuzzo[1], Lorenzo Mari[2], Stefano Miccoli[2], Renato Casagrandi[2], Stefano Merler[3], Marino Gatto[2], and Andrea Rinaldp[4,5]

[1]University Ca' Foscari of Venezia, Venice, Italy
[2]Politecnico di Milano, Milan, Italy
[3]Bruno Kessler Foundation, Trento, Italy
[4]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
[5]University of Padova, Padova, Italy
damiano.pasetto@unive.it

Abstract

The pandemic of SARS-CoV-2 that in few years caused more than 6'000'000 deaths worldwide prompted an urgency for the development of accurate epidemiological models to better understand the ongoing epidemic dynamics, anticipate the next phases of the pandemic, and analyse the impact of the implemented intervention strategies.

This talk will show how data assimilation, which is largely used in forecasting, is a fundamental tool to dynamically estimate the key parameters in compartmental-based epidemiological models. In particular, we consider a spatially-explicit model for the spread of SARS-CoV2 in Italy, which is based on a network of local communities connected by human mobility fluxes [1, 2]. In each community, disease transmission is described by a cascade of compartments that includes ad hoc infectious stages relevant to COVID-19 transmission dynamics and for describing the vaccination campaign [3]. The tracking of changes in the model parameters through an iterative particle filter [4] allows accounting for region-specific mobility restrictions during lockdown, presence of new variants, and possible behavioural change as a response to containment efforts and increased awareness. These kind of models are essential to produce quantitative estimates of the impact of the ongoing vaccination campaign and compute optimal vaccination strategies [4].

Keywords: Epidemiological model, Covid-19 epidemic in Italy, Iterative Particle Filtering, Data Assimilation

References

[1] M. Gatto, E. Bertuzzo, L. Mari, et al. (2020). *Spread and dynamics of the COVID-19 epidemic in Italy: Effects of emergency containment measures.* Proc Natl Acad Sci U S A. 12;117(19), 10484–10491. doi: 10.1073/pnas.2004978117.

[2] E. Bertuzzo, L. Mari, D. Pasetto, et al. (2020). *The geography of COVID-19 spread in Italy and implications for the relaxation of confinement measures.* Nat Commun 11, 4264, doi: 10.1038/s41467-020-18050-2.

[3] L. Mari, R. Casagrandi, E. Bertuzzo, et al. (2021). *The epidemicity index of recurrent SARS-CoV-2 infections.* Nat Commun 12, 2752 https://doi.org/10.1038/s41467-021-22878-7.

[4] J. C. Lemaitre, D. Pasetto, M. Zanon, et al. (2022). *Optimal control of the spatial allocation of COVID-19 vaccines: Italy as a case study.* PLOS Computational Biology 18(7): e1010237.doi: 10.1371/journal.pcbi.1010237.

Complex network near-synchronization for Lotka-Volterra predator-prey models

Cristiana J. Silva [*1, 2] and Guillaume Cantin[3]

[1]Department of Mathematics, ISCTE - Lisbon University Institute (ISCTE-IUL), Portugal
[2]Center for Research and Development in Mathematics and Applications (CIDMA), University of Aveiro, Portugal
[3]Laboratoire des Sciences du Numérique de Nantes, University of Nantes, France
cristiana.joao.silva@iscte-iul.pt; guillaume.cantin@univ-nantes.fr

Abstract

A complex network is proposed to model a heterogeneous geographical habitat of species which is perturbed by an anthropic extension, being fragmented in several patches, where the fragmentation is likely to alter the equilibrium of the ecological system. The complex network is constructed by coupling several patches on which interacting wild species are living and where, for each patch, the ecological inter-species dynamics are modeled by a Lotka-Volterra predator-prey model with Holling type II functional response. An important feature of the complex network is that each patch can admit its own dynamic and migrations of biological individuals in space, between each component of the fragmented environment, are taken into account by coupling the patches of the network. We prove sufficient conditions for the near-synchronization of the complex network, which guarantees that the complex network remains in a neighborhood of a synchronization state, provided the coupling strength is strong enough, even if the local behaviors are non-identical. This result allows us to modify the local dynamic of extinction of the species, by increasing the couplings with patches on which persistence, with or without oscillations, is ensured.

Keywords: Complex network, Non-identical systems, Near-synchronization.

References

[1] G. Cantin, C. J. Silva (2022). *Complex network near-synchronization for non-identical predator-prey systems*, AIMS Mathematics, 7(11), 19975-19997.

*This work was partially supported by Portuguese funds through CIDMA, The Center for Research and Development in Mathematics and Applications of University of Aveiro, and the Portuguese Foundation for Science and Technology (FCT–Fundação para a Ciência e a Tecnologia), within projects UIDB/04106/2020 and 2022.03091.PTDC.

Spatio-temporal models for immunological disorders leading to pattern formation

Romina Travaglini[1,2]

[1]Department of Mathematical, Physical and Computer Sciences, University of Parma, Italy
[2]Centre of Mathematics, University of Minho, Portugal
b13201@math.uminho.pt

Abstract

The study of systems involving a huge number of interacting agents (as particles, cells or individuals) can be described, at mesoscopic level, by means of kinetic equations [1]. We use these tools with the aim of extending the existing studies of anomalous immune response [2] in a spatio-temporal framework [3]. More precisely, we present a system of integro-differential equations that describes, on the one hand, interactions among different populations of human cells and, on the other hand, motion of immune cells stimulated by cytokines. We show how, assuming that processes considered occur at different time scales, it is possible to perform a formal hydrodynamic limit, obtaining macroscopic reaction-diffusion equations for the number densities of the constituents with a chemotaxis term. We then apply the procedure to a particular case of autoimmune disease, represented by Multiple Sclerosis. Finally, we study the system obtained, inquiring about the formation of spatial patterns (reproducing brain lesions characteristic of the pathology) through a Turing instability analysis of the problem and basing the discussion on microscopic parameters of the model.

Keywords: Kinetic theory, Multicellular systems, Chemotaxis, Turing instability, Pattern formation

References

[1] N. Bellomo, C. Bianca, M. Delitala (2009). *Complexity analysis and mathematical tools towards the modelling of living systems.* Phys. Life Rev., 6(3), 144-175.

[2] R. Della Marca, M. P. D. Machado Ramos, C. Ribeiro, A. J. Soares (2022). *Mathematical modelling of oscillating patterns for chronic autoimmune diseases.* Math.l Meth. Appl. Sci., 45(11), 7144–7161.

[3] J. Oliveira, A. J. Soares, R. Travaglini. *Kinetic models leading to pattern formation in the response of the immune system.* Special Issue of Rivista di Matematica dell'Università di Parma in memory of Giampiero Spiga. Accepted for publication

An integral boundary fractional model to the world population growth

Om Kalthoum Wanassi*[1] and Delfim F. M. Torres[1]

[1]Center for Research and Development in Mathematics and Applications (CIDMA), Department of Mathematics, University of Aveiro
{om.wanassi, delfim}@ua.pt

Abstract

We consider a fractional differential equation of order α, $\alpha \in (2, 3]$, involving a ψ-Caputo fractional derivative subject to initial conditions on function and its first derivative and an integral boundary condition that depends on the unknown function. As an application, we investigate the world population growth. We find an order α and a function ψ for which the solution of our fractional model describes given real data better than available models.

Keywords: ψ-Caputo fractional differential equations; integral boundary conditions; population growth model.

References

[1] O. K. Wanassi, D. F. M. Torres (2023). *An integral boundary fractional model to the world population growth*. Chaos Solitons Fractals, 168, Art. 113151, 4.

[2] Z. Baitiche, C. Derbazi, M. Benchohra (2020). *ψ-Caputo fractional differential equations with multi-point boundary conditions by topological degree theory*. Res. Nonlinear Anal. 3(4), 167–178.

[3] R. Almeida (2017). *What is the best fractional derivative to fit data?*. Appl. Anal. Discrete Math., 11(2), 358–368.

[4] R. Almeida (2017). *A Caputo fractional derivative of a function with respect to another function*. Commun. Nonlinear Sci. Numer. Simul., 44, 460–481.

[5] United Nations (1999). *The World at Six Billion Off Site*. Table 1, World Population From Year 0 to Stabilization, 5.

*The Center for Research and Development in Mathematics and Applications (CIDMA) and the Portuguese Foundation for Science and Technology (FCT), projects UIDB/04106/2020 and UIDP/04106/2020.

Fully 3D spatio-temporal resolved models of virus replication evaluated at realistic reconstructed cell geometries

Markus M. Knodel[1], Arne Nägel[2], Eva Herrmann[3], and Gabriel Wittum[4]

[1]Simulation in Technology, TechSim, Ölbronn-Dürrn, Germany
[2]MSQC, Universität Frankfurt a.M., Germany
[3]IBMM, Universität Frankfurt a.M., Germany
[4]MaS, CEMSE, KAUST, Saudi-Arabia
markus.knodel@techsim.org

Abstract

Virus pandemics and endemics cause enormous pain and costs. While the Covid19 pandemics induced obvious damages, the "silent" Hepatitis C virus (HCV) infection induced liver destruction is the main reason for liver transplants. HCV-generated virus genome replication factories are housed within virus-induced intracellular structures termed membranous webs (MW) which are derived from the Endoplasmatic Reticulum (ER). The ER is an interconnected intracellular membrane network. Our framework aims to mirror in vitro / in vivo experiments by means of fully spatio-temporal resolved diffusion-reaction partial differential equation (PDE) models describing the intracellular HCV viral RNA (vRNA) replication cycle. Our first qualitative model described the major components of virus replication by means of surface PDEs (sufPDEs) [3], as major processes are restricted to the 2D ER manifold. To improve the model, we introduced population dynamics inspired diffusion and reaction coefficients and different aggregate states for the components [1]. The combination of these new concepts with spatial resolution provoked questions for advanced experiments. Based on experimental data, we estimated the diffusion coefficient of a major viral protein [2]. Presently, we are merging effects restricted to 2D manifolds with others taking place in the full 3D volume. We couple sufPDEs with PDEs and use realistic coefficients to approach to quantitative reliable simulations. All simulations are performed at geometries which we reconstructed based on experimental data. Our simulations help understanding the relation of form and function of intracellular virus replication mechanisms. In the long run, our framework might help to facilitate the systematic development of efficient direct antiviral agents and vaccines.

Keywords: Computational virology; intracellular virus replication; PDEs; diffusion-reaction models; realistic reconstructed geometries; unstructured grids; vertex centered Finite Volumes; massively parallel multigrid solvers

References

[1] M. M. Knodel, P. Targett-Adams, A. Grillo, E. Herrmann, G. Wittum (2019). *Advanced Hepatitis C Virus Replication PDE Models within a Realistic Intracellular Geometric Environment.* Int. J. Environ. Res. Public Health, 16(3), 513. doi:10.3390/ijerph16030513

[2] M. M. Knodel, A. Nägel, S. Reiter, A. Vogel, P. Targett-Adams, J. McLauchlan, E. errmann, G. Wittum (2018). *Quantitative Analysis of Hepatitis C NS5A Viral Protein Dynamics on the ER Surface.* Viruses, 10, 28. doi:10.3390/v10010028

[3] M. M. Knodel, S. Reiter, P. Targett-Adams, A. Grillo, E. Herrmann, G. Wittum (2017). *3D Spatially Resolved Models of the Intracellular Dynamics of the Hepatitis C Genome Replication Cycle.* Viruses, 9, 282. doi:10.3390/v9100282

MS41 - Finite Element Methods for Constrained Problems

Least-squares finite elements for distributed optimal control problems

Thomas Führer[*1] and Michael Karkulik[†2]

[1]Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Santiago, Chile
[2]Departamento de Matemática, Universidad Técnica Federico Santa María, Valparaíso, Chile
tofuhrer@mat.uc.cl; michael.karkulik@usm.cl

Abstract

We present results of our recent work [2] where we introduce a framework for the numerical approximation of distributed optimal control problems with constraints imposed on the control. We derive and analyze a variational inequality where the PDE part is tackled by least-squares finite element methods [1]. The corresponding bilinear form is coercive. A reliable and efficient a posteriori error estimator based on a least-squares functional is derived for problems where box constraints are imposed on the control. It can be localized and therefore used to steer an adaptive algorithm. The abstract framework is applicable to a wide range of problems, including scalar second-order PDEs, the Stokes problem, and parabolic problems on space-time domains. We conclude the talk by presenting numerical examples for some selected problems.

Keywords: least-squares FEM, optimal control problem, variational inequality, a posteriori, parabolic equation

References

[1] P. Bochev, M. Gunzburger (2009). *Least-Squares Finite Element Methods*. Applied Mathematicas Sciences Vol. 166, Springer.

[2] T. Führer, M. Karkulik (2022). *Least-squares finite elements for distributed optimal control problmes*. In *arXiv.org* 2210.16377 (preprint).

[*]supported by ANID through FONDECYT project 1210391.
[†]supported by ANID through FONDECYT project 1210579.

Error estimates for a pointwise tracking optimal control problem of a semilinear elliptic equation

Alejandro Allendes*[1], Francisco Fuica†[2], and Enrique Otárola‡[1]

[1]Departamento de Matemática, Universidad Técnica Federico Santa María, Valparaíso, Chile
[2]Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna 4860, Santiago, Chile
{alejandro.allendes, francisco.fuica, enrique.otarola}@usm.cl

Abstract

We consider a pointwise tracking optimal control problem for a semilinear elliptic partial differential equation. We derive the existence of optimal solutions and analyze first and, necessary and sufficient, second order optimality conditions. We devise two strategies of discretization to approximate a solution of the optimal control problem: a semidiscrete scheme where the control variable is not discretized (the so-called variational discretization approach) and a fully discrete scheme where the control variable is discretized with piecewise constant functions. For both solution techniques, we analyze convergence properties of discretizations and derive error estimates.

Keywords: Optimal control, Semilinear equations, Dirac measures, Error estimates

References

[1] N. Behringer, D. Meidner, B. Vexler(2019). *Finite element error estimates for optimal control problems with pointwise tracking.* Pure Appl. Funct. Anal.,4, 177–204.

[2] E. Casas (2008). *Necessary and sufficient optimality conditions for elliptic control problems with finitely many pointwise state constraints.* ESAIM Control Optim. Calc. Var., 14, 575–589.

[3] E. Casas, M. Mateos (2017). *Optimal control of partial differential equations.* In *Computational mathematics, numerical analysis and applications*, SEMA SIMAI Springer Ser., Springer, Cham, Vol. 13, 3–59.

*The first author is partially supported by ANID through FONDECYT project 1210729.
†The second author is supported by ANID through FONDECYT postdoctoral project 3230126.
‡The third author is partially supported by ANID through FONDECYT project 1220156.

Nitsche-based finite element method for dynamic unilateral contact problems

Hao HUANG[1,2], Nicolas PIGNET[1], Guillaume Drouet[1], and Franz Chouly[2,3,4]

[1]ERMES, EDF Lab Paris-Saclay, France
[2]Institut de Mathématiques de Bourgogne, Université de Bourgogne Franche-Comté, France
[3]Center for Mathematical Modeling and Department of Mathematical Engineering, University of Chile and IRL 2807 - CNRS, Chile
[4]Departamento de Ingeniería Matemática, CI^{2}MA, Universidad de Concepción, Chile
{hao.huang, nicolas.pignet, guillaume.drouet}@edf.fr; franz.chouly@u-bourgogne.fr

Abstract

One of the main tools for numerical simulation for solid mechanic problems is the finite element method. In the industry, contact problems are omnipresent, and many traditional methods cannot provide acceptable solutions in the context of elastodynamics: they are too influenced by parasitic oscillations or do not conserve energy. A difficulty is that this type of problem has a non-linear boundary condition on the displacement field. The main existing methods for discretizing the Signorini contact conditions are the method of penalization, mixed/mortar methods, Nitsche's method, or the augmented Lagrangian method. Improvements in the accuracy and numerical robustness of these simulations are always expected by industry and researchers.

Usually, the time-space discretization involves the problems of choosing: (i) the finite element space; (ii) the enforcement of the contact condition, and (iii) the time-stepping scheme.

In this work, we focus on the evolution of the impact of an elastic body and a rigid obstacle. We want particularly to study how to combine time-marching schemes as HHT-α and TR-BDF2 schemes with contact via Nitsche's method, and its stability and convergence. We present then some simulation results with 1D and 3D benchmarks using different methods. By testing their performances, we are particularly interested in the influence of the numerical parameters, the parasitic oscillation associated with the contact surface due to the discontinuity in time, and the conservation or not of the total energy for the time-marching schemes. The new combinations applied in this work can eventually improve upon existing methods by providing better accuracy and numerical robustness for non-linear (and non-regular) dynamic problems.

Keywords: contact problem, Nitsche's method, finite elements, time-marching schemes.

References

[1] Hao Huang, Nicolas Pignet, Guillaume Drouet, Franz Chouly (2023). *HHT-α and TR-BDF2 schemes for dynamic contact problems.* ⟨hal-04021471v2⟩

Inf-sup condition of the $P^1_{nc} - (P^0 + P^1)$ mixed finite element

Erell Jamelot[1], Patrick Ciarlet, Jr[2], and Stefan Sauter[3]

[1]Université Paris-Saclay, CEA, Service de Thermo-hydraulique et de Mécanique des Fluides, 91191 Gif-sur-Yvette cedex, France
[2]POEMS, CNRS, INRIA, ENSTA Paris, Institut Polytechnique de Paris, 91120 Palaiseau, France
[3]Institut für Mathematik, Universität Zürich, Winterthurerstr 190, CH-8057 Zürich, Switzerland
[1]erell.jamelot@cea.fr; patrick.ciarlet@ensta-paris.fr; stas@math.uzh.ch

Abstract

There are different methods to solve Stokes problem. One of the most popular low order method is the nonconforming Crouzeix-Raviart mixed finite element method [1, Example 4], for which the discrete velocity is piecewise affine, continuous in the barycentre of the faces (let us say $\mathbf{P}^1_{nc}$); and the discrete pressure is piecewise constant, P^0. This method introduces some consistency error that may perturb the discrete velocity, which can lead to a non-physical solution when solving the Navier-Stokes equations, especially when the source field is a strong gradient. There are different cures, such that building a divergence free subspace of the discrete velocity space [4] or projecting the test function in the source term on some $\mathbf{H}(\mathrm{div})$-conforming space [6]. In the TrioCFD code [2, 5, 3], the discrete pressure space is generated by P^1-Lagrange plus P^0 basis functions. This leads to the $\mathbf{P}^1_{nc} - (P^0 + P^1)$ mixed finite element method. This method shows interesting numerical results. However, only an incomplete proof of inf-sup condition is available in [5, 3]. Our goal here is to gather and to clarify the evidence to exhibit the inf-sup condition. We will show that this finite element method shows accurate results in 2D. We will give numerical results to illustrate its efficiency.

Keywords: Stokes problem, nonconforming Crouzeix-Raviart finite element, inf-sup condition, pressure robust discretization

References

[1] M. Crouzeix, P.-A. Raviart (1973). *Conforming and nonconforming finite element methods for solving the stationary Stokes equations*, RAIRO, Sér. Anal. Numer., 7(33), 33–75.

[2] P. Emonot (1992). *Méthode de volumes éléments finis : applications aux équations de Navier-Stokes et résultats de convergence*. PhD thesis, Université Claude Bernard - Lyon I, France.

[3] T. Fortin (2006). *Une méthode éléments finis à décomposition* $\mathbf{L^2}$ *d'ordre élevé motivée par la simulation d'écoulement diphasique bas Mach*. Université Pierre et Marie Curie - Paris VI.

[4] F. Hecht (1981). *Construction d'une base de fonctions* P_1 *non conforme à divergence nulle dans* $\mathbb{R}^3$. RAIRO, Sér. Anal. Numér., 15(2), 119–150.

[5] S. Heib (2003). *Nouvelles discrétisations non structurées pour des écoulements de fluides à incompressibilité renforcée*. PhD thesis, Université Pierre et Marie Curie - Paris VI, France.

[6] A. Linke (2014). *On the Role of the Helmholtz-Decomposition in Mixed Methods for Incompressible Flows and a New Variational Crime*. Comput. Methods Appl. Mech. Engrg., 268, 782–800.

Recent extensions of efficient numerical iterative solvers for constrained variational phase-field fracture problems

Leon M. Kolditz[1], Thomas Wick[1,2], and Katrin Mang[3]

[1]Institute of Applied Mathematics, Leibniz Universität Hannover, Germany
[2]Université Paris-Saclay, LMPS - Laboratoire de Mecanique Paris-Saclay
[3]Institute of Structural Analysis, Leibniz Universität Hannover, Germany
{kolditz, wick}@ifam.uni-hannover.de

Abstract

In phase-field fracture simulation, a constraint variational inequality system, derived from the Francfort-Marigo energy functional [1] has to be solved. This problem is challenging due to two difficulties: Firstly, we have nonlinearities, which need to be treated. Secondly, it includes an inequality constraint that represents the irreversibility condition. The crucial nonlinearity can be resolved using an extrapolation depending on previous solutions to obtain a convex problem. The constraint can be treated with a primal-dual active set method. In a contribution from 2015 [2], Timo Heister, Mary Wheeler and Thomas Wick introduced a concept for solving phase-field fracture problems with a primal-dual active set method and the concept of extrapolation, which were later included in the `pfm-cracks` code from 2020 [3]. Combined with a Newton method for solving the nonlinear phase-field fracture problem, we obtain a solution algorithm which seeks to minimize the Newton residual while achieving convergence in the active set at the same time. This implementation has two drawbacks: on the one hand, the extrapolation leads to time-lagging fracture growing phenomena. On the other hand, the active set reveals slow convergence within the solution method. In this talk, we present an iteration on the extrapolation in order to iterate the problem to the monolithic limit. This neglects the time-lagging phenomena. Furthermore, three different suggestions for performance enhancements based on adjusting a constant, which takes a role during the computation of the active set. With a performance study, we substantiate the ideas by considering several quasi-static benchmarks in two or three dimensions.

Keywords: Phase-field fracture, complementarity system, primal-dual active set, modified Newton's method

References

[1] G.A. Francfort, J.-J. Marigo (1998). *Revisiting brittle fracture as an energy minimization problem.* Journal of the Mechanics and Physics of Solids, Vol. 8.

[2] T. Heister, M.F. Wheeler, T. Wick (2015). *A primal-dual active set method and predictor-corrector mesh adaptivity for computing fracture propagation using a phase-field approach.* Computer Methods in Applied Mechanics and Engineering, Vol. 290.

[3] T. Heister, T. Wick (2020). *pfm-cracks: A parallel-adaptive framework for phase-field fracture propagation.* Software Impacts, Vol. 6.

The augmented Lagrangian method as a framework for stabilised methods in computational mechanics

Erik Burman[1], Peter Hansbo[2], and Mats G. Larson[3]

[1]Department of Mathematics, University College London, UK
[2]Department of Mechanical Engineering, Jönköping University, Sweden
[3]Department of Mathematics and Mathematical Statistics, Umeå University, Sweden
mats.larson@unu.se

Abstract

In this talk, we present recent advances [1] in applying the augmented Lagrange multiplier method as a general approach for generating multiplier–free stabilized methods. The augmented Lagrangian method consists of a standard Lagrange multiplier method augmented by a penalty term, penalising the constraint equations, and is well known as the basis for iterative algorithms for constrained optimization problems. However, its use as a stabilization method in computational mechanics has only recently been appreciated. We first show how the method generates Galerkin/Least Squares type schemes for equality constraints and how it can be extended to develop new stabilized methods for inequality constraints. We present applications to different problems in computational mechanics.

Keywords: Augmented Lagrangian, Stabilized finite element method, Error estimates

References

[1] E. Burman, P. Hansbo, M. G. Larson (2023). *The augmented Lagrangian method as a framework for stabilised methods in computational mechanics*. Arch. Comput. Methods Eng., 30(4), 2579–2604.

On discrete ground states of rotating Bose–Einstein condensates

Mahima Yadav[1] and Patrick Henning[1]

[1]Department of Mathematics, Ruhr University Bochum
{mahima.yadav, patrick.henning}@rub.de

Abstract

The talk focuses on the study of ground states of Bose–Einstein condensates in a rotating frame. The ground states are described as the constrained minimizers of the Gross-Pitaevskii energy functional with an angular momentum term. The problem is discretized using Lagrange finite element spaces of arbitrary polynomial order. The approximation properties of discrete ground states are presented, taking into account the missing uniqueness of ground states which is mainly caused by the invariance of the energy functional under complex phase shifts. The error analysis is based on an Euler–Lagrange functional that we restrict to certain tangent spaces in which we have local uniqueness of ground states. Error estimates of optimal order are shown for the L^2- and H^1-norm, as well as for the ground state energy and chemical potential. We also present numerical experiments to illustrate various aspects of the problem structure.

Keywords: Constrained minimization problem, Gross-Pitaevskii equation, Bose–Einstein condensates, Finite element method.

References

[1] P. Henning, M. Yadav (2023). *On discrete ground states of rotating Bose-Einstein condensates.* ArXiv e-print 2303.00402.

MS42 - Nonsmooth and nonconvex optimization

Generalizing Adam to Manifolds by identifying a Global Tangent Space Representation

Benedikt Brantner[1] and Michael Kraus[1]

[1]Max-Planck-Institut für Plasmaphysik.
{benedikt.brantner, michael.kraus}@ipp.mpg.de

Abstract

One of the primary reasons behind the success of neural networks has been the emergence of an array of new, highly-successful optimizers, chief among them the Adam optimizer.

Another trend that is gaining increasing traction in the machine learning community is the introduction of manifolds (non-euclidean parameters) in neural network architectures. The motivation for doing so is twofold. First, it has been observed that architectures such as CNNs and transformers profit from enforced orthogonality constraints [1, 5]; this requires optimization on the Stiefel manifold. Second, many physics applications require enforcing constraints related to the system at hand; these require optimization on e.g. the symplectic Stiefel manifold, the Grassmann manifold and the symplectic Grassmann manifold [2]. This establishes a need to generalize optimizers to these structures.

Fruitful efforts have been made to do so in recent years [4, 3]. These existing optimizers do however not generalize all the aspects of the Adam algorithm to manifolds. In this work we propose a different approach based on the specific structure of the considered manifolds:

All of the manifolds mentioned above are "principal homogeneous spaces" that admit a global representation of the tangent space. This global representation can be used to perform all the operations in the Adam alorithm on manifolds and allows for faster and more efficient training of these general neural networks.

After discussing the theory behind these optimizers, an efficient implementation in `Julia` will be presented, together with numerical results.

Keywords: neural networks, manifold optimization, orthogonality constraints, structure-preservation.

References

[1] Nitin Bansal, Xiaohan Chen, and Zhangyang Wang. "Can we gain more from orthogonality regularizations in training deep networks?" In: *Advances in Neural Information Processing Systems* 31 (2018).

[2] Thomas Bendokat and Ralf Zimmermann. "Geometric Optimization for Structure-Preserving Model Reduction of Hamiltonian Systems". In: *IFAC-PapersOnLine* 55.20 (2022), pp. 457–462.

[3] Lingkai Kong, Yuqing Wang, and Molei Tao. "Momentum Stiefel Optimizer, with Applications to Suitably-Orthogonal Attention, and Optimal Transport". In: *arXiv preprint arXiv:2205.14173* (2022).

[4] Jun Li, Li Fuxin, and Sinisa Todorovic. "Efficient riemannian optimization on the stiefel manifold via the cayley transform". In: *arXiv preprint arXiv:2002.01113* (2020).

[5] Aston Zhang et al. "On orthogonality constraints for transformers". In: *Proceedings of the 59th Annual Meeting of the Association for Computational Linguistics and the 11th International Joint Conference on Natural Language Processing*. Vol. 2. Association for Computational Linguistics. 2021, pp. 375–382.

Variational Formulations for Solving PDEs with Non-Smooth Solutions using Non-Linear Surrogates

Juan Esteban Suarez[1]

[1]Center for Advanced Systems Understanding (CASUS), Görlitz, Germany.

Abstract

This talk intends to address the challenge of solving Partial Differential Equations (PDEs) with smooth or non-smooth solutions by formulating variational PDE formulations resulting in a soft-constrained optimization problem. The flexibility of the variational formulation enables us to use hybrid non-linear surrogates to approximate discontinuous shocks while solving forward or inverse PDE problems. We first explore general concepts and tools necessary for solving PDEs under a variational formulation with general non-linear surrogates and boundary conditions. We then compare the numerical performance of Physics Informed Neural Networks (PINNs) as surrogates against Polynomial Surrogate Models (PSMs). Our goal is to open up the discussion regarding the class of problems that genuinely require the use of Neural Networks. Our findings indicate that PSMs outperform PINNs by several orders of magnitude in both accuracy and runtime. Furthermore, we introduce a new method for approximating discontinuous functions using modified global spectral methods. We extend this method to solve PDEs with non-smooth solutions, providing an innovative solution to a highly challenging problem.

Keywords: Shock Approximation, Variational Formulation, PDEs

References

[1] J. E. S. Cardona,M. Hecht (2022). *Learning Partial Differential Equations by Spectral Approximates of General Sobolev Spaces.*

[2] J. E. S. Cardona,M. Hecht (2022). *Replacing Automatic Differentiation by Sobolev Cubatures fastens Physics Informed Neural Nets and strengthens their Approximation Power.*

On Solving Constrained Abs-smooth Optimization Problems Using a Frank-Wolfe Approach

Timo Kreimeier[1], Sebastian Pokutta[2], Andrea Walther[1], and Zev Woodstock[3]

[1]Department of Mathematics, Humboldt-Universität zu Berlin
[2]Zuse Institut Berlin & Technische Universität Berlin
[3]Zuse Institut Berlin
Timo.Kreimeier@hu-berlin.de

Abstract

In this talk we present an algorithm which appears to be the first bridge between the fields of conditional gradient methods, also known as Frank-Wolfe methods [1], and abs-smooth optimization [2]. The broad class of optimization tasks covered by this approach includes, e.g., the squared ℓ_2-error of a neural network with ReLU or hinge loss activation. Among others, these machine learning problems motivate our nonsmooth nonconvex problem setting.

For this purpose, we present a generalization to the traditional Frank-Wolfe gap and show that first-order minimality is achieved when it vanishes. Moreover, we will discuss a convergence rate for our algorithm which is identical to the smooth variant of the Frank-Wolfe algorithm [3].

Our method necessitates the solution of a piecewise linear subproblem which is more challenging than in the smooth case, where just a linear problem must be solved. To handle this nonsmoothness, we provide an efficient numerical method for its partial solution [4, 5], and we identify several applications, e.g., from machine learning, where our approach fully solves the subproblem. Numerical and theoretical convergence will be demonstrated, yielding several conjectures.

Keywords: Conditional gradient method, Frank-Wolfe algorithm, Abs-smooth optimization

References

[1] G. Braun, A. Carderera, C. W. Combettes, H. Hassani, A. Karbasi, A. Mokhtari, S. Pokutta (2022). *Conditional Gradient Methods*. arXiv: 2211.14103.

[2] A. Griewank (2013). *On stable piecewise linearization and generalized algorithmic differentiation*. Optimization Methods and Software, Taylor & Francis.

[3] T. Kreimeier, S. Pokutta, A. Walther, Z. Woodstock (2023). *On a Frank-Wolfe Approach for Abs-smooth Functions*. Submitted at Optimization Methods and Software, Taylor & Francis.

[4] A. Griewank, A. Walther (2019). *Finite convergence of an active signature method to local minima of piecewise linear functions*. Optimization Methods and Software, Taylor & Francis.

[5] T. Kreimeier, A. Walther, A. Griewank (2022). *An active signature method for constrained abs-linear minimization*. Available at https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/474.

First-order optimization without (much) geometry

Adrian S. Lewis[1], Siyu Kong[2], G. Lopez-Acedo[3], A. Nicolae[4], and Tonghua Tian[5]

[1]Operations Research and Information Engineering, Cornell
adrian.lewis@cornell.edu

Abstract

Two features characterize most classical optimization algorithms: variables are Euclidean (or perhaps live in a Hilbert space or manifold), and the objective is smooth, convex, or some composition thereof. This talk sketches some developments without one of these features. Starting with an outline of Kurdyka-Lojasiewicz-based complexity theory for optimization on metric spaces, the talk moves on to discuss alternating projections in geodesic metric spaces, and ends by analyzing the subgradient-oracle cost of nonconvexity in Lipschitz minimization.

Contributed Talks

Graph Based Semi-supervised Learning Using Spatial Segregation Theory

Farid Bozorgnia[1], Morteza Fotouhi,[2], Avetik Arakelyan[3], and Abderahim Elmoataz[4]

[1]Department of Mathematics, Instituto Superior Técnico, Lisbon
[2]Department of Mathematical Sciences, Sharif University of Technology
[3]Institute of Mathematics, NAS of Armenia
[4]GREYC, University of Caen Normandy
farid.bozorgnia@tecnico.ulisboa.pt

Abstract

In this talk, we briefly explain various models of Reaction-Diffusion Systems characterized by high competition rates. We investigate the existence and uniqueness of solutions for each model, and numerical approximation of their singular limit. Next, I address graph-based semi-supervised learning leverage the theory of these competitive-type systems of PDEs to classify data when only a few labels are available.

We define a discrete counterpart over connected graphs by using a direct analogue of the corresponding competitive system. Then we consider a model motivated by the recent numerical results on the spatial segregation of reaction-diffusion systems. Finally, we present some numerical experiments showing the efficiency of the method.

Keywords: Free boundary problems, Semi-supervised learning, Laplace learning.

References

[1] A. L. Bertozzi, A. Flenner (2012). *Diffuse interface models on graphs for classification of high dimensional data.* Multiscale Modeling and Simulation., 10(3), 1090-–1118.

[2] F. Bozorgnia, A. Arakelyan (2013). *Numerical algorithms for a variational problem of the spatial segregation of reaction-diffusion systems.* Applied Mathematics and Computation., 219 (17), 8863–8875.

[3] L. Caffarelli, F. Lin (2008). *Singularly perturbed elliptic systems and multi-valued harmonic functions with free boundaries.* J. Amer. Math. Soc. 21, no. 3, 847—862.

[4] J. Calder, B. Cook, M. Thorpe, and D. Slepčev (2020). *Poisson Learning: Graph based semi-supervised learning at very low label rates.* Proceedings of the 37th International Conference on Machine Learning. PMLR, 119, 1306-–1316.

Imposing slip conditions on curved boundaries for 3D incompressible flows with a very high-order accurate finite volume scheme on polygonal meshes

Ricardo Costa*[1], Stéphane Clain[2], Gaspar J. Machado[3], João M. Nóbrega[1], Hugo Beirão da Veiga[4], and Francesca Crispo[5]

[1]Institute for Polymers and Composites/Department of Polymer Engineering, University of Minho, Azurém *Campus*, 4804-058 Guimarães, Portugal
[2]Centre of Mathematics, University of Coimbra, 3000-143 Coimbra, Portugal
[3]Centre of Physics/Department of Mathematics, University of Minho, Azurém *Campus*, 4800-058 Guimarães, Portugal
[4]Department of Mathematics, University of Pisa, 56127 Pisa, Italy
[5]Department of Mathematics and Physics, University of Campania "Luigi Vanvitelli", 81100 Caserta, Italy

Abstract

The conventional no-slip boundary condition does not always hold in several fluid flow applications and must be replaced with appropriate slip conditions according to the wall and fluid properties. However, not only slip boundary conditions are still a subject of discussion among fluid dynamicists, but also their numerical treatment is far from being well-developed, particularly in the context of very high-order accurate methods. The complexity of these conditions significantly increases when the boundary is not aligned with the chosen coordinate system and, even more challenging, when the fluid slips along a curved boundary. The present work proposes a simple and efficient numerical treatment of general slip boundary conditions on arbitrary curved boundaries for three-dimensional fluid flow problems governed by the incompressible Navier-Stokes equations. In that regard, two critical challenges arise: (i) achieving very high-order of convergence with arbitrary curved boundaries for the classical no-slip boundary conditions and (ii) extending the developed numerical techniques to impose general slip boundary conditions. The conventional treatment of curved boundaries relies on generating curved meshes to eliminate the geometrical mismatch between the physical and computational boundaries and achieve high-order of convergence. However, such an approach requires sophisticated meshing algorithms, cumbersome quadrature rules on curved elements, and complex non-linear transformations. In contrast, the reconstruction for off-site data (ROD) method handles arbitrary curved boundaries approximated with linear piecewise elements, while employing polynomial reconstructions with specific linear constraints to fulfil the prescribed boundary conditions. For that purpose, the general slip boundary conditions are reformulated on a local orthonormal basis to allow a straightforward application of the ROD method with scalar boundary conditions. The Navier-Stokes equations are then discretised with a staggered finite volume method, and the numerical fluxes are computed solely on the polygonal mesh elements. Several benchmark test cases of fluid flow problems in non-trivial three-dimensional curved domains are addressed and confirm that the proposed method effectively achieves up to the eighth-order of convergence.

Keywords: Three-dimensional incompressible Navier-Stokes equations, Navier-slip boundary conditions, Finite volume method, Very high-order of convergence, Arbitrary curved boundaries, Piecewise-linear boundary approximation

*E-mail: rcosta@dep.uminho.pt

Subgrid Artificial Viscosity Modelling Based Defect-Deferred Correction Method for Fluid-Fluid Interaction

Medine Demir[1], Mustafa Aggul[2], and Songül Kaya[3]

[1]Weierstrass Institute
[2]Department of Mathematics, Hacettepe University
[3]Department of Mathematics, Middle East Technical University.
demir@wias-berlin.de; mustafaaggul@hacettepe.edu.tr;smerdan@metu.edu.tr

Abstract

Fluid-fluid interaction problem is of considerable interest especially in computational fluid dynamics simulations for different industrial and engineering applications. One of the common problem can be observed in atmosphere-ocean (AO) interactions. This work considers the approximate solutions of the equations of AO problem.

In this study, we propose a defect-deferred correction method of [1], increasing both temporal and spatial accuracy, for atmosphere-ocean interaction problem with the use of geometric averaging of [2] for decoupling terms at the nonlinear interface. In defect step, a different variant of SAV method essentially based on the one introduced in [3], where an effective VMS stabilization acts on only the small scales is employed for the numerical simulation of the AO problem. Instead of using projection operator for VMS stabilization, the stabilization is dealt with vorticity term and grad-div stabilization in the viscous term. An important aspect of this consideration is not only conforming mixed finite element approximation is produced, but also with the use of vorticity extra storage requirement is reduced. In the case of small viscosity, the use of only three variables instead of nine variables enables to improve the solution of the system. Then, a deferred step is combined with the defect step not only to eliminate dissipative influence of the artificial viscosity but also to increase temporal accuracy from first order to second. The unconditional stability and optimally convergent results of the resulting algorithm are investigated both analytically and numerically. Both theoretical and computational findings illustrate that the proposed vorticity based SAV method has advantages over gradient based SAV method for reducing computation cost.

Keywords: Atmosphere-ocean (AO) interactions, defect-deferred correction method, subgrid artificial viscosity (SAV) method, geometric averaging

References

[1] M. Aggul, S. Kaya (2021). *Defect-deferred correction method based on a subgrid artificial viscosity model for fluid-fluid interaction.* Appl. Numer. Math. 160, 178–191.

[2] J. Connors, J. Howell, W.J. Layton (2012). *Decoupled time stepping methods for fluid-fluid interaction.* SIAM J. Numer. Anal. 50(3), 1297–1319.

[3] K.J. Galvin (2011). *New subgrid artificial viscosity Galerkin methods for the Navier-Stokes equations.* Comput. Methods Appl. Mech. Engrg., 200, 242–250.

Path Planning for Space Debris Removal through Reinforcement Learning

Simon Gottschalk *and Matthias Gerdts

Institute of Applied Mathematics and Scientific Computing,
Department of Aerospace Engineering,
Universität der Bundeswehr München, 85577 Neubiberg, Germany
simon.gottschalk@unibw.de

Abstract

The question of how to remove space debris has become more important in recent years. On the one hand, this is due to the newly emerging challenges for satellite applications (e.g. communication systems). On the other hand, the number of satellite manufacturers and operators grows. Overall, this leads to a rise of the number of satellites in the orbit and increases the risk of collisions.

To tackle this problem, we focus on a robotic arm attached to a service satellite to grasp space debris. From a mathematical point of view, this leads to several challenges. One is the path planning for approaching and reaching the space debris with the robotic arm without any collision. Classical optimal control strategies (e.g. dynamic programming) struggle to solve the optimization problem with a high dimensional dynamical system and complex collision constraints in real time. For problems like this, Reinforcement Learning (RL), where a controller-like policy is trained in an offline phase based on simulated data, offers a solution. During the online phase, we then have a very fast policy, which is able to steer the dynamical system. However, for pure RL approaches, numerical tests reveal a long and inefficient training phase.

Therefore, we will present a hierarchical approach that benefits from both classical optimal control techniques and Reinforcement Learning. On a coarse level, RL manages path planning and collision avoidance by setting intermediate points. Then, an optimal control strategy can be used to steer the actual dynamical system from one point to the next one. In this way, the training phase of RL is shortened and more efficient since only a coarse planning is done. Moreover, the optimal control problem for classical approaches is simplified, since no collision constraints need to be considered.

Finally, we show the working principle and advantages by applying this strategy to a docking maneuver of two satellites.

Keywords: Reinforcement Learning, Optimal Control, Space Debris Removal, Path Planning

*This research has been conducted within the project frame of SeRANIS Seamless Radio Access Networks in the Internet of Space. The project is funded by dtec.bw Digitalization and Technology Research Center of the Bundeswehr, grant number 150009910.

On the inf-sup compatibility of raviart-thomas elements combined with conforming nodal elements

Pierre-Alain Goulm[1] and Fleurianne Bertrand[1]

[1]Fakultät für Mathematik, TU Chemnitz
[1]pierre.goulm@mathematik.tu-chemnitz.de;
fleurianne.bertrand@mathematik.tu-chemnitz.de

Abstract

The mixed finite element method has been widely utilized for solving elasticity problems, encompassing the development of several element pairs and various formulation types. In particular, mixed finite elements were introduce to allow for the robust implementation of constraints. Traditionally, an inf-sup condition is required to guarantee compatibility between finite element spaces. However, the recent contribution [1] shows existence and uniqueness of the solution can be obtained even though the numerical schemes is inf-sup unstable. This talks aims to investigate the stability of a corresponding coupled problem in poromechanics by closely examining the inf-sup condition for the continuous element pair $(RT_0)^2 \times (P_1)^2$ introduced in [2].

Keywords: inf-sup condition, mixed finite elements

References

[1] Daniele Boffi and Fleurianne Bertrand. A counterexample for the inf-sup stability of the RT^0/P^1 in $L_2H_1^0$ finite element combination for the mixed Poisson equation. Cambridge University Press, 2019

[2] Nils Viebahn, Karl Steeger, and Jörg Schröder. A simple and efficient Hellinger-reissner type mixed finite element for nearly incompressible elasticity. Computer Methods in Applied Mechanics and Engineering, 340:278–295, 201

Space-time parallel methods for parabolic problems

Iñigo Jimenez-Ciga[1], Andrés Arrarás[1], Francisco J. Gaspar[2], and Laura Portero[1]

[1]Department of Statistics, Computer Science, and Mathematics, Public University of Navarre
[2]Department of Applied Mathematics, University of Zaragoza
{inigo.jimenez, andres.arraras, laura.portero}@unavarra.es; fjgaspar@unizar.es

Abstract

In a context of increasingly complex computer architectures, parallel programming has become a remarkable tool for the solution of problems of different nature. The number of supercomputers has increased over the years, and this trend seems to continue in the future, due to the lack of speed improvement of each calculation core, which leads to a greater number of connected computers. In the context of differential equations, the concept of parallelization can be implemented for integrating evolutionary problems, in which space and time variables are involved. As a first approximation, parallelization in space can be suitable for certain problems, but, if a large number of calculation cores is available, time parallel time integrators are also required.

In this framework, we present two new space-time parallel methods based on the parareal algorithm. This time parallel time integrator considers two propagators, one of them cheap and fast and the other one expensive but more accurate that is used in a parallel way over the time windows (cf. [3]). The algorithm is combined with two time-splitting schemes, namely, the fractional implicit Euler scheme (as defined in [2]) and the Douglas-Rachford method (cf. [1]). These integrators can be parallelized in space, thus yielding combined methods which are parallel in space and time. The resulting algorithms permit us to integrate parabolic problems significantly faster by optimizing the use of available connected CPUs. We show stability and convergence properties for both methods, remarking the importance of choosing L-stable methods in order to obtain stable space-time parallel schemes with faster convergence, as suggested in [4]. Along with theoretical results, we propose some numerical experiments to confirm the power of the designed integrators, illustrating their potential when very fine meshes in time and space are needed.

Keywords: parabolic problems, parareal algorithm, space-time parallel methods, splitting methods

References

[1] J. Douglas Jr., H.H. Rachford (1956). *On the numerical solution of heat conduction problems in two and three space variables*. Trans. Amer. Math. Soc., 8(2): 421-439.

[2] W. Hundsdorfer, J. Verwer (2003). *Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations*. In Springer Ser. Comput. Math., vol. 33, Springer-Verlag, Berlin/Heidelberg.

[3] J.L. Lions, Yvon Maday, G. Turinici (2001). *Résolution d'EDP par un schéma en temps "pararéel"*. C. R. Acad. Sci. (1) - Math., 332(7), 661–668.

[4] G.A. Staff, E.M. Rønquist (2005). *Stability of the parareal algorithm*. In T.J. Barth et al., editors, *Domain Decomposition Methods in Science and Engineering*. Lect. Notes Comput. Sci. Eng., vol. 40. Springer, Berlin/Heidelberg, 449–456.

Low-Dissipation Central-Upwind Schemes

Alexander Kurganov[1]

[1]Department of Mathematics, Southern University of Science and Technology, Shenzhen, China

Abstract

The talk will be focused on central-upwind schemes, which are simple, efficient, highly accurate and robust Godunov-type finite-volume methods for hyperbolic systems of conservation and balance laws. I will first briefly go over the main three steps in the derivation of central-upwind schemes. First, we assume that the computed solution is realized in terms of its cell averages, which are used to construct a global in space piecewise polynomial interpolant. We then evolve the computed solution according to the integral form of the studied hyperbolic system. The evolution is performed using a nonsymmetric set of control volumes, whose size is proportional to the local speeds of propagation: this allow one to avoid solving any (generalized) Riemann problems. Once the solution is evolved, it must be projected back onto the original grid as otherwise the number of evolved cell averages would double every time step and the scheme would become impractical. The projection should be carried out in a very careful manner as the projection step may bring an excessive amount of numerical dissipation into the resulting scheme as was the case in previous versions of the central-upwind schemes.

In order to more accurately project the solution, we have recently introduced a new way of making the projection. A major novelty of the new approach is that we use a subcell resolution and reconstruct the solution at each cell interface using two linear pieces. This allows us to perform the projection in the way, which would be extremely accurate in the vicinities of linearly degenerate contact waves. This leads to the new second-order semi-discrete low-dissipation central-upwind schemes, which clearly outperform their existing counterparts as confirmed by a number of numerical experiments conducted for both the 1-D and 2-D Euler equations of gas dynamics in both single- and multifluid settings.

The accuracy of the low-dissipation central-upwind schemes can be further increased in two ways. First, we develop a scheme adaption strategy: we automatically detect "rough" parts of the computed solution and apply an overcompessive slope limiter in these areas at the piecewise linear reconstruction step. The adaptive low-dissipation central-upwind schemes achieve a superb resolution in a variety of challenging numerical examples. Second, we utilize the new low-dissipation central-upwind numerical fluxes to construct new fifth-order finite-difference A-WENO schemes, which outperfom their existing A-WENO counterparts based on less accurate central-upwind numerical fluxes.

Keywords: Finite-volume methods, central-upwind schemes, Euler equations of gas dynamics, compressible multifluids

Sound radiation from double wall structure with poroelastic layers: variational formulation and finite element results

Walid Larbi[1]

[1]Laboratoire de Mécanique des Structures et des Systèmes Couplés (LMSSC), Conservatoire national des arts et métiers (Cnam), 2 rue Conté, 75003 Paris, France
walid.larbi@lecnam.net

Abstract

Double-walled structures separated by an acoustic cavity are widely used in many applications for sound insulation purposes. Their sound transmission loss is estimated by calculating the ratio between the incident sound power on the first wall and the radiated sound power by the second [1, 2]. The introduction of a poroelasic layers brings a better sound insulation against external noise. In this context, this work deals with the numerical prediction of the sound radiation from double-walled structure with poroelastic layers. The proposed approach is based on the use of the finite element method for the modeling of the different solid and fluid domains of the problem. A mixed displacement-pressure variational formulation of the Biot poroelasticity equations is used to model the poroelastic domain [3]. The structure is excited by a diffuse field represented by a superposition of plane waves with random phases and directions. The acoustic power radiated by the second wall is calculated by applying the Rayleigh integral method [4]. The results show the importance of optimizing the position of the porous layers to maximize the sound insulation.

Keywords: Sound transmission, Variational formulation, Finite Element, Poroelastic, Double wall

References

[1] W. Larbi, J.-F. Deü and R. Ohayon (2016). *Vibroacoustic analysis of double-wall sandwich panels with viscoelastic core*. Computers & Structures, 174, 92–103.

[2] W. Larbi, J.-F. Deü, R. Ohayon (2016). *Finite element reduced order model for noise and vibration reduction of double sandwich panels using shunted piezoelectric patches*. Applied Acoustics, 108, 40–49.

[3] J.F. Allard and N. Atalla (2009). *Propagation of Sound in Porous Media: Modelling Sound Absorbing Materials*. Second Edition, John Wiley & Sons.

[4] F. Fahy, P. Gardonio (2006). *Sound and Structural Vibration, Radiation, Transmission and Response*. 2nd Edition, Academic Press.

Semiclassical numerical modeling of gain materials with a high order Dicontinuous Galerkin time-domain solver

C. Legrand[1], S. Lanteri[2], and S. Descombes[2]

[1]Atlantis, INRIA d'Université Côte d'Azur
cedric.legrand@inria.fr; stephane.lanteri@inria.fr; stephane.descombes@unice.fr

Abstract

This talk is concerned on the interaction between an electromagnetic field and a gain medium in the context of laser physics, with the goal of modelling the gain process that results in an increase in optical power. To achieve this, we focus on the atomic structure of the gain medium, specifically the behavior of its electrons, and explore their interaction with the electromagnetic field. This phenomenon can be modelled by a four-level atomic system model that combines Maxwell's equations and a set of non-linear Ordinary Differential Equations (ODEs) to describe the electronic density evolution for each energy level. Most of the existing works dealing with this model consider teh FDTD method as seen in [1]. In this talk, we will present a novel numerical modeling leveraging the Discontinuous Galerkin Time-Domain scheme in 3D that we have set up to solve this model.

Based on the work done in [2], we have established a leap-frog 2 temporal scheme for this problem. For the DG scheme, we had to make approximations for the nonlinear terms present in the ODEs. A theoretical study of the problem and the schemes were carried out, and we defined a continuous and discrete energy for this problem, inspired by the work done in [3], which we estimated in both cases. Finally, the DG scheme was implemented in 3D and validated using manufactured solutions. We will present these results, including orders of numerical convergence obtained and the application of this numerical method to a physical case.

Keywords: Laser physics, gain medium, time-domain Maxwell equations, rate equations, Discontinuous Galerkin method.

References

[1] Amit S. Nagra, and A. York (1998). *FDTD Analysis of Wave Propagation in Nonlinear Absorbing and gain Media.*

[2] Vrushali A. Bokil, Yingda Cheng, Yan Jiang, and Fengyan Li (2017). *Energy stable discontinuous Galerkin methods for Maxwell's equations in nonlinear optical media.*

[3] L. Fezoui, S. Lantéri, S. Lohrengel, and S. Piperno (2005). *Convergence and stability of a discontinuous Galerkin time-domain method for the 3D heterogeneous Maxwell equations on unstructured meshes.*

Model order reduction for reaction-advection problems using an optimally stable Petrov-Galerkin scheme

Lukas Renelt*, Christian Engwer, and Mario Ohlberger

Institute for Analysis and Numerics, University of Münster, Germany

lukas.renelt@uni-muenster.de

Abstract

A known challenge in the field of model order reduction is the application of established techniques to hyperbolic problems. Taking the linear transport equation as a simple example, it has been shown that the approximability - measured by the Kolomogorovo n-width - decays slowly and thus linear techniques are bound to perform poorly [3].

However, in many real-world-applications the advection field is often constant as it is either analytically known/measured or given as the solution to i.e. the Darcy- or the Navier-Stokes-equation. We examine the case of reactive transport in a catalytic filter with a parametrized reaction coefficient and parametrized inflow conditions while the velocity field is constant and given as the Darcy-flow. We were able to prove that in this setting the Kolomogorov n-width decays exponentially.

For the discretization we adapt the construction introduced by Brunken et al. [1] and recently also employed by Henning et al. [2] yielding an optimally-stable scheme using non-standard function spaces [4]. We discuss the advantages of this approach for (localized) model order reduction, as well as its challenges. Numerical experiments using a greedy-type algorithm confirm the exponential convergence of the approximation error.

Keywords: Model order reduction, transport dominated problems, optimal stability

References

[1] J. Brunken, K. Smetana, and K. Urban. (Parametrized) first order transport equations: realization of optimally stable Petrov-Galerkin methods. *SIAM J. Sci. Comput.*, 41(1):A592–A621, 2019.

[2] J. Henning, D. Palitta, V. Simoncini, and K. Urban. An ultraweak space-time variational formulation for the wave equation: Analysis and efficient numerical solution. *ESAIM: M2AN*, 56(4):1173–1198, 2022.

[3] M. Ohlberger and S. Rave. Reduced basis methods: Success, limitations and future challenges. In *Proceedings of ALGORITMY*, pages 1–12, 2016.

[4] L. Renelt, M. Ohlberger, and C. Engwer. An optimally stable approximation of reactive transport using discrete test and infinite trial spaces, 2023, math.NA/2303.15943.

*The authors acknowledge funding by the BMBF under contract 05M20PMA and by the Deutsche Forschungsgemeinschaft under Germany's Excellence Strategy EXC 2044 390685587, Mathematics Münster: Dynamics – Geometry – Structure.

Data-parallelism based deep learning approach for the model order reduction of parametric partial differential equations

Nirav Vasant Shah *[1], Chris Richardson[2], and Garth N. Wells[1]

[1]Department of Engineering, University of Cambridge
[2]Department of Earth Sciences, University of Cambridge
{nvs31, cnr12, gnw20}@cam.ac.uk

Abstract

Deep learning based model order reduction of parametric partial differential equations has gained traction in recent years. Deep learning based methods can be non-intrusive in nature and may not require access to source code used to solve high-fidelity model. In the case of offline-online two stage procedure, deep learning methods are quicker in the online phase. However during the offline phase, they suffer from severe computational cost associated to generation of training data and training of artificial neural network. On exascale systems, such approaches require more careful numerical implementation due to heterogeneous mixed CPU/GPU devices. In this context, we introduce data-parallelism based distributed training of the artificial neural network in order to address the issue of high offline cost. We also introduce `PyTorch-RBniCSx-FEniCSx` based open source package, `DLRBniCSx`, for deep learning based reduced order modelling.

Keywords: Geometric parametrisation, Reduced order modelling, Artificial neural network, Data-parallelism

References

[1] N. V. Shah, M. Girfoglio, P. Quintela, G. Rozza, A. Lengomin, F. Ballarin, P. Barral (2022). *Finite element based Model Order Reduction for parametrized one-way coupled steady state linear thermo-mechanical problems*. Finite Elements in Analysis and Design. Vol. 212, 103837.

[2] L. Meneghetti, N. Shah, M. Girfoglio, N. Demo, M. Tezzele, A. Lario, G. Stabile, G. Rozza (2022). *Chapter 20: A Deep Learning Approach to Improving Reduced Order Models*. In *Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics*, eds.: G. Rozza, G. Stabile, and F. Ballarin. SIAM, Philadelphia, PA, 19104.

*This work is supported by United Kingdom Research and Innovation under the project "SysGenX: Composable software generation for system-level simulation at exascale".

Adaptive solution of a model for the drying of porous solids

María González Taboada*[1] and Hiram Varela†[1]

[1]Department of Mathematics and CITIC, University of A Coruña (Spain)
maria.gonzalez.taboada@udc.es; hiram.varela@udc.es

Abstract

In this talk, we discuss the adaptive solution of a model for porous media flow based on the Darcy-Forchheimer equations. We will consider an adaptive algorithm based on an a posteriori error indicator of residual type, reliable and locally efficient. Then, we will present the application of this numerical method to the simulation of the drying of porous solids, like wood and wood composites.

Keywords: Darcy-Forchheimer equations, a posteriori error estimates, mixed finite element, drying, porous solids

References

[1] V. Girault, M.F. Wheeler (2008). *Numerical discretization of a Darcy-Forchheimer model.* Numer. Math., 110, 161–198.

[2] E.U. Schlünder (2004). *Drying of porous material during the constant and the falling rate period: A critical review of existing hypotheses.* Drying Technology, 22, 1517–1532.

[3] F. Hecht (2012). *New Developments in FreeFEM++.* J. Numer. Math, 20, 251–265.

[4] J.J. Salas, H. López, B. Molina (2011). *An analysis of a mixed finite element method for a Darcy-Forchheimer model.* Math Comput. Model, 57, 2325–2338.

*M.G.T. wishes to acknowledge the financial support of Xunta de Galicia through grant ED431C 2022/47 and the support received from CITIC through Xunta de Galicia and the European Regional Development Fund (grant ED431G 2019/01).

†H.V. acknowledges the financial support of the Spanish Ministerio de Educación through grant FPU18/06125, Xunta de Galicia (grant ED431C 2022/47) and CITIC through Xunta de Galicia and the European Regional Development Fund (grant ED431G 2019/01).

High-Order-Integration for Regular Closed Surfaces

Gentian Zavalani[1], Oliver Sander[2], and Michael Hecht[3]

[1,3]Center for Advanced Systems Understanding (CASUS), D-02826 Görlitz
[1,3]Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany
[1,2]Technische Universität Dresden, D-01062 Dresden, Germany
[1]g.zavalani@hzdr.de

Abstract

In this talk, we present high-order surface quadratures (HOSQ) approximating regular surface integrals on closed surfaces. HOSQ rests on curved surface triangulations realised due to k^{th}-order interpolation of the closest point projection $\pi : \mathcal{M}_h \longrightarrow \mathcal{M}$, extending initial linear surface approximations $\mathcal{M}_h$ of mesh size $h > 0$. The surface quadratures rest on a novel diffeomorphic square-triangle transformation yielding an alternative to Duffy's transformation, termed square-squeezing. Square-Squeezing enables to pull-back interpolation and integration tasks to the standard square, suppressing Runge's phenomenon when choosing Chebyshev–Lobatto interpolation nodes. For regular initial linear surface approximations $\mathcal{M}_h$, we provide algebraic approximation rates scaling purely with the interpolation degree, $\deg = k$, and not, as most common, with the mesh size $h > 0$.

Consequently, instead of applying mesh-refinements, high-accurate surface integral approximations for coarse meshes can be reached by choosing high interpolation degrees. We will present numerical results for a wide variety of regular surface integrals, demonstrating the approximation power of the HOSQ method and its applicability to numerical differential geometry.

Keywords: high-order accuracy, numerical integration, surface integrals, square squeezing transformation, closest point projection

Poster Presentations

Parallel training of deep neural networks

Samuel A. Cruz Alegría[1,2], Ken Trotti[1], Alena Kopaničáková[1,3], and Rolf Krause[1,2]

[1]Università della Svizzera Italiana, Switzerland
[2]UniDistance Suisse, Switzerland
[3]Brown University, United States
samuel.adolfo.cruz.alegria@usi.ch, ken.trotti@usi.ch;
Alena_Kopanicakova@brown.edu;
rolf.krause@usi.ch

Abstract

Deep neural networks (DNNs) have vast applications across academic disciplines. The precision and versatility of DNNs depend on the amount of parameters and training data. As network size and data volume continue to increase, it is crucial to develop new scalable and distributed training methods. Our proposed approach employs non-linear domain-decomposition techniques on the data space, with demonstrated convergence and scalability through benchmark problems. Compared to the stochastic gradient descent (SGD) method, our approach significantly reduces the number of iterations and execution time. Ultimately, we demonstrate the scalability of our PyTorch-based training framework by leveraging CUDA and NCCL technologies.

Keywords: Neural networks, Domain decomposition, Training

A reduced model technique for the Darcy problem in a fractured porous media that ensure local mass conservation

Alessio Fumagalli[1] and Wietse M. Boon[1]

[1]MOX, Department of Mathematics, Politecnico di Milano, Italy
alessio.fumagalli@polimi.it; wietsemarijn.boon@polimi.it

Abstract

Constructing fast solution schemes often involves deciding which errors are acceptable and which approximations can be made for the sake of computational efficiency. Herein, we consider a mixed formulation of Darcy flow and take the perspective that the physical law of mass conservation is significantly more important than the constitutive relationship, i.e. Darcy's law. Within this point of view, we propose a three-step solution technique that guarantees local mass conservation.

In the first step, an initial flux field is obtained by using a locally conservative method, such as the TPFA Finite Volume Method. Although this scheme is computationally efficient, it lacks consistency and therefore requires a suitable correction. Since this correction is divergence-free, the Helmholtz decomposition ensures that it is given by the curl of a potential field. The second step therefore employs an H(curl)-conforming discretization to compute the correction potential and update the flux field. The pressure field is computed in the final step by using the same TPFA system from the first step.

The procedure guarantees local mass conservation regardless of the quality of the computed correction. Thus, we relax this computation using tools from reduced order modeling. We introduce a reduced basis method that is capable of rapidly producing a potential field for given permeability fields. By applying the curl to this field, we ensure that the correction is divergence-free and mass conservation is not impacted.

Finally, we extend the method to solving Darcy flow in fractured porous media. We rewrite the equations in terms of mixed-dimensional differential operators and identify the problem as a mixed-dimensional Darcy flow system. In turn, the proposed three-step solution procedure directly applies using the mixed-dimensional curl to ensure local mass conservation.

Keywords: Porous media flow, Reduced basis method

Modeling of the child's lower urinary system

Lisa Grandjean[1], Nadia Boudaoud[2], Guillaume Dollé[1], Stéphanie Salmon[1], and Marie-Laurence Poli-Merol[2]

[1]LMR UMR CNRS 9008, University of Reims, France
[2]American Memorial Hospital of Reims, France
lisa.grandjean@univ-reims.fr; nadia.boudaoud.laghmani@gmail.com;
guillaume.dolle@univ-reims.fr, stephanie.salmon@univ-reims.fr,
mpolimerol@chu-reims.fr

Abstract

The bladder is the organ in the urinary system which has the function of receiving the urine produced by the kidneys, keep it and then evacuate. In this research, we build with paediatric surgeons a simple numerical model of the child's bladder to study the mechanism of filling and voiding in order to better understand how the fluid interacts with the wall. The different models are based on real data provided by surgeons, such as volumes, flows, urodynamic data or medical images like cystography.

During the urination, the bladder wall deforms and the size of bladder decrease. To represent this phenomenon, we use the Arbitrary Lagrangian Eulerian (ALE) method to solve the Navier-Stokes equations with a free surface, using FreeFem++ [1],

$$\begin{cases} \dfrac{\partial \vec{u}}{\partial t} + (\vec{u} - \vec{c}).\nabla \vec{u} - \nu \Delta \vec{u} + \nabla p = 0 \ , \quad \nabla . \vec{u} = 0 \quad \text{in } \Omega^t \\ \nu \dfrac{\partial \vec{u}}{\partial \vec{n}} - p\vec{n} = -p_e \vec{n} - \sigma(\kappa)\vec{n} \quad \text{on } \Gamma^t_{free} \end{cases} \tag{1}$$

where $\vec{u}$ is the fluid velocity, ν its kinematic viscosity, p the pressure, p_e is the abdominal pressure, σ is the surface tension coefficient, κ is the curvature of the free surface and $\vec{c}$ represent the domain velocity.

The upper wall (Γ_{free}), called bladder dome, become deformed when the urine is flowing towards the urethra and goes out. The lower part of the wall is fixed because the bladder trigone and the pelvis prevent the deformation of this zone. The domain velocity $\vec{c}$ is calculated by the harmonic extension of $\vec{u}$ on Γ_{free}, like in [2]. Results obtained are satisfactory, reproducing a physiological behavior.

Regarding the filling of the bladder, urine gradually enters through the ureters and pushes the bladder dome until it reaches the maximum capacity. We first impose the movement of the dome to reproduce the displacement observed in the images of cystography. We will show different fluid-structure interaction models that would allow us to obtain the same results.

Keywords: Navier-Stokes equations, ALE formulation, Free surface, Fluid-structure interactions

References

[1] F. Hecht (2012). *New development in FreeFem++*. J. Numer. Math., 20, 3-4, 251–265, `https://freefem.org/`

[2] B. Maury (1995). *Characteristics ALE Method for the Unsteady 3D Navier-Stokes Equations with a Free Surface*. Research article.

Numerical methods for electromagnetic cartography in medical imaging

Charlotte Milano[1], Stephanie Lohrengel[1], and Stéphanie Salmon[1]

[1]LMR UMR CNRS 9008 University Reims Champagne Ardenne, France
charlotte.milano@univ-reims.fr, stephanie.lohrengel@univ-reims.fr,
stephanie.salmon@univ-reims.fr

Abstract

It is well known that electrical properties (EPs), i.e. conductivity and permittivity, of biological tissues of human body can provide information about pathological and healthy tissues. On the other hand, the precise knowledge of EPs is necessary in numerical simulation of magnetic resonance imaging (MRI) which is highly recommended to guarantee the international safety standards of the patient during the medical exam. We will present here a method called "contrast source inversion" that aims to recover the EPs of tissues from measurements of the radio frequency magnetic field performed by MRI scanners.

To this end, synthetical measurements have been obtained by the two-dimensional simulation of the electromagnetic field in a MRI birdcage coil. The two-dimensional transverse magnetic mode of Maxwell's equations reduces the electric field problem into a scalar Helmholtz problem:

$$\begin{cases} -\Delta E^{sc} - k^2 E^{sc} = -k^2 w \text{ in } \Omega \\ E^{sc} = 0 \text{ on } \partial\Omega \end{cases} \tag{1}$$

where $E^{sc} = E - E^b$, in which E and E^b are, respectively, the total electric field in presence of the body and the background field generated by the same source field J. Moreover, $w = \chi E$ is the contrast source with $\chi = 1 - \epsilon_r$, the contrast of the body (where ϵ_r represents the relative permittivity depending on both EPs).

The contrast source inversion method reformulates the inverse problem as the minimization of a cost functional, which is weighted of the data and state errors:

$$F[w,\chi] = \frac{\eta}{2}\|f_{data} - (G^D \circ \mathcal{L}_b)[w]\|_D^2 + \frac{\eta_D}{2}\|\chi E^b - w + \chi((G^D \circ \mathcal{L}_b)[w])\}\|_D^2$$

where η and η_D are the weights, $\|\cdot\|_D$ denotes the L^2 norm on the domain D where the data f_{data} are collected, and G^D is the restriction on D.

Finally, $\mathcal{L}_b$ refers to the following problem:

$$\mathcal{L}_b : L^2(D) \to H_0^1(\Omega) \qquad w \mapsto \mathcal{L}_b[w] = E^{sc}$$

where E^{sc} is the solution of the problem (1) which is solved using finite element method.

Keywords: Inverse problem, Maxwell's equations, Finite element method

References

[1] P. van den Berg, A. Abubakar (1997). *A contrast source inversion method*, Inverse Problems, 13(6), 1607–1620.

[2] A. Arduino, L. Zilberti, M. Chiampin, O. Bottauscio (2017). *CSI-EPT in Presence of RF-Shield for MR-Coils*. IEEE Trans. Med. Imaging, 36(7), 1396–1404.

Blocked sampling method

Evie Nielen[1], Karen Veroy-Grepl[1], and Oliver Tse[1]

[1]Department of Mathematics and Computer Science, Eindhoven University of Technology, Netherlands
e.t.e.nielen@tue.nl, o.t.c.tse@tue.nl, k.p.veroy@tue.nl

Abstract

In the last two decades, model order reduction has been established as an important tool for the solution of high-dimensional parametrized partial differential equations. However, even with the development and success of new methods that exploit machine learning tools, the problem of offline sampling remains. Most methods still rely on a random sampling of the parameter space, which especially in high-dimensional parameter spaces necessitates large amounts of training data. We explain a novel method to determine where to sample, therefore reducing the number of samples required.

Keywords: Parametrized PDEs, High-dimensional parameter space, Reduced basis, Greedy sampling, Block sampling

References

[1] A. Quarteroni, A. Manzoni, F. Negri (2016). *Reduced basis methods for partial differential equations an introduction.* Springer International Publishing.

[2] L. Iapichino, S. Volkwein (2015). *Optimization strategy for parameter sampling in the reduced basis method.* IFAC-PapersOnLine, 48(1), 707–712.

Parameter identification on time-dependent domains using adaptive finite cell methods

Annika Osmers[1] and Andreas Rademacher[1]

[1]Center for Industrial Mathematics (ZeTeM), University of Bremen, Germany
aosmers@uni-bremen.de, arademac@uni-bremen.de

Abstract

Motivated by an industrial drilling process, we consider a time-dependent domain $\Omega(t) \subset \mathbb{R}^d$, $d \in \{2, 3\}$ and a time interval $I = [0, T]$ with end point $T > 0$. We aim for the control-state tuple (q, u), which satisfies the following parabolic optimization problem:

$$\min J(q, u) := \int_I J_1(u(t)) \, \mathrm{dt} + J_2(u(T)) + \frac{\alpha}{2}\|q\|^2$$

subject to

$$\begin{aligned} \dot{u}(x,t) + Au(x,t) &= f(x,t) && \text{in } \Omega(t) \times I \\ u(\cdot, 0) &= u_0 && \text{in } \Omega(0) \\ \partial_n u(x,t) &= q(x,t) && \text{on } \Gamma(t) \times I, \end{aligned}$$

where J_1 and J_2 are suitable functionals. Alternatively, it is possible to formulate the problem as an optimality system. To this end, necessary and sufficient optimality conditions of first order are derived by means of the Lagrangian.

In order to deal with the time dependence of the domain, a fictitious domain (FD) approach is used. It is characterized by the fact that the complicated domain $\Omega(t)$ is embedded into a fictitious domain $\tilde{\Omega} \subset \mathbb{R}^d$ of constant shape. Therefore, we have to penalize those solution components that are not generated on the actually existing domain $\Omega(t)$ by means of a very small FD-parameter $\epsilon > 0$. It is realized by incorporating a regularized cut-off function in the spatial quasilinear differential operator A of second order. For the numerical solution, a space-time finite element discretization is realized; together with the FD approach it forms the so-called finite cell method (FCM). The discontinuous temporal test functions enable the formulation of the discrete problem equations as time stepping schemes.

The next step will be the derivation of a posteriori error estimators, which evaluate the error between the solutions of the continuous and the discrete optimization problems. Here, the error arises from the five error sources: FD approach, space and time discretization, quadrature and numerics. For the a posteriori error control the so-called dual weighted residuals (DWR) method will be used. Afterwards, we will develop an adaptive FCM algorithm based on the derived a posteriori error estimators, which balances the different error components in an appropriate way.

Keywords: Optimal control, Time-dependent domains, Fictitious domain approach, Finite cell method

References

[1] D. Meidner (2008). *Adaptive space-time finite element methods for optimization problems governed by nonlinear parabolic systems*. PhD thesis, Ruprecht Karl University of Heidelberg.

[2] K. Rosin (2019). *Adaptive finite element methods for contact problems embedded in a fictitious domain – simulation and optimal control*. PhD thesis, Technische Universität Dortmund.

Accurate error estimation in CG and CG-like methods

Jan Papež[1]

[1]Institute of Mathematics of the Czech Academy of Sciences, Czech Republic
papez@math.cas.cz

Abstract

In [1], we presented an adaptive estimate for the energy norm of the error in the conjugate gradient (CG) method. The estimate is very cheap to evaluate and numerically reliable in finite-precision computations. Additionally, following [2], we show the extension of the estimate for other methods (CGLS, CGNE, LSQR, and CRAIG) for solving linear approximation problems with a general rectangular matrix. The estimate can be used also for preconditioned variants of the methods and can be easily implemented into existing codes.

The poster is based on joint work with G. Meurant and P. Tichý.

Keywords: System of linear algebraic equations, Conjugate gradient method, Error estimate

References

[1] G. Meurant, J. Papež, P. Tichý (2021). *Accurate error estimation in CG*. Numer. Algorithms, 88, 1337–1359.

[2] J. Papež, P. Tichý. *Estimating the error in CG-like algorithms for least-squares and least-norm problems*. (in preparation)

Improved Crouzeix-Raviart scheme for the Stokes and Navier-Stokes problem

Andrew Peitavy*[1], Erell Jamelot[1], Christophe Le Potier[1], and Eric Chénier[2]

[1]Université Paris-Saclay, CEA, Service de Thermo-hydraulique et de Mécanique des Fluides, 91191 Gif-sur-Yvette, France.
[2]Université Gustave Eiffel, Université Paris Est Creteil, CNRS, UMR 8208, MSME, F-77454 Marne-la-Vallée, France.
{andrew.peitavy, erell.jamelot, christophe.le-potier}@cea.fr; eric.chenier@u-pem.fr

Abstract

The TrioCFD code is a computational fluid dynamics (CFD) simulation software developed at the CEA. It solves Navier-Stokes equations and it is dedicated to the numerical simulation of turbulent flows for scientific and industrial applications, particularly in the nuclear field. An effective way to solve the equations is to use the first-order non-conforming Crouzeix-Raviart finite element method that we call the $\mathbf{P}^1_{nc} - P^0$ scheme. This finite element method is convenient since they induce local mass conservation and leads to a linear system that is cheap to solve. However spurious velocities may appear and damage the approximation. An improved version (by adding pressure degree of freedom at the vertices) is implemented in TrioCFD code for simplicial meshes, that we call the $\mathbf{P}^1_{nc} - (P^0 + P^1)$ scheme [1], and reduces the spurious velocities in $2D$. It is also efficient in $3D$, except when the source term is a strong gradient. To obtain the same accuracy in $3D$ as in $2D$, one must increase the number of degrees of freedom of the discrete pressure space, which leads to a more expensive numerical scheme. We aim to develop a new numerical scheme that would reduce the spurious velocities both in $2D$ and $3D$, but at a lower cost.

We propose a scheme, that allows ones to reduce the spurious velocities without adding degrees of freedom. We present a new discretization for the gradient of pressure based on the symmetric MPFA scheme (Finite volume MultiPoint Flux Approximation [2, 3]). This scheme has been encoded in Octave and TrioCFD and has been compared to the other alternatives. It gives promising results by being a good compromise between $\mathbf{P}^1_{nc} - P^0$ scheme and $\mathbf{P}^1_{nc} - (P^0 + P^1)$ scheme.

Keywords: Navier-Stokes equations, MPFA scheme, Spurious velocities, Crouzeix-Raviart FEM

References

[1] S. Heib (2003). *Nouvelles discrétisations non structuées pour des écoulements de fluides à incompressibilité renforcé.* PhD thesis, Université Pierre et Marie Curie Paris 6.

[2] L. Agelas and R. Masson (2008). *Convergence of the finite volume MPFA O scheme for heterogeneous anisotropic diffusion problems on general meshes.* In *Acad. Sci. Paris*, Ser. I 346.

[3] C. Le Potier (2005). *A finite volume method for the approximation of highly anisotropic diffusion operators on unstructured meshes.* In *Comptes rendus Mathématiques de l'Académie des Sciences*, 340.

*I thank Robert Eymard for his academic collaboration

Least-squares solutions to the Monge-Ampère equation in optical design

A. H. van Roosmalen[1], M. J. H. Anthonissen[1], J. H. M. ten Thije Boonkkamp[1], and W. L. IJzerman[1,2]

[1]CASA, Department of Mathematics and Computer Science, Eindhoven University of Technology
[2]Signify Research
a.h.v.roosmalen@tue.nl

Abstract

An inverse problem in optical design consists of finding an optical system that shapes a given light distribution $f : \mathcal{X} \to [0, \infty)$ into a desired target distribution $g : \mathcal{Y} \to [0, \infty)$. Our goal is to find a function u, defining the optical system. The target coordinates of a ray are linked to its source coordinates through the optical map $\boldsymbol{m} : \mathcal{X} \to \mathcal{Y}$. For many systems, the ray path is governed by an equation of the form $u(\boldsymbol{x}) = G(\boldsymbol{x}, \boldsymbol{y}, z)$, for an auxiliary function z. We define H as the inverse of G w.r.t. z, such that

$$u(\boldsymbol{x}) = G\big(\boldsymbol{x}, \boldsymbol{y}, z(\boldsymbol{y})\big) \iff z(\boldsymbol{y}) = H\big(\boldsymbol{x}, \boldsymbol{y}, u(\boldsymbol{x})\big). \tag{1}$$

We can find a unique solution pair $(u, \boldsymbol{m})$ by assuming that u is G-convex [2]. We define $H^*(\boldsymbol{x}, \boldsymbol{y}) = H\big(\boldsymbol{x}, \boldsymbol{y}, u(\boldsymbol{x})\big)$ and obtain the necessary condition $\nabla_{\boldsymbol{x}} H^*(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{0}$. Substituting $\boldsymbol{y} = \boldsymbol{m}(\boldsymbol{x})$ and differentiating w.r.t. $\boldsymbol{x}$ gives

$$\boldsymbol{P}(\boldsymbol{x}) = \boldsymbol{C}(\boldsymbol{x}, \boldsymbol{m}(\boldsymbol{x}), u(\boldsymbol{x}))\mathrm{D}\boldsymbol{m}(\boldsymbol{x}), \tag{2}$$

where $\boldsymbol{P} := -\mathrm{D}_{\boldsymbol{xx}} H^*$ and $\boldsymbol{C} := \mathrm{D}_{\boldsymbol{xy}} H^*$. The conservation of energy relation leads to a Monge-Ampère-type equation of the form

$$\det(\mathrm{D}\boldsymbol{m}(\boldsymbol{x})) = \frac{f(\boldsymbol{x})}{g(\boldsymbol{m}(\boldsymbol{x}))} =: F(\boldsymbol{x}, \boldsymbol{m}(\boldsymbol{x})), \tag{3}$$

giving us $\det \boldsymbol{P} = F \det \boldsymbol{C}$. We have to find a u and $\boldsymbol{m}$ that satisfy Eq. (2) and (3) combined with the boundary condition $\boldsymbol{m}(\partial\mathcal{X}) = \partial\mathcal{Y}$. We solve this iteratively with a least-squares solver. First find a $\boldsymbol{P}$ by minimizing a functional that minimizes the deviation from Eq. (2), constrained with $\det \boldsymbol{P} = F \det \boldsymbol{C}$. We then find a projection $\boldsymbol{b}$ from $\boldsymbol{m}(\partial\mathcal{X})$ to $\partial\mathcal{Y}$. Solving Eq. (2) in a least-squares sense for $\boldsymbol{m}$ leads to two coupled elliptic equations that are discretized with the finite volume method. The final step computes u from $\nabla_{\boldsymbol{x}} H(\boldsymbol{x}, \boldsymbol{y}, u(\boldsymbol{x}))|_{\boldsymbol{y}=\boldsymbol{m}(\boldsymbol{x})} = \boldsymbol{0}$ in a least-squares sense, leading to a Neumann problem, which is again discretized with the finite volume method.

Keywords: Illumination optics, Computational optics

References

[1] A. H. van Roosmalen, J. H. M. ten Thije Boonkkamp, M. J. H. Anthonissen and W. L. IJzerman (2021). *Design of a freeform two-reflector system to collimate and shape a point source distribution.* Opt. Express 29, 25605-25625.

[2] L. B. Romijn, J. H. M. ten Thije Boonkkamp, M. J. H. Anthonissen and W. L. IJzerman (2021). *An Iterative Least-Squares Method for Generated Jacobian Equations in Freeform Optical Design.* SIAM, Vol 43, B298-B322.

Numerical Identification of Friction Parameters in Contact Problems

Magdalena Thode[1] and Prof. Dr. Andreas Rademacher[1]

[1]University of Bremen, Center for Industrial Mathematics (ZeTeM), Germany
{m.thode, arademac}@uni-bremen.com

Abstract

Friction plays a significant role in many mechanical processes. The simulation of such a process depends strongly on the choice of the friction model. Friction models are determined by one or more friction model parameters. As these parameters cannot be measured directly, we identify them numerically.

For linear-elastic, unilateral contact, the displacement u can be obtained by solving Signorini's problem numerically (see [2]). The setting yields a variational inequality in the weak form. Restricting the choice of feasible displacements can be avoided by adding a term that penalizes the violation of the contact condition. Friction is included for the tangential direction on the contact boundary. We discretize the problem using finite elements.

The numerical parameter identification problem is given by

$$J(p^*) = \inf_p J(p), \qquad J(p) = \frac{1}{2}\int_{\Gamma_C} (u(p) - u_{\text{exp}})^2 \mathrm{d}o + \frac{\alpha}{2}\int_{\Gamma_C} p^2 \mathrm{d}o, \quad \alpha \text{ const},$$

governed by Signorini's problem with friction and penalty. We consider measured and simulated displacements, u_{exp} and u, on the contact boundary Γ_C and friction model parameters p.

Friction comprises both sticking and slipping phases. The distinction of the two phases leads to a non-differentiable term for the friction and thus to a non-smooth parameter-to-state operator. To make gradient-based optimization methods applicable, we have to smoothen the problem by regularizing the friction term. This results in a family of regularized parameter identification problems governed by a variational equation, which can be solved by standard techniques (see e. g. [1]).

For the frictionless Signorini problem with penalty, the convergence of the solutions with respect to the penalty parameter has been studied in [3]. Convergence considerations will now be extended to the problem with regularized friction. This involves numerical experiments for the simulation and the parameter identification.

We aim at developing an adaptive algorithm that balances the influence of the regularizations. To that end, the dual weighted residual method (DWR) will be applied to derive a goal-oriented error estimator that includes estimators for the penalization error and the friction regularization error.

The frictional contact in bolt-nut connections is discussed as an example.

Keywords: parameter identification, frictional contact, penalty method, adaptive finite elements

References

[1] F. Tröltzsch (2010). *Optimal Control of Partial Differential Equations.* AMS, Providence, RI.

[2] N. Kikuchi, J. T. Oden (1988). *Contact Problems in Elasticity.* SIAM, Philadelphia, PA.

[3] A. Rademacher, K. Rosin (2018). *Adaptive Optimal Control of Signorini's Problem.* Computational Optimization and Applications, 70(2), 531–569.

Approximating fluid-structure interaction using finite element method: comparison of Taylor-Hood and Scott-Vogelius elements

Karel Vacek[1] and Petr Svacek[1]

[1]Department of Technical Mathematics, Czech Technical University in Prague, Czech Republic
karel.vacek@fs.cvut.cz, petr.svacek@fs.cvut.cz

Abstract

The fluid-structure interaction problem is a very interesting phenomenon with many important applications, e.g. the flutter of aircraft wings, the operating life of compressors or a design of wind turbine blades. This paper focuses on finite element approximation of fluid-structure interaction problems. A simplified two-dimensional problem of incompressible fluid flow interacting with a vibrating cylinder with one degree of freedom is considered. In this case, it is necessary to deal with the time change of the computational fluid domain. The arbitrary Lagrangian-Eulerian (ALE) method is employed and the Navier-Stokes equations in ALE formulation are numerically approximated using the finite element method, see [1]. Two representatives of the FE family satisfying Babuška-Brezzi (BB) inf-sup condition, which guarantees numerical stability, are chosen: the classical Taylor-Hood (TH) finite element and the Scott-Vogelius (SV) finite element. The SV element, which approximates pressure by a discontinuous function, satisfies strongly the divergent-free constraint, and thus it delivers better theoretical a priori error estimates, see [2].

In the end, we compare in-house implementations of both TH and SV elements on the vibrating cylinder benchmark. The resonance of cylinder vibrations appears for certain inlet velocities and they are compared with the reference data.

Keywords: Finite element method, Fluid-structure interaction, ALE method, Taylor-Hood element, Scott-Vogelius element

References

[1] N. Takashi, T. J. Hughes (1992). *An arbitrary Lagrangian-Eulerian finite element method for interaction of fluid and a rigid body.* Comput. Methods Appl. Mech. Eng., 95, 115–138.

[2] N. R. Gauger, A. Linke, P. W. Schroeder (2019). *On high-order pressure-robust space discretisations, their advantages for incompressible high Reynolds number generalised Beltrami flows and beyond.* SMAI j. comput. math., 5, 89–129.

https://enumath2023.com/

FCT project: UIDB/04621/2020 (CEMAT)

cemat center for computational and stochastic mathematics

fct Fundação para a Ciência e a Tecnologia

U LISBOA | UNIVERSIDADE DE LISBOA

TÉCNICO LISBOA

ISEG Lisbon School of Economics & Management

Springer

ENUMATH 2019

CIMA

CIM CENTRO INTERNACIONAL DE MATEMÁTICA

CEMAPRE

Turismo de Lisboa