# BOOK OF ABSTRACTS

# Preface

The Seventh Chilean Workshop on Numerical Analysis of Partial Differential Equations (WONAPDE 2024), organized by the Center for Research in Mathematical Engineering ($CI^2MA$) of the Universidad de Concepción, Concepción, Chile, takes place from January $15^{st}$ to $19^{th}$, 2024, and aims at continuing a series of conferences that are carried on every three years.

The main goal of the Workshop is to present recent developments in Numerical Analysis of Partial Differential Equations, for which plenary lectures and minisymposia have been organized. **The present volume contains the abstracts of all contributions, which are placed following the order of the presentations in the conference programme.**

The list of minisymposia and corresponding organizers is:

**MS1: Recent Advances in polytopic methods**

MICHELLE BOTTI, Politecnico di Milano, Milano, Italy, e-mail: michele.botti@polimi.it

LORENZO MASCOTTO, University of Milano-Bicoca, Milano, Italy, e-mail: lorenzo.mascotto@unimib.it

**MS2: Approximation and analysis of partial differential equations with singular data**

ENRIQUE OTÁROLA, Universidad Técnica Federico Santa María, Santiago, Chile, e-mail: enrique.otarola@usm.cl

ABNER SALGADO, University of Tennessee, Knoxville, USA, e-mail: asalgad1@utk.edu

**MS3: Boundary integral equations in coupled physical system**

CHRISTOPHER COOPER, Universidad Técnica Federico Santa María, Valparaíso, Chile, e-mail: christopher.cooper@usm.cl

ELWIN VAN 'T WOUT, Pontificia Universidad Católica de Chile, Santiago, Chile, e-mail: e.wout@uc.cl

**MS4: Computational electromagnetis**

RODOLFO RODRÍGUEZ, Universidad de Concepción, Concepción, Chile, e-mail: rodolfo@ing-mat.udec.cl

PILAR SALGADO, Universidade de Santiago de Compostela, Santiago de Compostela, Spain, e-mail: mpilar.salgado@usc.es

PABLO VENEGAS, Universidad del Bío Bío, Concepción, Chile, e-mail: pvenegas@ubiobio.cl

**MS5: Effective solvers for innovative discretizations of multiphysics phenomen**

NICOLÁS BARNAFI, Universidad de Chile, Santiago, Chile, e-mail: nbarnafi@cmm.uchile.cl

SIMONE SCACCHI, Università degli Studi di Milano, Milano, Italy, e-mail: simone.scacchi@unimi.it

**MS6: From BEM to DPG: a minisymposium dedicated to the 60th birthday of prof. Norbert Heue**

THOMAS FÜHRER, Pontificia Universidad Católica de Chile, Santiago, Chile, e-mail: tofuhrer@mat.uc.cl

MICHAEL KARKULIK, Universidad Técnica Federico Santa María, Valparaíso,Chile, e-mail: michael.karkulik@usm.cl

**MS7: Full and reduced-order modeling of multiphysics problem**

ERNESTO CASTILLO, Universidad de Santiago de Chile, Santiago, Chile, e-mail: ernesto.castillode@usach.cl

FELIPE GALARCE, Pontificia Universidad Católica de Valparaiso, Valparaíso, Chile, e-mail: felipe.galarce@pucv.cl

**MS8: Mathematical modelling in biomedicine with cardiac application**

MATTHIAS GSELL, Medical University of Graz, Graz, Austria, e-mail: matthias.gsell@medunigraz.at

ELIAS KARABELAS, Karl-Franzens-University Graz, Graz, Austria, e-mail: elias.karabelas@uni-graz.at

ARGYRIOS PETRAS, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, e-mail: argyrios.petras@ricam.oeaw.ac.at

**MS9: Neural networks for partial differential equation**

IGNACIO MUGA, Universidad de Santiago de Chile, Santiago, Chile, e-mail: ignacio.muga@pucv.cl

DAVID PARDO, University of the Basque Country, Leioa, Spain, e-mail: david.pardo@ehu.es

PAULINA SEPÚLVEDA, Pontificia Universidad Católica de Valparaiso, Valparaíso, Chile, e-mail: paulina.sepulveda@pucv.cl

**MS10: Nonlinear hyperbolic PDE: numerical techniques and related model**

ELISABETTA CARLINI, Sapienza Università di Roma, Roma, Italy, e-mail: carlini@mat.uniroma1.it

ADRIANO FESTA, Politecnico di Torino, Torino, Italy, e-mail: adriano.festa@polito.it

LUIS MIGUEL VILLADA, Universidad del Bío Bío, Concepción, Chile, e-mail: lvillada@ubiobio.cl

**MS11: Numerical approximation of eigenvalue problems of PDE**

FELIPE LEPE, Universidad del Bío Bío, Concepción, Chile, e-mail: flepe@ubiobio.cl

GONZALO RIVERA, Universidad de Los Lagos, Osorno, Chile, e-mail: gonzalo.rivera@ulagos.cl

JESÚS VELLOJÍN, Universidad del Bío Bío, Concepción, Chile, e-mail: jvellojin@ubiobio.cl

**MS12: Numerical methods for fluid-membrane interactio**

RICARDO OYARZÚA, Universidad del Bío-Bío, Concepción, Chile, e-mail: royarzua@ubiobio.cl

**MS13: Numerical methods for mineral processing, wastewater treatment, and related application**

FERNANDO BETANCOURT, Universidad de Concepción, Concepción, Chile, e-mail: fbetancourt@udec.cl

RAIMUND BÜRGER, Universidad de Concepción, Concepción, Chile, e-mail: rburger@ing-mat.udec.cl

**MS14: Numerical methods for particulate and non-newtonian flow**

YURI SOBRAL, Universidade de Brasília, Brasília, Brazil, e-mail: ydsobral@Unb.br

**MS15: Recent advances in (hybridizable) discontinuous Galerkin methods and application**

MANUEL SÁNCHEZ, Pontificia Universidad Católica, Santiago, Chile, e-mail: manuel.sanchez@uc.cl

PATRICK VEGA, Universidad de Santiago de Chile, Santiago, Chile, e-mail: patrick.vega@usach.cl

**MS16: Recent advances in BEM for complex domain**

PAUL ESCAPIL-INCHAUSPÉ, Data Observatory Foundation, Santiago, Chile, e-mail: paul.escapil@dataobservatory.net

JOSÉ PINTO, Universidad Adolfo Ibañez, Santiago, Chile, e-mail: jose.pinto@uai.cl

**MS17: Session of Communications**

VERÓNICA ANAYA, Departamento de Matemática, Facultad de Ciencias, Universidad del Bío-Bío, Concepción, Chile, e-mail: vanaya@ubiobio.cl

**MS18: Structure preserving methods for nonlinear conservation equation**

JEAN-LUC GUERMOND, Department of Mathematics, TAMU, Texas, USA, e-mail: guermond@tamu.edu

**MS19: Theoretical and numerical advances for mixed-dimensional 3d-1d couplin**

LUCA FORMAGGIA, Politecnico di Milano, Milano, Italy, e-mail: luca.formaggia@polimi.it

ALESSIO FUMAGALLI, Politecnico di Milano, Milano, Italy, e-mail: alessio.fumagalli@polimi.it

MIROSLAV KUCHTA, Simula Research Laboratory, Oslo, Norway, e-mail: miroslav@simula.no

The organizers acknowledge financial support from:

- Center for Mathematical Modelling (CMM), Universidad de Chile, and Center for Research in Mathematical Engineering (CI$^2$MA), Universidad de Concepción, through project Basal FB210005, ANID-Chile.

- Anillo project Dsalt, ACT210087, ANID-Chile.
- Anillo project ACT210030, ANID-Chile
- Presidency, Universidad de Concepción.
- Vice Presidency for Research and Development, Universidad de Concepción.

In addition, the organizers express their sincere gratitude to Mrs. **Lorena Carrasco** for her dedicated work in most of the organizational aspects of the conference.

Concepción, January 2024

ORGANIZING COMMITTEE
Raimund Bürger, Universidad de Concepción
Jessika Camaño, Universidad Católica de la Santísima Concepción
Gabriel N. Gatica Universidad de Concepción
Ricardo Oyarzúa, Universidad del Bío Bío
Manuel Solano Universidad de Concepción

# Contents

## MS2: Approximation and analysis of partial differential equations with singular data



## MS3: Boundary integral equations in coupled physical systems



## MS4: Computational electromagnetism

**MS7: Full and reduced-order modeling of multiphysics problems**



**MS8: Mathematical modelling in biomedicine with cardiac applications**



**MS9: Neural networks for partial differential equations**

**MS10: Nonlinear hyperbolic PDE: numerical techniques and related models**



**MS11: Numerical approximation of eigenvalue problems of PDEs**

**MS13: Numerical methods for mineral processing, wastewater treatment, and related applications**



**MS14: Numerical methods for particulate and non-newtonian flows**

**MS18: Structure preserving methods for nonlinear conservation equations**

**MS19: Theoretical and numerical advances for mixed-dimensional 3d-1d coupling**



**Author Index**

# Plenary talks

# On skeletal muscle: modeling and simulation

Nilima Nigam[1]

Department of Mathematics, Simon Fraser University, Canada
nigam@math.sfu.ca

**Summary.** Skeletal muscles exhibit fascinating structural and mechanical properties. Skeletal muscle is composed of cells collectively referred to as fibers, which themselves contain contractile proteins arranged longtitudinally into sarcomeres. These latter respond to signals from the nervous system, and contract; unlike cardiac muscle, skeletal muscles can respond to voluntary control. Muscles react to mechanical forces - they contain connective tissue and fluid, and are linked via tendons to the skeletal system - but they also are capable of activation via stimulation (and hence, contraction) of the sacromeres. The restorative along-fibre force introduce strong mechanical anisotropy, and depend on departures from a characteristic length of the sarcomeres; diseases such as cerebral palsy cause this characteristic length to change, thereby impacting muscle force.

In the 1910s, A.V. Hill [1] observed muscles heat when they contract, but not when they relax. Based on experiments on frogs he posited a mathematical description of skeletal muscles which approximated muscle as a 1-dimensional nonlinear and massless spring. This has been a remarkably successful model, and remains in wide use. Yet skeletal muscle is three dimensional, has mass, and a fairly complicated structure. Are these features important? What insights are gained if we include some of this complexity in our models? Many mathematical questions of interest in skeletal muscle mechanics arise: how to model this system, how to discretize it, and what theoretical properties does it have?

In this talk, we survey recent work on the modeling, simulation and validation of a fully 3-D continuum elasticity approach for skeletal muscle dynamics. Skeletal muscle is modelled as a fibre- reinforced nonlinear elastic material, with other connective tissues such as aponeurosis and tendon being similarly described. These fibres are capable of nonlinear activation. We use a three-field formulation [2, 6] After discretization (semi-implicit in time, FEM in space), the model is validated against physiological data, and then used to understand the impact of muscle architecture, mass and tissue properties on questions of physiological interest [4, 5].

This is joint work based on a long-standing collaboration with James Wakeling (Dept. of Biomedical Physiology and Kinesiology, SFU).

**Keywords**: Nonlinear elasticity, skeletal muscle mechanics, three-field formulation.

## References

1. A. V. Hill. *The heat of shortening and the dynamic constants of muscle.* Proceedings of the Royal Society of London, Series B- Biological Sciences,1938.
2. J. Simo, R. Taylor and K. Pister, *Variational and projection methods for the volume constraint in finite deformation elastoplasticity*, Computer Methods in Applied Mechanics and Engineering, v.51, 1985.
3. Blemker, S.S., Delp, S.L. *Three- Dimensional Representation of Complex Muscle Architectures and Geometries*, Annals of Biomedical Engineering, 33, 661–673 (2005)
4. J. Wakeling, S. Ross, D. Ryan, B. Bolsterlee, B. Konno, S. Domínguez and N. Nigam *The Energy of Muscle Contraction. I. Tissue Force and Deformation During Fixed-End Contractions* Frontiers in Physiology,v.11, 2020.
5. R.Konno,N. Nigam, J. Wakeling, and S. Ross. *The Contributions of Extracellu- lar Matrix and Sarcomere Properties to Passive Muscle Stiffness in Cerebral Palsy* Frontiers in Physiology,v.12, 2022
6. J. Almonacid, S. Dominguez-Rivera, R. Konno, N. Nigam, S.A. Ross, C. Tam and J. Wakeling, *A three-dimensional model of skeletal muscle tissues* SIAM Journal of Applied Mathematics, 2023.

# Transmission Eigenvalues, Non-scattering Phenomena and the Inverse Problem

Fioralba Cakoni[1]

Department of Mathematics, Rutgers University, New Brunswick, New Jersey, USA
fc292@math.rutgers.edu

**Summary.** Transmission eigenvalues are inherent to the scattering theory for inhomogeneous media. They are related to frequencies at which there exist time harmonic incoming waves that are not scattered by a given inhomogeneity; in other words, the inhomogeneity is invisible to probing by such waves. The transmission eigenvalue problem is non-selfadjoint with a challenging and interesting mathematical structure, which has prompted a significant amount of recent research [1]. Existence of infinitely many real transmission eigenvalues is proven for a large class of inhomogeneities. It is also shown that real transmission eigenvalues can be determined from scattering data, hence they are important for the inverse problem. In this talk we discus the role of transmission eigenvalues in understanding essential properties of the relative scattering operator, and as a fundamental building block of methods for solving the inverse scattering problem. We show some recent theoretical results on transmission eigenvalues and non-scattering phenomena [4, 5] as well as a general approach for introducing new interior eigenvalue problems in a similar framework of nonscattering [1]. We present several applications which clearly indicate the versatile potential of these measurable eigenvalues as target signatures for the identification of changes and faults in the interrogating media and their unexpected imaging capabilities [2, 3]. The talk highlights some open theoretical and computational questions related to this active research area in inverse scattering.

**Keywords**: inverse scattering, transmission eigenvalues, non-scattering phenomenon, scattering theory, inhomogeneous media

**Mathematics Subject Classifications (2010)**: 35A01, 35A15, 78A25, 78A46

## References

1. F. Cakoni, D. Colton, and H. Haddar. *Inverse Scattering Theory and Transmission Eigenvalues*. Second Edition, CBMS Series, SIAM Publications, **98** 2023.
2. F. Cakoni, S. Cogar, and P. Monk. A spectral approach to non-destructive testing via electromagentic waves. IEEE, *Transactions on Antennas and Propagation* **69**, no 12, 8689-8697 (2021).
3. F. Cakoni, P. Monk, and Y. Zhang. Target signatures for thin surfaces. *Inverse Problems* **38** 025011 (2022)
4. F. Cakoni, and M. Vogelius. Singularities almost always scatter: Regularity results for non-scattering inhomogeneities, *Communication on Pure and Applied Mathematics*, (appeared online).
5. F. Cakoni, M. Vogelius, and J. Xiao. On the Regularity of Non-Scattering Anisotropic Inhomogeneities. *Arch. Ration. Mech. Anal.* **247** no 3, paper 31, (2023).

# Divergence Preserving Cut Finite Element Methods

Sara Zahedi[1]

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

**Summary.** I will give an introduction to Cut Finite Element Methods (CutFEM) for interface problems and present our recent development that results in pointwise divergence-free velocity approximations of incompressible flows.

I will first introduce 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. I will then based on $\mathbf{H}^{\text{div}}$-conforming finite elements present cut finite element methods for the Stokes equations [2]. These methods exhibit optimal convergence order for the velocity, pointwise divergence-free velocity fields, and well-posed linear systems, independently of the position of the boundary/interface relative to the computational mesh. In cut finite element methods Dirichlet boundary conditions are imposed weakly, which gives rise to some challenges that I will discuss.

**Keywords**: mass conservation, mixed finite element methods, unfitted finite element methods, weak imposition of boundary conditions

**Mathematics Subject Classifications (2010)**: 65N30, 65N85, 65N22.

## References

1. T. Frachon, P. Hansbo, E. Nilsson, S. Zahedi. A divergence preserving cut finite element method for Darcy flow. arXiv:2205.12023, 2023.
2. T. Frachon, E. Nilsson, S. Zahedi. Divergence-free cut finite element methods for Stokes flow. arXiv:2304.14230, 2023.

# Nonconforming Virtual Element Methods

Ilaria Perugia[1]

Faculty of Mathematics, University of Vienna
ilaria.perugia@univie.ac.at

**Summary.** The Virtual Element Method (VEM) is an extension of the finite element method to polytopic meshes. Test and trial spaces are made up of functions that are solutions to local problems related to the PDE to be approximated. They generally contain polynomials of a given maximum degree, as well as nonpolynomial functions, which need not be explicitly known. In order to impose conformity conditions in the global spaces, the local VEM spaces and their degrees of freedom are defined in such a way as to impose continuity either of the traces at interelement boundaries (conforming VEM), or of a certain number of moments at the mesh facets (nonconforming VEM). Unlike conforming VEM, nonconforming VEM can be presented in a unified framework for any dimension, which considerably simplifies its analysis and implementation.

I will discuss two applications of nonconforming VEM discretizations. The first one is to the Helmholtz problem, where the VEM is constructed in terms of plane wave functions, and the nonconforming setting allows for local orthogonalization and elimination of degrees of freedom, resulting in improved efficiency. The second one is to the heat equation in a space-time variational formulation. In this case, I will emphasize the advantages of the nonconforming approach, particularly in handling incompatible data and mesh adaptivity. This talk is based on [1], [2], [3], and [4].

**Keywords**: virtual element methods, Helmholtz equation, plane waves, heat equation, space–time methods, polytopic meshes

**Mathematics Subject Classifications (2010)**: 35J05, 35K05, 65N12, 65N30.

## References

1. L. Mascotto, I. Perugia and A. Pichler. A nonconforming Trefftz virtual element method for the Helmholtz problem. *Math. Models Methods Appl. Sci.*, 29 (2019), 1619-1656.
2. L. Mascotto, I. Perugia and A. Pichler. A nonconforming Trefftz virtual element method for the Helmholtz problem: numerical aspects. *Comp. Meth. Appl. Mech. Engrg.*, 347 (2019), 445-476.
3. S. Gómez, L. Mascotto, A. Moiola and I. Perugia. Space-time virtual elements for the heat equation. accepted for publication in *SIAM J. Numer. Anal.* (arXiv:2212.05343 [math.NA]).
4. S. Gomez, L. Mascotto and I. Perugia. Design and performance of a space-time virtual element method for the heat equation on prismatic meshes. *Comput. Methods Appl. Mech. Engrg.*, 418 (2024) 116491.

# Weights and applications in numerics

Abner J. Salgado[1]

Department of Mathematics, University of Tennessee, Knoxville, TN 37996, USA.
asalgad1@utk.edu

**Summary.** The use of weights and weighted norm inequalities has a rich history in harmonic analysis and the study of regularity properties to solutions of partial differential equations (PDE). Starting from classical results, we will present an overview of the application of some of these ideas to the numerical analysis of PDEs. Our main attention will be on some recent results concerning the use of weights in fractional diffusion, problems with singular data and some degenerate/singular PDE problems. Although these seem as disparate and unrelated applications, it is remarkable that the only structural assumption on the weight is that it belongs to a so-called Muckenhoupt $A_p$ class, which has been thoroughly studied in harmonic analysis since the 1970's.

**Keywords**: Muckenhoupt weights, weighted estimates, singular sources, fractional diffusion.

**Mathematics Subject Classifications (2020)**: 65N30, 65N80, 65N12, 65N15, 35Q35, 35Q30, 35R06, 35J70, 35J75.

# Non-local conservation laws: theory, numerics and applications

Paola Goatin[1]

Université Côte d'Azur, Inria, CNRS, LJAD
paola.goatin@inria.fr

**Summary.** In this talk, I will revise recent results on well-posedness and numerical approximation of conservation laws with integral dependencies in the flux function, typically in the form of convolution products. This type of equations arises in a variety of physical, engineering and biological applications, where integral terms account for non-local interaction phenomena. In this setting, the main challenges are represented by the analytical characterization of solutions, the treatment of boundary conditions and the reduction of numerical simulation costs. These are functional to the solution of optimal control problems arising in applications. In particular, I will focus on applications to vehicular and pedestrian traffic modeling.

**Keywords**: non-local conservation laws; high-order finite volume schemes; macroscopic flow models; PDE constrained optimization

**Mathematics Subject Classifications (2010)**: 35L65, 65M08, 90B20.

## References

1. A. Aggarwal, R.M. Colombo and P. Goatin. Nonlocal systems of conservation laws in several space dimensions. SIAM *J. Numer. Anal.*, 53(2) (2015), 963-983.
2. S. Blandin and P. Goatin. Well-posedness of a conservation law with non-local flux arising in traffic flow modeling. *Numer. Math.*,132(2) (2016), 217-241.
3. R. Bürger, P. Goatin, D. Inzunza and L.M. Villada. A non-local pedestrian flow model accounting for anisotropic interactions and domain boundaries. *Math. Biosci. Eng.*, 17(5) (2020), 5883-5906.
4. C. Chalons, P. Goatin and L.M. Villada. High order numerical schemes for one-dimension non-local conservation laws. SIAM *J. Sci. Comput.*, 40(1) (2018), A288-A305.
5. F.A. Chiarello, P. Goatin and E. Rossi. Stability estimates for non-local scalar conservation laws. *Nonlinear Anal. Real World Appl.*, 45 (2019), 668-687.
6. F.A. Chiarello, P. Goatin and L.M. Villada. Lagrangian-Antidiffusive Remap schemes for non-local multi-class traffic flow models. *Comput. Appl. Math.*, 39, 60 (2020).
7. P. Goatin, D. Inzunza and L.M. Villada. Nonlocal macroscopic models of multi-population pedestrian flows for walking facilities optimization. Preprint hal-04191630.
8. P. Goatin and E. Rossi. Well-posedness of IBVP for 1D scalar non-local conservation laws. *Z. Angew. Math. Mech.*, 99(11) (2019).

# Applied Mathematics for some Separation Processes

Stefan Diehl[1]

Centre for Mathemtical Sciences, P.O. Box 22100, Lund University, Sweden
stefan.diehl@math.lth.se

**Summary.** The five stages of applied mathematics — modelling, analysis of the direct problem, analysis of the inverse problem, construction and analyses of numerical schemes, and dissemination of the results by simulation and validation against real data — will be exemplified for some industrial separation processes driven by gravity. Particles and dissolved substances that are either valuable or harmful are separated from a liquid by sedimentation, flotation or filtration in mineral processing, waste- and drinking-water treatment, and chemical industries.

Results in the applied fields often only describe stationary situations or contain ad hoc numerical methods for dynamic simulations. Some reasons for this insufficiency can be found in the mathematical challenges that arise already with balance-law multi-phase models in one dimension expressed by systems of nonlinear convection-diffusion-reaction PDEs with spatially discontinuous coefficients and terms that make the systems degenerate from parabolic to hyperbolic depending on the solution. The mathematical and numerical analysis of such systems constitute challenges with the aim of having reliable and efficient numerical schemes, but also tools for model calibration and control or optimization of the processes.

The talk focuses on the five applied-mathematics stages for sedimentation of particles in a liquid [2, 3, 4, 5, 6, 10], whereas the analogous development for column flotation in mineral processing [1, 7, 8, 9] is detailed in the minisymposium *Numerical methods for mineral processing, wastewater treatment, and related applications*, where also a new biofilm-growth model with numerical scheme of slow sand filtration is presented.

**Keywords**: conservation law, discontinuous flux, degenerate parabolic, inverse problem, sedimentation, flotation

**Mathematics Subject Classifications (2010)**: 35K57, 35L65, 35Q35, 65M06

## References

1. F. Betancourt, R. Bürger, S. Diehl, L. Gutiérrez, M. C. Martí and Y. Vásquez. A model of froth flotation with drainage: simulations and comparison with experiments. *Minerals*, 13, 344, 2023.
2. R. Bürger, J. Careaga and S. Diehl. Flux identification of scalar conservation laws from sedimentation in a cone. *IMA J. Appl. Math.* 83, 526—552, 2018.
3. R. Bürger, J. Careaga, and S. Diehl. A method-of-lines formulation for a model of reactive settling in tanks with varying cross-sectional area. *IMA J. Appl. Math.*, 86(3):514–546, 2021.
4. R. Bürger, J. Careaga, S. Diehl, R. Merckel and J. Zambrano: Estimating the hindered-settling flux function from a batch test in a cone. *Chem. Eng. Sci.* 192, 244—253, 2018.
5. R. Bürger, J. Careaga, S. Diehl and R. Pineda. A moving-boundary model of reactive settling in wastewater treatment. Part 1: Governing equations. *Appl. Math. Modelling*, 106:390–401, 2022.
6. R. Bürger, J. Careaga, S. Diehl and R. Pineda. A moving-boundary model of reactive settling in wastewater treatment. Part 2: Numerical scheme. *Appl. Math. Modelling*, 111:247–269, 2022.
7. R. Bürger, J. Careaga, S. Diehl and R. Pineda. A model of reactive settling of activated sludge: Comparison with experimental data. *Chem. Eng. Sci.*, 267:118244, Mar. 2023.
8. R. Bürger, S. Diehl, M. C. Martí and Y. Vásquez. A degenerating convection-diffusion system modelling froth flotation with drainage. *IMA J. Appl. Math.*, 87(6):1151–1190, 2022.
9. R. Bürger, S. Diehl, M. C. Martí and Y. Vásquez. A difference scheme for a triangular system of conservation laws with discontinuous flux modeling three-phase flows. *Netw. Heterog. Media*, 18:140–190, 2023.
10. J. Careaga and S. Diehl. Entropy solutions and flux identification of a scalar conservation law modelling centrifugal sedimentation. *Math. Meth. Appl. Sci.* 1–28, 2020.

# Mathematical ultrasonics: Analysis and Simulation

Vanja Nikolić[1]

Department of Mathematics, Radboud University, 6525 AJ Nijmegen, The Netherlands
vanja.nikolic@ru.nl

**Summary.** Research in ultrasonics is fueled by a growing number of high-intensity ultrasound applications in medicine and industry. Sound evolution is quasilinear at high intensities or frequencies, and in tissue-like media, nonlocal effects of time-fractional type may come into play. This application field gives rise to many interesting mathematical questions involving such nonlinear and nonlocal wave equations, including discretizations under realistic (smallness) assumptions on the data and dealing with singular behavior in the vanishing limit of medium parameters. In this talk, I will give an overview of these questions and then present recent work on the robust mathematical and numerical analysis of singularly perturbed nonlinear acoustic wave equations. In particular, acoustic equations of Westervelt and Kuznetsov type with (non)local dissipation will be discussed. Here, one can draw parallels from their uniform treatment in the continuous setting, as both rest upon devising appropriate energy functionals that remain stable in the zero parameter limit.

The talk is based on joint works [1]–[4], and [5].

**Keywords**: mathematical ultrasonics, asymptotic-preserving methods

**Mathematics Subject Classifications (2010)**: 65M12, 65M15, 35L72, 65M60

## References

1. B. Dörich and V. Nikolić, Robust fully discrete error bounds for the Kuznetsov equation in the inviscid limit, *in preparation*.
2. B. Kaltenbacher and V. Nikolić, Parabolic approximation of quasilinear wave equations with applications in nonlinear acoustics. SIAM *Journal of Mathematical Analysis*, 54(2): 1593–1622, 2022.
3. Mostafa Meliani and V. Nikolić, Mixed approximation of nonlinear acoustic equations: Well-posedness and a priori error analysis. *Applied Numerical Mathematics*, to appear.
4. V. Nikolić and B. Wohlmuth, A priori error estimates for the finite element approximation of Westervelt's quasilinear acoustic wave equation. SIAM *Journal on Numerical Analysis*, 57(4):1897–1918, 2019.
5. V. Nikolić, Asymptotic-preserving finite element analysis of Westervelt-type wave equations. *arXiv:2303.10743*, 2023.

# Mixed Finite Element Methods for Fluid-Poroelastic Structure Interaction

Sergio Caucao[1], Tongtong Li[2], and Ivan Yotov[3]

Universidad Católica de la Santísima Concepción
scaucao@ucsc.cl
Dartmouth College
tongtong.li@dartmouth.edu
University of Pittsburgh
yotov@math.pitt.edu

**Summary.** The Stokes-Biot model describes the interaction between a free fluid and a fluid in a poroelastic material. The two regions are coupled via suitable interface conditions, including balance of forces, continuity of normal velocity, and no-slip or slip with friction tangential velocity condition. We develop a fully mixed formulation for the Stokes-Biot model. It is based on weakly symmetric deviatoric stress, velocity, and vorticity for Stokes, weakly symmetric stress, displacement, and rotation for elasticity, and mixed velocity and pressure for Darcy flow. This formulation exhibits multiple advantages, including local conservation of mass for the Darcy fluid, local poroelastic and Stokes momentum conservation, accurate approximations with continuous normal components for the Darcy velocity, the poroelastic stress, and the free fluid stress, locking-free behavior, and robustness with respect to the physical parameters. Well posedness of the variational formulation and its mixed finite element approximation is established. Stability and error analysis is performed for the numerical method. Furthermore, we employ a multipoint stress mixed finite element method for the discretization of the Stokes and elasticity equations, as well as a multipoint flux mixed finite element method for the Darcy flow. The method allows for local elimination of the stresses, Darcy velocity, vorticity, and rotation, resulting in a symmetric and positive definite cell centered system involving only the Stokes velocity, displacement, and Darcy pressure. Numerical results are presented to illustrate the performance of the method, including its flexibility and robustness for several geoscience applications.

**Keywords**: fluid-poroelastic structure interaction, Stokes-Biot model, mixed finite element methods, multipoint flux methods

**Mathematics Subject Classifications (2010)**: 76S05, 76D07, 74F10, 35M33, 65M60, 65M12

## References

1. S. Caucao, T. Li, and I. Yotov. A multipoint stress-flux mixed finite element method for the Stokes-Biot model. *Numerische Mathematik*, 152:411-473, 2022.

# Numerical analysis of a porous natural convection system with vorticity and viscous dissipation

Russel Demos[1], Ricardo Ruiz-Baier[2], and Segundo Villa-Fuentes[3]

School of Mathematics, Monash University, 9 Rainforest Walk, Melbourne 3800 VIC, Australia
rdem0006@student.monash.edu
School of Mathematics, Monash University, 9 Rainforest Walk, Melbourne 3800 VIC, Australia
ricardo.ruizbaier@monash.edu
School of Mathematics, Monash University, 9 Rainforest Walk, Melbourne 3800 VIC, Australia
segundo.villafuentes@monash.edu

**Summary.** We propose and analyse a new formulation and pointwise divergence-free mixed finite element methods for the numerical approximation of Darcy–Brinkman equations in vorticity–velocity–pressure form, coupled with a transport equation for thermal energy with viscous dissipative effects and mixed Navier-type boundary conditions. The solvability analysis of the continuous and discrete problems hinges on Banach spaces needed to properly control the advective and dissipative terms in the non-isothermal energy balance equation. Error estimates in appropriate norms are derived, and a few representative numerical examples are provided.

**Keywords**: Flow–transport coupling; Highly permeable porous media; Vorticity-based formulation; Mixed finite element methods; Analysis in Banach spaces; Viscous dissipation.

**Mathematics Subject Classifications (2010)**: 65N30, 65N15, 35Q30, 35K05.

## References

1. M. Amara, E. Chacón Vera, and D. Trujillo. Vorticity–velocity–pressure formulation for Stokes problem. *Math. Comp.*, **73**(248) (2004) 1673–1697.
2. C. Amrouche and I. Boussetouan. Vector potentials with mixed boundary conditions. Application to the Stokes problem with pressure and Navier-type boundary conditions. *SIAM J. Math. Anal.*, **53**(2) (2021) 1745–1784.
3. V. Anaya, M. Bendahmane, D. Mora, and R. Ruiz-Baier, On a vorticity-based formulation for reaction-diffusion-Brinkman systems. *Netw. Heterog. Media*, **13**(1) (2018) 69–94.
4. C.I. Correa and G.N. Gatica. On the continuous and discrete well-posedness of perturbed saddle-point formulations in Banach spaces. *Comput. Math. Appl.*, **117** (2022) 14–23.
5. V. Maz'ya and J. Rossmann. Lp estimates of solutions to mixed boundary value problems for the Stokes system in polyhedral domains. *Math. Nachr.*, **280**(7) 751–793.

## MS1: Recent Advances in polytopic methods

# A deeper investigation on Virtual Element accuracy: the role of bulk and boundary approximations

Lourenco Beirão da Veiga[1] and Giuseppe Vacca[2]

University of Milano-Bicocca
lourenco.beirao@unimib.it
University of Bari
giuseppe.vacca@uniba.it

**Summary.** The Virtual Element Method (VEM) was introduced in [1] as a generalization of the finite element method (FEM) that is able to cope with general polytopal meshes; since its introduction, the VEM enjoyed a large success in the numerical analysis and engineering communities.

The present talk, based on [2], will not deal with advanced applications of the method but rather with its foundations, and may be of interest in general for schemes making use of polygonal meshes. Standard h-interpolation (and convergence) estimates for shape regular meshes in FEM and VEM involve the diameter $h_E$ of elements as the main grid parameter; in the presence of triangular (or quadrilateral) shape regular meshes this gives a complete picture. Instead, in the presence of more general meshes one may wonder if polygons with many small edges (and an associated "richer" discrete space such as those used in VEM or Polygonal FEM) can yield, in some sense, better interpolation properties and if this will reflect also on the final error among the discrete and exact solutions. Basically, the answer is no, but the investigation allows to shed more light on the matter and develop an interesting variant.

Looking into the interpolation capabilities of the VEM space, by a refined analysis we show that the $H^1$ interpolation error on each element (polygon) $E$ can be split into a boundary contribution and a bulk contribution. Although for basic VEM spaces the bulk contribution will dominate the error, this investigation leads to the following idea: if one increases the degree of the VEM only inside the element then the bulk approximation order improves. For such "enriched" VEM, elements with small edges indeed lead to more accurate interpolation in a sense that we will make precise.

In the VEM setting, in order for such refined interpolation property to reflect also on an improved convergence property, one needs also to ameliorate the stability estimates of the scheme. Indeed, standard VEM stabilization estimates assume a bounded number of edges, an hyphotesis that we are able to eliminate leading to final convergence estimates that show an improvement in the presence of many small edges (with respect to standard estimates looking only at the element diameter). Furthermore, we will show some numerical test both for quadrilateral/Voronoi meshes with edge subdivision and on meshes generated by an agglomeration procedure.

**Keywords**: Virtual element method, bubble enrichment, interpolation and stability estimates

**Mathematics Subject Classifications (2010)**: 65N12

## References

1. L. Beirao da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L.D. Marini, A. Russo. Basic principles of the Virtual Element Method. SIAM *Math. Mod. Meth. in Appl. Sci.*, 23:199-214, 2013.
2. L. Beirao da Veiga, G. Vacca. Sharper Error Estimates for Virtual Elements and a Bubble-Enriched Version. *Siam J. Numer. Anal.*, 60:1853-1878, 2022.

# Mixed variational formulations of virtual elements for the polyharmonic operator $(-\Delta)^n$

Franco Dassi[1], David Mora[2], Carlos Reales[3], and Iván Velásquez[4]

Dipartimento di Matematica e Applicazioni, Università degli studi di Milano - Bicocca
franco.dassi@unimib.it
Departamento de Matemáticas, Universidad del Bío-Bío
dmora@ubiobio.cl
Departamento de Matemáticas y Estadística, Universidad de Córdoba
creales@correo.unicordoba.edu.co
Departamento de Ciencias Básicas, Universidad del Sinú-Elías Bechara Zainúm
ivanvelasquez@unisinu.edu.co

**Summary.** In this talk we will present a virtual element method to approximate the solution of a three-dimensional polyharmonic problem $(-\Delta)^n u = g$. The idea behind the proposed approach is to consider $m+1$ or $m$ auxiliary unknowns when $n = 2m+1$ or $n = 2m$, respectively. In the former case, $n = 2m+1$, we will solve $m$ fourth-order problems and a second order one, while, in the latter case, $m$ fourth-order problems have to be solved. To achieve this goal, we use $C^1$ and $C^0$ conforming virtual element spaces for fourth and second order problems, respectively. We also provide the convergence and error estimates for both cases. Finally, we will show a series of numerical tests for $n = 3,4$ and 7, to verify the theoretical results.

**Keywords**: Polyharmonic equation; Ciarlet-Raviart method; virtual element method; polytopal meshes; error estimates.

**Mathematics Subject Classifications (2010)**: 35M30 and 65M99.

# A nonconforming stream virtual element discretization for the Navier-Stokes equations

Dibyendu Adak[1], David Mora[2], and Alberth Silgado[3]

GIMNAP, Departamento de Matemática, Universidad del Bío-Bío, Concepción, Chile.
dadak@ubiobio.cl
GIMNAP, Departamento de Matemática, Universidad del Bío-Bío, Concepción, Chile and CI$^2$MA, Universidad de Concepción, Concepción, Chile
dmora@ubiobio.cl
GIMNAP, Departamento de Matemática, Universidad del Bío-Bío, Concepción, Chile.
asilgado@ubiobio.cl

**Summary.** In this talk, we develop a Morley-type virtual element method for solving the Navier-Stokes problem in stream-function formulation. A stability and error analysis by employing an enriching operator is developed. More precisely, by employing such operator, we provide new discrete Sobolev embeddings, which allow to establish the well-posedness of the discrete formulation and obtain optimal error bounds in broken $H^2$-, $H^1$- and $L^2$-seminorms, under minimal regularity condition on the weak solution. Some important variables such as the velocity, pressure and vorticity are obtained through postprocessing algorithms from the discrete stream-function. Finally, we report several numerical experiments on different polygonal meshes.

**Keywords**: nonconforming virtual element methods, Navier-Stokes equations, stream-function form, discrete Sobolev embeddings, optimal error estimates.

**Mathematics Subject Classifications (2010)**: 65N30, 65N12, 76D05, 65N15.

## References

1. Adak, D. Mora, and A. Silgado. The Morley-type virtual element method for the Navier-Stokes equations in stream-function form on general meshes, arXiv preprint; arXiv:2212.02173.
2. P.F. Antonietti, G. Manzini, and M. Verani. The fully nonconforming virtual element method for biharmonic problems, Math. Models Methods Appl. Sci., **28**(2):387–407, 2018.
3. J. Zhao, B. Zhang, S. Chen and S. Mao. The Morley–type virtual element for plate bending problems. J. Sci. Comput., **76**(1):610–629, 2018.

# Virtual Element Methods for large-scale simulations in complex geometries: polytopal mesh adaptivity

Stefano Berrone[1], Gioana Teora[2], and Fabio Vicini[3]

Politecnico di Torino
stefano.berrone@polito.it
Politecnico di Torino
gioana.teora@polito.it
Politecnico di Torino
fabio.vicini@polito.it

**Summary.** In this presentation, we will discuss key aspects of using Virtual Element Methods (VE methods) to simulate real-world problems. VE methods are gaining attention due to their flexibility in mesh generation for complex geometries. We will start by exploring a new approach that combines mesh generation and refinement from a basic geometric description, particularly focusing on polygonal mesh refinement to address quality preservation and improvement challenges in complex domains.

A novel refinement technique tailored for convex cells will be introduced, incorporating properties conducive to addressing convergence and optimality concerns within adaptive methods. Key aspects in refining general convex polygons encompass a cell refinement strategy contingent solely upon the marked cells for refinement at each step, a partial enhancement of mesh quality, or, at the very least, the maintenance of non-degenerate mesh quality throughout refinement iterations, and a constraint on the number of unknowns in the discrete problem relative to the number of cells in the mesh.

Lastly, our discussion will encompass the simulation of flux within fractured and porous-fractured media, a geological application characterized by exceedingly complex geometric features. Fractures are often modeled as polygons, intersecting within three-dimensional space, while fractured media models are typically stochastically generated, employing probabilistic distributions for fracture density, orientation, and size. The stochastic nature of fractures and their intersections naturally introduces geometric challenges within the simulation domains. Moreover, the large number of fractures and the demand for precise simulations on extensive domains pose mesh generation as a paramount challenge, where the incorporation of polygonal or polyhedral elements, including hanging nodes, greatly simplifies the process, albeit occasionally resulting in the inclusion of elements with suboptimal quality.

**Keywords**: Polygonal mesh generation

**Mathematics Subject Classifications (2010)**: 65N30, 65N50

## References

1. S. Berrone, and A. D'Auria, A new quality preserving polygonal mesh refinement algorithm for Virtual Element Methods, *Finite Elements in Analysis and Design*, Vol. 207, pp. 103502, 2022.
2. S. Berrone, A. Borio, and A. D'Auria, Refinement strategies for polygonal meshes applied to adaptive VEM discretization, *Finite Elements in Analysis and Design*, Vol. 186, pp. 103502, 2021.
3. S. Berrone, and A. Borio, A Residual A Posteriori error estimate for the Virtual Element Method, *Mathematical Models and Methods in Applied Sciences*, Vol. 27, pp. 1423-1458, 2017.
4. S. Berrone, A. Raeli, Efficient partitioning and reordering of conforming virtual element discretizations for large scale Discrete Fracture Network flow parallel solvers, *Engineering Geology*, vol. 306, 106747, 2022.

# Self-stabilized Virtual Element Method

Alessandro Russo[1]

Department of Mathematics and Applications, University of Milano-Bicocca, Italy
and IMATI CNR, Pavia, Italy
alessandro.russo@unimib.it

**Summary.** The Virtual Element Method (VEM) is a recent generalization of classical Finite Element Method to general polygonal and polyhedral meshes. Standard VEM discrete bilinear forms are the sum of a singular part maintaining consistency on polynomials and a stabilizing form enforcing coercivity. The stabilization term has been extensively studied, however it remains a somehow arbitrarily chosen component of VEM with several possible overall effects on the practical applicability of the method.

The aim of this talk is to present some techniques to automatically compute a stabilization term for the Virtual Element Method in simple cases. Shortcoming and benefits of this approach will be discussed.

**Keywords**: finite element method, virtual element method

**Mathematics Subject Classifications (2010)**: 65N30.

## References

1. M. Cremonesi, A. Lamperti, C. Lovadina, U. Perego, A. Russo. Analysis of a self-stabilized quadrilateral virtual element for 2D linear elasticity in the Hu–Washizu formulation. To appear in *Computers & Mathematics with Applications*.

# A lowest order stabilization-free mixed Virtual Element Method

Andrea Borio[1], Carlo Lovadina[2], Francesca Marcon[3], and Michele Visinoni[4]

Politecnico di Torino
andrea.borio@polito.it
University of Milan
carlo.lovadina@unimi.it
Politecnico di Torino
francesca.marcon@polito.it
University of Milan
michele.visinoni@unimi.it

**Summary.** In these years, the study of numerical methods for solving partial differential equations on polygonal and polyhedral meshes has been experiencing a growing interest in the scientific community. One of them, the Virtual Element Method (VEM), gained more and more attention thanks to its great flexibility and robustness in treating elements with arbitrary and highly distorted shapes. The core idea behind VEM consists of using local approximation spaces of functions whose analytical expression is not known, suitable polynomial projections, and particular bilinear forms stabilizing the method. Unfortunately, in some specific cases, the choice of stabilization term can affect the results. Therefore, there is a strong interest in developing self-stabilized virtual elements that preserve the advantages of the VEM.

In this talk, we present a lowest-order self-stabilized VE scheme for the Poisson problem in mixed form. The idea, to avoid the stabilization term, is to use a suitable projection operator over the gradients of harmonic polynomials of suitable degree. A complete theoretical analysis of the stability and convergence is developed in the case of quadrilateral meshes. Some numerical tests are provided in order to show the validity and the potential of our analysis [1].

**Keywords**: Virtual element method, Mixed formulation, Quadrilateral meshes, Poisson problem

**Mathematics Subject Classifications (2010)**: 65N12, 65N30

## References

1. A. Borio, C. Lovadina, F. Marcon, M. Visinoni. A lowest order stabilization-free mixed Virtual Element Method, *Submitted for publication*, 2023.

# Stabilization-free Virtual Element Methods in primal form

Stefano Berrone[1], Andrea Borio[2], Francesca Marcon[3], and Gioana Teora[4]

Politecnico di Torino
stefano.berrone@polito.it
Politecnico di Torino
andrea.borio@polito.it
Politecnico di Torino
francesca.marcon@polito.it
Politecnico di Torino
gioana.teora@polito.it

**Summary.** In the framework of polygonal and polyhedral methods for the solution of partial differential equations, Virtual Element Methods (VEM) play a central role, since they enlarge the class of shapes that can be used in the computational mesh and thus increase the flexibility in handling geometrically complex domains. VEM schemes are based on the definition of local spaces of functions whose analytical expression is not known and suitable polynomial projections of basis functions are used to build consistent discrete bilinear forms, while coercivity is attained introducing a stabilizing operator.

In this talk we introduce a new flavour of VEM in primal form, designed to avoid the use of an arbitrary stabilization term by making use of projections of basis functions on higher order polynomial spaces. These methods preserve the structure of the exact bilinear form and are thus particularly suitable for the solution of problems characterized by anisotropies. We show the theoretical results about the well-posedness of the numerical scheme and display some numerical results highlighting the main features of the method.

**Keywords**: Virtual Element Methods, polygonal meshes, stabilization

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N30

## References

1. S. Berrone, A. Borio, and F. Marcon. Comparison of standard and stabilization free virtual elements on anisotropic elliptic problems. *Applied Mathematics Letters*, 129:107971, 2022.
2. S. Berrone, A. Borio, and F. Marcon. Lowest order stabilization free virtual element method for the 2d poisson equation, 2023. arXiv:2103.16896
3. S. Berrone, A. Borio, F. Marcon, and G. Teora. A first-order stabilization-free virtual element method. *Applied Mathematics Letters*, 142:108641, 2023.
4. A. Borio, M. Busetto, and F. Marcon. SUPG-stabilized stabilization-free VEM: a numerical investigation. Submitted.

# Adaptive virtual element methods: Convergence and optimality

Lourenco Beirão da Veiga[1], Claudio Canuto[2], Ricardo H. Nochetto[3], Giuseppe Vacca[4], and Marco Verani[5]

Dipartimento di Matematica e Applicazioni, Università degli Studi di Milano Bicocca, Via Roberto Cozzi 55 - 20125 Milano, Italy
lourenco.beirao@unimib.it
Dipartimento di Scienze Matematiche G.L. Lagrange, Politecnico di Torino, Corso Duca degli Abruzzi 24 - 10129 Torino, Italy
claudio.canuto@polito.it
Department of Mathematics and Institute for Physical Science and Technology, University of Maryland, College Park - 20742, MD, USA
rhn@math.umd.edu
Dipartimento di Matematica, Università degli Studi di Bari, Via Edoardo Orabona 4 - 70125 Bari, Italy
giuseppe.vacca@uniba.it
MOX-Laboratory for Modeling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano, Piazza Leonardo da Vinci 32 - 20133 Milano, Italy
marco.verani@polimi.it

**Summary.** We design an adaptive virtual element method (AVEM) of lowest order over non-conforming triangular meshes with hanging nodes in 2d, which are treated as polygons. The proposed AVEM [3] concatenates two modules, GALERKIN and DATA. The former deals with piecewise constant data and is shown to be a contraction between consecutive iterates. The latter approximates general data by piecewise constants to a desired accuracy. AVEM hinges on the stabilization-free a posteriori error estimators derived in [2]. We show that AVEM is convergent and quasi-optimal, in terms of error decay versus degrees of freedom, for solutions and data belonging to appropriate approximation classes.

**Keywords**: virtual element method, nonconforming meshes, a posteriori error analysis, stabilization

**Mathematics Subject Classifications (2010)**: 65N30, 65N50

## References

1. A. Cangiani, E. H. Georgoulis, T. Pryer, and O. J. Sutton. A posteriori error estimates for the virtual element method. Numer. Math., 137(4):857-893, 2017.
2. L. Beirão da Veiga, C. Canuto, R. H. Nochetto, G. Vacca, M. Verani, Adaptive VEM: Stabilization-Free A Posteriori Error Analysis. SIAM J. Numer. Anal., 61(2):399-494 (2023).
3. L. Beirão da Veiga, C. Canuto, R. H. Nochetto, G. Vacca, M. Verani, Adaptive VEM for variable data: convergence and optimality. Submitted (2023).

# Polynomial–degree–robust a posteriori estimates for the virtual element method

Théophile Chaumont-Frelet[1], Joscha Gedicke[2], and Lorenzo Mascotto[3]

Inria, Univ. Lille, CNRS, UMR 8524 – Laboratoire Paul Painlevé
theophile.chaumont@inria.fr
Institut für Numerische Simulation, Universität Bonn
gedicke@ins.uni-bonn.de
Dipartimento di Matematica e Applicazioni, Università di Milano Bicocca
lorenzo.mascotto@unimib.it

**Summary.** The virtual element method (VEM) is becoming increasingly popular to discretize PDEs due to its ability to operate on general polytopal meshes and its structure-preserving properties [1]. To reliably assess the error associated with the VEM approximation and efficiently adapt the mesh, *a posteriori* error estimators have been proposed in the literature; see, e.g., [2, 3, 4]. The estimators developed therein are residual-based and have two shortcomings: the constants in the inequalities linking the estimator to the error depend on (i) the polynomial degree of the discretization and (ii) the choice of stabilization. In contrast, for standard finite element (FEM) and discontinuous Galerkin discretizations, equilibrated estimators have been proposed to alleviate these limitations [7]. Although the framework proposed in [7] is fairly general, it cannot be immediately applied to the VEM, due to the nature of the stabilization and the fact that the shape functions are virtual [6]. In this talk, I will present *a posteriori* error estimates that are robust with respect to the polynomial degree and the choice of stabilization [5]. Beyond its intrinsic interest, the development of the estimator introduces new tools that may be helpful for other aspects of the numerical analysis of the VEM.

**Keywords**: a posteriori error estimates; flux-equilibration; high-order methods, virtual element methods.

**Mathematics Subject Classifications (2010)**: 65L60, 65N15.

## References

1. L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L.D. Marini, and A. Russo. Basic principles of virtual element methods. *Mathematical Models and Methods in Applied Sciences*, 23(1):199-214, 2013.
2. L. Beirão da Veiga and G. Manzini. Residual a posteriori error estimation for the virtual element method for elliptic problems. ESAIM *Mathematical Modelling and Numerical Analysis*, 49(2):577-599, 2015.
3. S. Berrone and A. Borio. A residual a posteriori error estimate for the virtual element method. *Mathematical Models and Methods in Applied Sciences*, 27(8), 1423-1458, 2007.
4. A. Cangiani, E.H. Georgoulis, T. Pryer, and O.J. Sutton. A posteriori error estimates for the virtual element method. *Numerische Mathematik*, 137(4):857-893, 2017.
5. T. Chaumont-Frelet, J. Gedicke and L. Mascotto. Generalized gradients for virtual elements and applications to a posteriori error analysis. *In preparation*, 2023.
6. F. Dassi, J. Gedicke and L. Mascotto. Adaptive virtual element methods with equilibrated fluxes. *Applied Numerical Mathematics*, 173:249-278, 2022.
7. A. Ern and M. Vohralík. Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations. SIAM *Journal on Numerical Analysis*, 53(2):1058-1081, 2015.

# Positivity-preserving discretisations in general meshes

Gabriel R. Barrenechea[1]

University of Strathclyde
gabriel.barrenechea@strath.ac.uk

**Summary.** In this talk I will present a method that enforces bound-preservation (at the degrees of freedom) of the discrete solution (recently presented in [1]). The method is built by first defining an algebraic projection onto the convex closed set of finite element functions that satisfy the bounds given by the solution of the PDE. Then, this projection is hardwired into the definition of the method by writing a discrete problem posed for this projected part of the solution. Since this process is done independently of the shape of the basis functions, and no result on the resulting finite element matrix is used, this process guarantees bound-preservation independently of the underlying mesh. The core of the talk will be devoted to explaining the main idea in the context of linear (and nonlinear) reaction-diffusion equations. Then, I will explain the main difficulties encountered when extending this method to convection-diffusion equations, and, more importantly, to a finite element method defined in polytopal meshes. The results in this talk have been carried out in collaboration with Abdolreza Amiri (Strathclyde, UK), Emmanuil Geourgoulis (Heriot-Watt, UK and Athens, Greece), Tristan Pryer (Bath, UK), and Andreas Veeser (Milan, Italy).

**Keywords**: positivity preservation; polyhedral meshes; physical consistency.

## References

1. G.R. Barrenechea, E. Georgoulis, T. Pryer, and A. Veeser, A nodally bound-preserving finite element method. arXiv:2304.01067, *IMA Journal on Numerical Analysis*, to appear.

# High-order interpolatory/quasi-interpolatory serendipity virtual element method for semilinear parabolic problems

Sergio Gómez[1]

University of Milano-Bicocca
sergio.gomezmacias@unimib.it

**Summary.** We present an efficient virtual element method [1] for the numerical approximation of a general class of semilinear parabolic problems of the form

$$\partial_t u - \Delta u + r(u) = 0.$$

The proposed approach exploits the properties of the serendipity version of the virtual element method (VEM), which allows for the elimination of some internal-moment degrees of freedom (DOF) on each element. More precisely, we approximate the nonlinear reaction term $r(u)$ in the problem by its DOF interpolant $\mathscr{I}_h r(u_h)$ in the serendipity VEM space. Such an approximation is computable from the DOF of the discrete solution $u_h$ with a low computational cost. This technique can be easily extended to nonlinear reaction-difussion systems.

The accuracy and efficiency of the proposed method when combined with a second order Strang operator splitting time discretization is illustrated with several numerical experiments.

**Keywords**: semilinear parabolic problem; serendipity; virtual element method; interpolation operator.

**Mathematics Subject Classifications (2010)**: 65M60; 65M12; 35K57; 35K58.

## References

1. S. Gómez. High-order interpolatory serendipity virtual element method for semilinear parabolic problems. Calcolo, 59(3), 25, 2022.

# Parallel multilevel preconditioners for virtual element discretizations of saddle point problems

Tommaso Bevilacqua[1], Franco Dassi[2], Stefano Zampini[3], and Simone Scacchi[4]

Università degli Studi di Milano, Italy
tommaso.bevilacqua@unimi.it
Università degli Studi di Milano-Bicocca, Italy
franco.dassi@unimib.it
King Abdullah University of Science and Technology, Saudi Arabia
stefano.zampini@kaust.edu.sa
Università degli Studi di Milano, Italy
simone.scacchi@unimi.it

**Summary.** The Virtual Element Method (VEM) is a recent technology for the numerical approximation of partial differential equations on computational grids constituted by polygonal or polyhedral elements of very general shape. The aim of this work is to develop effective linear solvers for general order VEM approximations of three-dimensional scalar elliptic equations in mixed form and Stokes equations. To this end, we consider block algebraic multigrid preconditioners and balancing domain decomposition by constraints (BDDC) preconditioners. The latter allow us to use conjugate gradient iterations, although the algebraic linear systems resulting from the discretization of the differential problems are indefinite.

**Keywords**: Virtual Element Method; Saddle-point linear systems; Parallel computing; Domain Decomposition; BDDC method.

**Mathematics Subject Classifications (2010)**: 65F08; 65N30; 65N35; 65N55

## References

1. F. Dassi and S. Scacchi. Parallel solvers for virtual element discretizations of elliptic equations in mixed form. *Computers & Mathematics with Applications*, 79 (7): 1972–1989, 2020.
2. F. Dassi, S. Zampini and S. Scacchi. Robust and scalable adaptive BDDC preconditioners for virtual element discretizations of elliptic partial differential equations in mixed form. *Computer Methods in Applied Mechanics and Engineering*, 391: 114620, 2022.
3. T. Bevilacqua and S. Scacchi. BDDC Preconditioners for Divergence Free Virtual Element Discretizations of the Stokes Equations. *Journal of Scientific Computing*, 92 (2): 63, 2022.

# Nodal auxiliary space preconditioners for mixed virtual element methods

Wietse M. Boon[1] and Erik Nilsson[2]

Politecnico di Milano, Milano, Italy
wietsemarijn.boon@polimi.it
KTH Royal Institute of Technology, Stockholm, Sweden
erikni6@kth.se

**Summary.** This work extends the Hiptmair-Xu nodal space preconditioner for $H(\mathrm{div})$ and $H(\mathrm{curl})$ conforming finite elements to the virtual element framework. For its construction, we first derive regular decompositions of the virtual element spaces on polytopal grids using (tuples of) nodal virtual element spaces. Canonical projection operators are introduced to map from these spaces to facet and edge virtual element spaces. Using the framework of auxiliary space preconditioning, combined with suitable multigrid methods, we derive efficient preconditioners for problems posed in $H(\mathrm{curl})$ and $H(\mathrm{div})$. The preconditioners are particularly robust if elements with large aspect ratios are present in the mesh.

**Keywords**: Virtual Element Methods, preconditioning, robustness

**Mathematics Subject Classifications (2010)**: 65N12, 65N30

# Virtual element approximations for the poroelasticity/elasticity interface problem on polygonal meshes

Sarvesh Kumar[1], David Mora[2], Ricardo Ruiz-Baier[3], and Nitesh Verma[4]

Department of Mathematics, Indian Institute of Space Science and Technology, Thiruvananthapuram 695 547, Kerala, India.
sarvesh@iist.ac.in
GIMNAP, Departamento de Matemática, Universidad del Bío-Bío, Casilla 5-C, Concepción, Chile; and CI$^2$MA, Universidad de Concepción, Chile.
dmora@ubiobio.cl
School of Mathematical Sciences and Victorian Heart Institute, Monash University, 9 Rainforest Walk, Melbourne 3800 VIC, Australia; and World-Class Research Center "Digital biodesign and personalized healthcare", Sechenov First Moscow State Medical University, Moscow, Russia; and Universidad Adventista de Chile, Casilla 7-D, Chillán, Chile.
ricardo.ruizbaier@monash.edu
Departamento de Matemática, Universidad del Bío-Bío, Casilla 5-C, Concepción, Chile.
nverma@ubiobio.cl

**Summary.** In this talk, we propose, analyse and implement a virtual element discretisation for an interfacial poroelasticity/elasticity consolidation problem. The formulation of the time–dependent poroelasticity equations uses displacement, fluid pressure and total pressure, and the elasticity equations are written in displacement-pressure formulation. The construction of the virtual element scheme does not require Lagrange multipliers to impose the transmission conditions (continuity of displacement and total traction, and no–flux for the fluid) on the interface. We show the stability and convergence of the virtual element method for different polynomial degrees, and the error bounds are robust with respect to delicate model parameters (such as Lamé constants, permeability, and storativity coefficient). Finally we provide numerical examples that illustrate the properties of the scheme.

**Keywords**: Biot equations, virtual element methods, time-dependent problems, a priori error analysis.

**Mathematics Subject Classifications (2010)**: 65M60, 74F10, 35K57, 74L15.

## References

1. L. Beirão da Veiga, C. Lovadina, and G. Vacca. Divergence free virtual elements for the Stokes problem on polygonal meshes. ESAIM: Mathematical Modeling in Numerical Analysis, 51(2), 509–535, 2017.
2. R. Bürger, S. Kumar, D. Mora, R. Ruiz-Baier, and N. Verma. Virtual element methods for the three-field formulation of time-dependent linear poroelasticity. Advances in Computational Mathematics, 47: 2021.
3. V. Girault, G. Pencheva, M. F. Wheeler, and T. Wildey. Domain decomposition for poroelasticity and elasticity with DG jumps and mortars. Mathematical Models and Methods in Applied Sciences, 21: 169–213, 2011.
4. V. Girault, M.F. Wheeler, B. Ganis, and M.E. Mear. A lubrication fracture model in a poro-elastic medium. Mathematical Models and Methods in Applied Sciences, 25: 587–645, 2015.

# A $C^1$-conforming arbitrary-order two-dimensional Virtual Element Method for the fourth-order phase-field equation

Gianmarco Manzini[1], Dibyendu Adak[2], Yu Leng[3], Jeeyon N. Plohr[4], and Hashem Mourad[5]

Applied Mathematics and Plasma Physics, T-5, Theoretical Division,
Los Alamos National Laboratory, Los Alamos, NM, USA
gmanzini@lanl.gov
Applied Mathematics and Plasma Physics, T-5, Theoretical Division,
Los Alamos National Laboratory, Los Alamos, NM, USA
dadak@lanl.gov
Fluid Dynamics and Solid Mechanics, T-3, Theoretical Division,
Los Alamos National Laboratory, Los Alamos, NM, USA
yleng@lan.gov
Materials and Physical Data, XCP-5, Computational Physics Division,
Los Alamos National Laboratory, Los Alamos, NM, USA
jplohr@lanl.gov
Fluid Dynamics and Solid Mechanics, T-3, Theoretical Division,
Los Alamos National Laboratory, Los Alamos, NM, USA
mourad@lanl.gov

**Summary.** We present a conforming virtual element method [1] for the two-dimensional High-Order Phase Field (HOPF) equation [2]. This equation is a fourth-order equation and our numerical approximation relies on the design of an arbitrary order accurate, virtual element space with $C^1$ global regularity. Such regularity is guaranteed by taking the values of the virtual element functions and their full gradient at the mesh vertices as degrees of freedom. High-order accuracy requires also edge polynomial moments of the trace of the virtual element functions and their normal derivatives. A set of representative test cases assess the behavior of the method.

**Keywords**: High-order Phase-Field (HOPF) model, virtual element method, high-regular conforming method

**Mathematics Subject Classifications (2010)**: 65M12, 65M15, 65M60

## References

1. L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, and A. Russo. Basic principles of virtual element methods. *Math. Models Methods Appl. Sci.*, 23(1):199–214, 2013.
2. D. Adak, G. Manzini, H. M. Mourad, J. N. Plohr, L. Svolos A C1-conforming arbitrary-order two-dimensional virtual element method for the fourth-order phase-field equation. Los Alamos Technical Report N. LA-UR 21-31995

# A Reynolds semi-robust and pressure-robust Hybrid High-Order method for the solution of the incompressible Navier–Stokes equations on general meshes

Daniel Castanon Quiroz[1] and Daniele A. Di Pietro[2]

Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas, Universidad Nacional Autónoma de México, México.
daniel.castanon@iimas.unam.mx
IMAG, Univ Montpellier, CNRS, Montpellier, France.
daniele.di-pietro@umontpellier.fr

**Summary.** In this presentation we introduce and analyze a novel Reynolds semi-robust and pressure-robust Hybrid High-Order method for the time dependent incompressible Navier–Stokes equations on general meshes. A numerical scheme is called "Reynolds semi-robust" if its velocity error estimates are independent of the Reynolds number (or $\nu^{-1}$). On the other hand, pressure robustness means that the velocity error estimates are independent of the pressure. The importance of the pressure robustness property is that gives a proper momentum balance for the numerical simulation of the Navier–Stokes equations which is crucial when large rotational body forces are present. The proposed method supports arbitrary approximation orders, and is (relatively) inexpensive thanks to the possibility of statically condensing a subset of the unknowns at each time iteration. In particular, using polynomials of degree $k \geq 0$ at mesh faces, and polynomials of degree $(k+1)$ at mesh elements, we formally prove a velocity error estimate in the $L^\infty(L^2(\Omega))$-norm of order $h^{k+\frac{1}{2}}$ which equals to the best known velocity error estimate on simplicial meshes.

**Keywords**: hybrid high-order methods; time-dependent incompressible flow; general meshes; Re-semi-robust error estimates; pressure robustness

**Mathematics Subject Classifications (2010)**: 35Q30, 65M15, 65M60, 76D17, 76M10

# Symplectic Hamiltonian finite element methods for semilinear wave propagation

Manuel A. Sánchez[1] and Joaquín Valenzuela[2]

Institute for Mathematical and Computational Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile
manuel.sanchez@uc.cl
School of Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile
javalenzuela3@uc.cl

**Summary.** This paper presents Hamiltonian finite element methods for approximating a class of semilinear wave propagation problems, including the nonlinear Klein-Gordon and sine-Gordon equations. The aim is to obtain accurate high-order approximations while conserving physical quantities of interest such as energy. To achieve conservation properties at a discrete level, we propose semidiscrete schemes based on two Hamiltonian structures of the equation. These include Mixed finite element methods, discontinuous Galerkin methods, and hybridizable discontinuous Galerkin methods (HDG). In particular, we propose a new class of DG methods using time operators to define the numerical traces resulting in an energy-conserving scheme. Symplectic explicit-partitioned, and diagonally-implicit Runge Kutta schemes are used for time discretization. We present numerical examples illustrating the approximations' accuracy and energy conservation of the approximations and the simulation of soliton cloning.

**Keywords**: hybridizible discontinuous Galerkin, Hamiltonian systems, semilinear wave

**Mathematics Subject Classifications (2010)**: Numerical Analysis (math.NA)

*M.A. Sánchez was partially supported by FONDECYT Iniciación grant n. 11180284 and FONDECYT Regular N. 1221189 and by Centro Nacional de Inteligencia Artificial CENIA, FB210017, Basal ANID Chile. J. Valenzuela was partially supported by FONDECYT Iniciación grant n. 11180284 and FONDECYT Regular N. 1221189.

# An Incomplete Balancing Domain Decomposition Method based on Polynomial Finite Element Spaces

Daisuke Tagami[1]

Institute of Mathematics for Industry (IMI), Kyushu University
tagami@imi.kyushu-u.ac.jp

**Summary.** A Balancing Domain Decomposition (BDD) method is originally proposed by Mandel [1], and is regarded as the preconditioner of linear iterative solvers for artificial boundary problems appearing in Domain Decomposition Methods (DDM) based on finite element methods; see, for example, Glowinski, et al. [2]. There exist many literatures on the application of BDD into large-scale computational models; see, for example in case of elastic problems, Ogino, et al. [3].

On the other hand, we have already computed ultra large-scale computational models derived from finite element methods for magnetic field problems by using iterative DDM; see, for example, Sugimoto, et al. [4]. However, in [4], we have used a simplified diagonalization as the preconditioner. Therefore, we require more effective preconditioner to reduce computational costs much more, and try to apply a BDD method into the preconditioner of an iterative DDM for magnetic field problems, where the magnetic vector potential is regarded as an unknown function.

When using a BDD method, we need to set a coarse space, which includes the kernel of the coefficient matrix of resultant linear system derived from a corresponding artificial boundary problem. In case of magnetic field problems, the number of the Degrees Of Freedom (DOF) of the coarse space is equal to the number of nodal points of triangulation. This fact leads BDD methods for magnetic field problems can keep the condition number of the coefficient matrix of resultant linear system, but we cannot expect to reduce their computational costs.

Now, to reduce the number of DOF of coarse spaces in BDD methods and their computational costs, Polytopal Element Methods (PEM; see Di Pietro, et al. [5]) is introduced, and is used for approximations of the coarse space with Domain-by-Domain methods. We call the method *incomplete BDD*. Owing to the approximation of coarse spaces, we can expect to reduce computational costs to solve coarse-space problems as well as to keep the condition number of the coefficient matrix of resultant linear system.

**Keywords**: balancing domain decomposition, discrete de Rham sequence, polytopal element, perturbed magnetostatic problem, polyhedral mesh

**Mathematics Subject Classifications (2010)**: 65N55, 78M10, 78M25

## References

1. Mandel, J. “Balancing domain decomposition,” *Commun. Numer. Methods Engrg.*, vol. 9, no. 3, pp. 233–241, 1993.
2. Glowinski, R., Dinh, Q., and Periaux, J. “Domain decomposition methods for nonlinear problems in fluid dynamics,” *Compt. Meths. Appl. Mech. Engrg.*, vol. 40, no. 1, pp. 27–109, 1983.
3. Ogino, M., Shioya, R., and Kanayama, H. “An inexact balancing preconditioner for large-scale structural analysis,” *J. Comput. Sci. Tech.*, vol. 2, pp. 150–161, 2008.
4. Sugimoto, S., Tagami, D., Ogino, M., Takei, A., and Kanayama, H. “Improvement of convergence in time-harmonic Eddy current analysis with hierarchical domain decomposition method,” *Trans. Japan Soc. Simul. Tech.*, vol. 7, no. 1, pp. 11–17, 2015.
5. Di Pietro, D. A. and Droniou, J. “An arbitrary-order method for magnetostatics on polyhedral meshes based on a discrete de Rham sequence,” *J. Comput. Phys.*, vol. 429, Article-ID 109991, 2021.

# A locking-free polygonal staggered DG method for the Biot system of poroelasticity

Lina Zhao[1], Eric Chung[2], and Eun-Jae Park[3]

Department of Mathematics, City University of Hong Kong, Kowloon Tong, Hong Kong SAR, China.
linazha@cityu.edu.hk
Department of Mathematics, The Chinese University of Hong Kong, Hong Kong SAR, China.
tschung@math.cuhk.edu.hk
School of Mathematics and Computing (Computational Science and Engineering), Yonsei University, Seoul 03722, Korea.
ejpark@yonsei.ac.kr

**Summary.** In this talk, we present a staggered discontinuous Galerkin method for a five-field formulation of the Biot system of poroelasticity on general polygonal meshes. Elasticity is equipped with stress-displacement-rotation formulation with weak stress symmetry for arbitrary polynomial orders, which extends the piecewise constant approximation developed in (L. Zhao and E.-J. Park, SIAM J. Sci. Comput. 42:A2158-A2181,2020). The proposed method is locking free and can handle highly distorted grids possibly including hanging nodes, which is desirable for practical applications. We prove the convergence estimates for the semi-discrete scheme and fully discrete scheme for all the variables in their natural norms. In particular, the stability and convergence analysis do not need a uniformly positive storativity coefficient. Moreover, to reduce the size of the global system, we propose a five-field formulation based fixed stress splitting scheme, where the linear convergence of the scheme is proved. Several numerical experiments are carried out to confirm the optimal convergence rates and the locking-free property of the proposed method.

**Keywords**: Staggered DG, General polygonal mesh, Locking-free, Fixed stress splitting, Weak symmetry, Biot system, Poroelasticity

## References

1. L. Zhao and E.-J. Park A staggered cell-centered DG method for linear elasticity on polygonal meshes. *SIAM J. Sci. Comput.*, 42, A2158-A2181, 2020.
2. L. Zhao, E. Chung, and E.-J. Park Locking free staggered DG method for the Biot system of poroelasticity on general polygonal meshes *IMA Journal of Numerical Analysis*, 43, 2777-2816, 2023.

# MS2: Approximation and analysis of partial differential equations with singular data

# Source regularization through projection in dual norms for nonconforming finite element discretizations

Ignacio Muga[1], Sergio Rojas[2], Kristoffer G. van der Zee[3], and Patrick Vega[4]

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile
ignacio.muga@pucv.cl
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile
sergio.rojas.h@pucv.cl
School of Mathematical Sciences, University of Nottingham, UK
KG.vanderZee@nottingham.ac.uk
Departamento de Matemática y Ciencia de la Computación, Universidad de Santiago de Chile, Chile.
patrick.vega@usach.cl

**Summary.** We propose an adaptive projection method for the regularization of continuous linear functionals acting on Sobolev spaces. We focus on projections onto finite element spaces, computing the best approximation measured in a dual norm. Irregular functionals act in more regular spaces, so the number of degrees of freedom associated with conforming finite element spaces increases, motivating the use of nonconforming discretizations as an extension of their conforming counterpart [1]. Working with nonconforming finite elements is non-trivial if the source term is not in the dual of the finite element space, making our approach particularly useful in this context [2], since the regularization belongs to such a dual space. This approach also computes a residual representative as an additional unknown in an equivalent mixed variational formulation, which, together with the projections, are computed through an adaptive mesh refinement procedure driven by the residual representative. For computability reasons, we use a discrete dual norm that supremizes over a nonconforming finite element space. We propose nonconforming compatible pairs and, therefore, obtain quasi-optimal convergent methods. Finally, we show how our projection method can efficiently compute nonconforming approximations to partial differential equations with (ultra) rough data.

**Keywords**: projection in dual norms, adaptive regularization, a posteriori error analysis, residual minimization, nonconforming discretizations.

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N22, 65N30, 65N50.

**Funding**: IM was supported by the Chilean National Agency for Research and Development (ANID) through FONDECYT project 1230091. SR was supported by the Chilean grant ANID FONDECYT 3210009. K. G. vdZ was partially funded by the Engineering and Physical Sciences Research Council (EPSRC), UK, under Grant EP/W010011/1. PV was funded by the Chilean grant ANID FONDECYT 3220858.

## References

1. F. Millar, I. Muga, S. Rojas, and K. G. van der Zee. Projection in negative norms and the regularization of rough linear functionals. *Numerische Mathematik*, 150, 1087-1121, 2022.
2. I. Muga, S. Rojas, K. G. van der Zee, and P. Vega. Source regularization through projection in dual norms for nonconforming finite element discretizations. *In preparation*, 2023.

# Goal-oriented adaptive multilevel quasi-Monte Carlo for elliptic random PDEs

Joakim Beck[1], Yang Liu[2], Erik von Schwerin[3], and Raúl Tempone[4]

Computer, Electrical and Mathematical Sciences and Engineering, 4700 King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia.
joakim.beck@kaust.edu.sa
Computer, Electrical and Mathematical Sciences and Engineering, 4700 King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia.
yang.liu.3@kaust.edu.sa
Computer, Electrical and Mathematical Sciences and Engineering, 4700 King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia.
erik.vonschwerin@kaust.edu.sa
Computer, Electrical and Mathematical Sciences and Engineering, 4700 King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia and Alexander von Humboldt Professor in Mathematics for Uncertainty Quantification, RWTH Aachen University, 52062 Aachen, GERMANY.
raul.tempone@kaust.edu.sa

**Summary.** We present our work titled "Goal-oriented adaptive multilevel quasi-Monte Carlo (MLQMC) for elliptic random PDEs," building upon [Beck, Joakim, et al., "Goal-oriented adaptive finite element multilevel Monte Carlo with convergence rates." Computer Methods in Applied Mechanics and Engineering (2022)] and other ongoing research. Our objective is to solve an elliptic partial differential equation (PDE) with lognormal random input data, when the PDE model faces geometry-induced singularity.

Earlier research [Moon, K-S., et al. "Convergence rates for an adaptive dual weighted residual finite element algorithm." BIT Numerical Mathematics 46.2 (2006)] established convergence rates for a goal-oriented adaptive algorithm. This algorithm utilized isoparametric d-linear quadrilateral finite element approximations and the dual weighted residual error representation in a deterministic context. Notably, this algorithm refines the mesh based on the error's impact on the Quantity of Interest (QoI).

Our current work seeks to merge MLMC/MLQMC with the adaptive finite element solver. Unlike traditional Multilevel Monte Carlo methods, where each sample is determined using a discretization-based numerical method (with resolution tied to the level), our adaptive MLMC (AMLMC) algorithm employs a series of tolerances as its levels. Specifically, for a particular realization of the input coefficient and a set accuracy level, the AMLMC formulates its approximate sample using the initial mesh from the sequence of deterministic, non-uniform meshes. These meshes are produced by the previously mentioned adaptive algorithm and meet the sample-dependent bias constraint. Additionally, the incorporation of QMC enhances the convergence rate.

**Keywords**: Multilevel quasi-Monte Carlo, Goal-oriented adaptivity, Computational complexity, Finite elements, Partial differential equations with random data, Lognormal diffusion

**Mathematics Subject Classifications (2010)**: 65C05 65N50 65N22 35R60

## References

1. J. Beck, Y. Liu, E. von Schwerin and R. Tempone. Goal-oriented adaptive finite element multilevel Monte Carlo with convergence rates. *Computer Methods in Applied Mechanics and Engineering*, 402:115582, 2022.
2. K-S. Moon, E. von Schwerin, A. Szepessy and R. Tempone. Convergence rates for an adaptive dual weighted residual finite element algorithm. BIT *Numerical Mathematics*, 46:367-407, 2006.

# Bilinear optimal control for the fractional Laplacian: error estimates on Lipschitz domains

Francisco Bersetche[1], Francisco Fuica[2], Enrique Otárola[3], and Daniel Quero[4]

Universidad Técnica Federico Santa María
bersetche@gmail.com
Pontificia Universidad Católica de Chile
Francisco.fuica@mat.uc.cl
Universidad Técnica Federico Santa María
enrique.otarola@usm.cl
Universidad Técnica Federico Santa María
daniel.quero@alumnos.usm.cl

**Summary.** Given a desired state $u_\Omega \in L^2(\Omega)$ and a regularization parameter $\lambda > 0$, we introduce the cost functional

$$J(u,q) = \frac{1}{2}\|u - u_\Omega\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|q\|^2_{L^2(\Omega)}. \tag{1}$$

Let $f \in L^2(\Omega)$ be a fixed function. We shall be concerned with the following optimal control problem: Find $\min J(u,q)$ subject to the fractional elliptic PDE

$$(-\Delta)^s u + qu = f \text{ in } \Omega, \quad u = 0 \text{ in } \Omega^c, \tag{2}$$

where $\Omega^c = \mathbb{R}^d \setminus \Omega$, and the control constraints

$$q \in \mathbb{Q}_{ad}, \quad \mathbb{Q}_{ad} := \{v \in L^\infty(\Omega) : a \leq v(x) \leq b \text{ for a.e. } x \in \Omega\}. \tag{3}$$

Here, the control bounds $a$ and $b$ are such that $0 < a < b$ and $(-\Delta)^s$ corresponds to the integral definition of the fractional Laplace operator, namely:

$$(-\Delta)^s w(x) := C(d,s)\text{p.v.} \int_{\mathbb{R}^d} \frac{w(x) - w(y)}{|x-y|^{d+2s}} \mathrm{d}y, \quad C(d,s) := \frac{2^{2s} s \Gamma(s + \frac{d}{2})}{\pi^{\frac{d}{2}} \Gamma(1-s)},$$

where p.v. stands for the Cauchy principal value and $C(d,s)$ is a normalization constant.

In this work we establish the existence of optimal solutions and analyze first and, necessary and sufficient, second order optimality conditions. Regularity estimates for optimal variables are also analyzed. We devise two strategies of finite element discretization: a semidiscrete scheme where the control variable is not discretized 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, fractional diffusion, integral fractional Laplacian, first and second order optimality conditions, regularity estimates, finite elements, convergence, error estimates.

**Mathematics Subject Classifications (2010)**: 35R11, 49J20, 49K20, 49M25, 65K10, 65N15, 65N30.

## References

1. F. Bersetche, F. Fuica, E. Otarola, and D. Quero, *Bilinear optimal control for the fractional laplacian: error estimates on lipschitz domains*, 2023. arXiv:2112.07114.
2. C. Kenne, G. Mophou, and M. Warma, *Bilinear optimal control for a fractional diffusive equation*, arXiv e-prints, (2022), p. arXiv:2210.17494.
3. A. Kröner and B. Vexler, *A priori error estimates for elliptic optimal control problems with a bilinear state equation*, J. Comput. Appl. Math., 230 (2009), pp. 781–802.

# A pointwise tracking optimal control problem for the stationary Navier–Stokes equations

Francisco Fuica[1] and Enrique Otárola[2]

Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna 4860, Santiago, Chile.
francisco.fuica@mat.uc.cl
Departamento de Matemática, Universidad Técnica Federico Santa María, Valparaíso, Chile.
enrique.otarola@usm.cl

**Summary.** We study a pointwise tracking optimal control problem for the stationary Navier–Stokes equations; control constraints are also considered. The problem entails the minimization of a cost functional involving point evaluations of the state velocity field, thus leading to an adjoint problem with a linear combination of Dirac measures as a forcing term in the momentum equation, and whose solution has reduced regularity properties. We analyze the existence of optimal solutions and derive first and, necessary and sufficient, second order optimality conditions in the framework of regular solutions for the Navier–Stokes equations. We develop two discretization strategies: a semidiscrete strategy in which the control variable is not discretized, and a fully discrete scheme in which the control variable is discretized with piecewise constant functions. For each solution technique, we analyze convergence properties of discretizations and derive a priori error estimates.

**Keywords**: optimal control problem, Navier–Stokes equations, Dirac measures, first and second order optimality conditions, finite element approximations, convergence, error estimates.

**Mathematics Subject Classifications (2010)**: 35Q30, 35Q35, 35R06, 49J20, 49K20, 49M25, 65N15, 65N30.

## References

1. A. Allendes, F. Fuica, and E. Otárola. Error estimates for a pointwise tracking optimal control problem of a semilinear elliptic equation. *SIAM Journal on Control and Optimization*, 60(3):1763–1790, 2022.
2. E. Casas, M. Mateos, and J.-P. Raymond. Error estimates for the numerical approximation of a distributed control problem for the steady-state Navier-Stokes equations. *SIAM Journal on Control and Optimization*, 46(3):952–982, 2007.
3. E. Casas and K. Kunisch. Optimal control of the two-dimensional stationary Navier-Stokes equations with measure valued controls. *SIAM Journal on Control and Optimization*, 57(2):1328–1354, 2019.

# Computational polyconvexification of isotropic functions

Timo Neumeier[1], Malte A. Peter[2], Daniel Peterseim[3], and David Wiedemann[4]

Institute of Mathematics, University of Augsburg, Universitatsstr. 12a, 86159 Augsburg, Germany
timo.neumeier@uni-a.de
Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences (CAAPS), University of Augsburg, Universitätsstr. 12a, 86159 Augsburg, Germany
malte.peter@uni-a.de
Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences (CAAPS), University of Augsburg, Universitätsstr. 12a, 86159 Augsburg, Germany
daniel.peterseim@uni-a.de
Institute of Mathematics, University of Augsburg, Universitatsstr. 12a, 86159 Augsburg, Germany
david.wiedemann@uni-a.de

**Summary.** Based on the characterization of the polyconvex envelope of isotropic functions by their signed singular value representations, we propose a simple algorithm for the numerical approximation of the polyconvex envelope. Instead of operating on the dxd-dimensional space of matrices, the algorithm requires only the computation of the convex envelope of a function on a d-dimensional manifold, which is easily realized by standard methods. The significant speedup associated with the dimension reduction from dxd to d is demonstrated in a series of numerical experiments

# Curvature and the HHJ Method

Shawn W. Walker[1]

Louisiana State University
walker@math.lsu.edu

**Summary.** This talk presents some recent advances in extending the classic Hellan–Herrmann–Johnson (HHJ) finite element to surfaces for approximation of bending problems and computing curvature. We give a brief review of the surface version of the HHJ method which leads to a convergent method to solve the surface Kirchhoff plate problem on surfaces embedded in $\mathbb{R}^3$, along with numerical examples. We also describe a post-processing technique for approximating the surface Hessian of a scalar function from discrete data. We show how this scheme is easily extended to give convergent approximations of the *full shape operator* of the underlying surface, even for piecewise linear triangulations. Several numerical examples are given on non-trivial surfaces to illustrate the method. Lastly, we describe on-going work on how the surface HHJ scheme can be modified for computing Willmore flow.

**Keywords**: surface finite elements, surface Hessian, Kirchhoff plate, bending, shape operator, non-conforming method.

**Mathematics Subject Classifications (2010)**: 65D18, 65N30, 35J40

## References

1. Douglas N. Arnold and Shawn W. Walker. The Hellan–Herrmann–Johnson Method with Curved Elements. SIAM *Journal on Numerical Analysis*, 58(5):2829-2855, 2020.
2. Shawn W. Walker. The Kirchhoff Plate Equation on Surfaces: The Surface Hellan–Herrmann–Johnson Method. IMA *Journal of Numerical Analysis*, 42(4):3094-3134, 2021.
3. Shawn W. Walker. Approximating the Shape Operator with the Surface HHJ Element. *in review*, 2023.

## MS3: Boundary integral equations in coupled physical systems

# Runge-Kutta convolution quadrature based on Gauss methods

Lehel Banjai[1] and Mateo Ferrari[2]

Maxwell Institute for Mathematical Sciences, Department of Mathematics, Heriot-Watt University Edinburgh, EH14 4AS, United Kingdom
l.banjai@hw.ac.uk
Dipartimento di Scienze Matematiche G.L. Lagrange Politecnico di Torino, Torino, 10129, Italy
matteo.ferrari@polito.it

**Summary.** In this talk, we delve into a discretization technique for time-domain boundary integral operators, Convolution Quadrature (CQ) combined with Galerkin BEM or spatial collocation.

We present an error analysis of Runge-Kutta CQ based on Gauss methods applied to hyperbolic operators. The order of convergence relies heavily on the parity of the number of stages, a more favourable situation arising for the odd cases than the even ones. Moreover, for particular situations the order of convergence is higher than for Radau IIA or Lobatto IIIC methods when using the same number of stages.

We further investigate an application to transient acoustic scattering where, for certain scattering obstacles, the favourable situation occurs in the important case of the exterior Dirichlet-to-Neumann map. Numerical experiments and comparisons show the performance of the method.

**Keywords**: Runge-Kutta Gauss methods, convolution quadrature, wave equation, Dirichlet-to-Neumann

**Mathematics Subject Classifications (2010)**: 65R20 , 65L06 , 65M15

## References

1. L. Banjai, M. Ferrari. Runge-Kutta convolution quadrature based on Gauss methods. arXiv:2212.07170, 2022.

# Bridging boundaries in molecular electrostatics: towards leveraging BEM-based tools into scientific communities

Christopher D. Cooper[1]

Universidad Técnica Federico Santa María
christopher.cooper@usm.cl

**Summary.** In the domain of computational chemistry, the Poisson-Boltzmann equation stands as a pillar for understanding the electrostatic properties of biomolecules immersed in aqueous environments. Our work explores into the application of the Boundary Element Method (BEM) to solve this equation, offering a precise and versatile numerical framework. This presentation elucidates the unique advantages of BEM in this context, highlighting its accuracy describing the molecular geometry and charges, and treatment of boundary conditions at infinity, and also its limitations in terms of the linear approximation and variation of material parameters in space.

We go beyond the theoretical foundations to discuss practical applications where the boundary integral representation of equations provides a significant advantage over alternative methods. However, our journey does not end with mathematical rigor; it extends into the realm of software development. We introduce the Poisson-Boltzmann & Jupyter (PBJ) code as evidence to our commitment to building robust, sustainable, and user-friendly numerical tools. We stress the importance of making these advanced tools accessible to the computational chemistry community, recognizing that the path to community adoption is fraught with challenges.

Join us in exploring the boundaries of molecular electrostatics, where mathematics, software development, and community engagement converge in pursuit of a common goal: advancing our understanding of the intricate world of biomolecular interactions.

**Keywords**: boundary element method, Poisson-Boltzmann, molecular electrostatics, Jupyter

**Mathematics Subject Classifications (2010)**: 92E10, 92C40, 45A05

## References

1. C.D. Cooper, J.P: Bardhan, and L.A. Barba biomolecular electrostatics solver using Python, GPUs and boundary elements that can handle solvent-filled cavities and Stern layers *Computer Physics Communications*, 185 (3): 720-729, 2014.
2. S.D. Search, C.D. Cooper, and E. van't Wout Towards optimal boundary integral formulations of the Poisson–Boltzmann equation for molecular electrostatics *Journal of Computational Chemistry*, 43 (10): 674-691, 2022.
3. I. Addison-Smith, H.V. Guzmán, and C.D. Cooper Accurate Boundary Integral Formulations for the Calculation of Electrostatic Forces with an Implicit-Solvent Model *Journal of Chemical Theory and Computation*, 19 (10):2996-3006, 2023.

# Enhancing Predictive Accuracy in Molecular Electrostatics: Coupling Finite and Boundary Elements with Variable Permittivity

Mauricio Guerrero[1] and Christopher Cooper[2]

Universidad Tecnica Federico Santa Maria
mauricio.guerrero.14@sansano.usm.cl
Universidad Tecnica Federico Santa Maria
christopher.cooper@usm.cl

**Summary.** In the domain of molecular biophysics, electrostatic interactions hold a pivotal role in diverse applications, ranging from the analysis of molecular interactions to drug design. Calculating solvation and binding energies is a common practice in these studies, often facilitated by continuous models that simplify complex molecular structures and computational costs. These models delineate the domain into two regions, the solute and solvent, separated by an interface, and apply the Poisson-Boltzmann equation across these regions.

However, a challenge arises when accurately representing the region proximate to the solute-solvent interface, where the constant permittivity description employed by the boundary element method, which we use, may falter in capturing the intricacies of the electrostatic field.

In response to this challenge, we present an innovative approach that couples finite and boundary elements while incorporating variable permittivities. Instead of abrupt changes in permittivity, we introduce a refined technique aimed at smoothing the transition zone. This approach enables us to enhance predictive accuracy in molecular electrostatics.

Computational implementation of this method is realized using state-of-the-art software tools such as Dolfin and Bempp, facilitating the seamless integration of finite and boundary elements.

Our results demonstrate significant improvements in predictive accuracy, particularly in the calculation of solvation and binding energies. We compare our findings with established datasets, underscoring the superior predictive capabilities of our approach.

In conclusion, our work offers a promising avenue for advancing predictive accuracy in molecular electrostatics. By coupling finite and boundary elements with variable permittivity, we mitigate the limitations of existing models and provide a valuable tool for researchers in the field. Our participation in this conference seeks to foster discussion and collaboration, opening doors to further refinement and broader applications of this innovative approach.

**Keywords**: BEM, FEM, Poisson-Boltzmann, Molecular electrostatics.

**Mathematics Subject Classifications (2010)**: 92E10, 92C40, 45A05

## References

1. Wang, S., Alexov, E., and Zhao, S. On regularization of charge singularities in solving the Poisson-Boltzmann equation with a smooth solute-solvent boundary *Mathematical biosciences and engineering: MBE*, 18 (2): 1370, 2021.
2. Yoon, B. J., and Lenhoff, A. M. A boundary element method for molecular electrostatics with electrolyte effects *Journal of Computational Chemistry*, 11 (9), 1080-1086, 1990.
3. Shaw, P. B. Theory of the Poisson Green's function for discontinuous dielectric media with an application to protein biophysics *Physical Review A*, 32 (4), 2476, 1985.

# Parametric Shape Holomorphy of Boundary Integral Operators: Applications to Operator Learning and Multifidelity Bayesian Inversion

Fernando Henríquez[1], Ivan Bioli[2], and Jürgen Dölz[3]

MCSS, Chair of Computational Mathematics and Simulation Science, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland
fernando.henriquez@epfl.ch,ivan.bioli@epfl.ch
Institute for Numerical Simulation, University of Bonn, Friedrich-Hirzebruch-Allee 7, 53115 Bonn, Germany.
doelz@ins.uni-bonn.de
Institute for Numerical Simulation, University of Bonn, Friedrich-Hirzebruch-Allee 7, 53115 Bonn, Germany.
doelz@ins.uni-bonn.de

**Summary.** We consider a family of boundary integral operators supported on a collection of parametrically defined bounded Lipschitz boundaries. These operators depend on parametric variables, giving rise to a parameter-to-operator map. In the first part of this talk, we discuss the analytic or holomorphic dependence of said boundary integral operators upon the parametric variables, i.e., of the parameter-to-operator map. As a direct consequence we also establish holomorphic dependence of solutions to boundary integral equations, i.e., holomorphy of the parameter-to-solution map. The established parametric holomorphy results have been identified as a key property to derive best N-term approximation rates to overcome the so-called curse of dimensionality in the approximation of parametric maps with distributed, high-dimensional inputs.

In the second part of this talk, we illustrate the practical relevance of our findings by examining the sound-soft Helmholtz acoustic scattering problem and its frequency-robust boundary integral formulations. We are interested in exploring the relevance of this result in data-driven approaches to forward and inverse uncertainty quantification in acoustic scattering problems. More precisely, we consider:

(i) Data-driven learning of the parameter-to-solution map using the reduced basis method.
(ii) Multifidelity learning tailored for Bayesian problems, particularly in the small noise and large data limits.

We present a comprehensive mathematical analysis of both approaches, leveraging the parametric holomorphy result. Finally, we provide numerical experiments showcasing the advantages of these data-driven techniques over traditional methods in terms of efficiency, accuracy, and scalability.

**Keywords**: Parametric Holomorphy; Boundary Integral Operators; Operator Learning; Multifidelity Learning; Bayesian Inverse Problems.

**Mathematics Subject Classifications (2010)**: 5P05, 32D05, 35A20, 62F15.

## References

1. Jürgen Dölz and Fernando Henríquez. Parametric Shape Holomorphy of Boundary Integral Operators with Applications. arXiv preprint arXiv:2305.19853 (2023)
2. Jan S. Hesthaven and Stefano Ubbiali. Non-intrusive reduced order modeling of nonlinear problems using neural networks. *Journal of Computational Physics* 363 (2018): 55-78.

# Stable adaptive least-squares space-time BEM for the wave equation

Daniel Hoonhout[1], Richard Löscher[2], Olaf Steinbach[3], and Carolina A. Urzúa-Torres[4]

Delft University of Technology
D.M.Hoonhout@tudelft.nl
Graz University of Technology
Loescher@math.tugraz.at
Graz University of Technology
O.Steinbach@tugraz.at
Delft University of Technology
C.A.UrzuaTorres@tudelft.nl

**Summary.** We consider space-time boundary element methods for the weakly singular operator $\mathsf{V}$ corresponding to transient wave problems. In particular, we restrict ourselves to the one-dimensional case and work with prescribed Dirichlet data and zero initial conditions. We begin by revisiting two approaches: energetic BEM [1] and the more recent formulation proposed in [3], for which the weakly singular operator is continuous and satisfies inf-sup conditions in the related spaces. However, numerical evidence suggests that it is unstable when using low-order Galerkin-Bubnov discretisations. As an alternative, it was shown in [4] that one obtains ellipticity -and thus stability- by composing $\mathsf{V}$ with the modified Hilbert transform [5].

In this talk, we reformulate these variational formulations as minimisation problems in $L^2$. For discretisation, the minimisation problem is restated as a mixed saddle point formulation. Unique solvability can be established by combining conforming nested boundary element spaces for the mixed formulation such that the first-kind variational formulation is discrete inf-sup stable. We will analyse under which conditions the discrete inf-sup stability is satisfied, and, moreover, we will show that the mixed formulation provides a simple error estimator, which can be used for adaptivity. The theory is complemented by several numerical examples.

**Keywords**: Wave equation, Boundary Element Methods, Space-time, Least-squares

**Mathematics Subject Classifications (2010)**: 35L05 49J20 65M38 65M50

## References

1. A. Aimi, M. Diligenti, C. Guardasoni, and S. Panizzi. A space-time energetic formulation for wave propagation analysis by BEMs. *Riv. Mat. Univ. Parma* (7), **8**:171–207, 2008
2. D. Hoonhout, R. Löscher, O. Steinbach, C. Urzúa–Torres. (2023). *Stable least-squares space-time boundary element methods for the wave equation.* [Unpublished Manuscript]
3. O. Steinbach, C. Urzúa–Torres. A new approach to space-time boundary integral equations for the wave equation. *SIAM Journal on Math- ematical Analysis*, **54**(2):1370–1392, 2022.
4. O. Steinbach, C. Urzúa–Torres, M. Zank: Towards coercive boundary element methods for the wave equation. *J. Integral Equations Appl.* **34** (2022) 501–515.
5. O. Steinbach, M. Zank, Coercive space-time finite element methods for initial boundary value problems, *Electron. Trans. Numer. Anal.*, **52**:154-194 (2020)

# Boundary Element Methods for Focused Ultrasound Treatment in Biomedical Engineering

Elwin van 't Wout[1], Reza Haqshenas[2], and Pierre Gélat[3]

Institute for Mathematical and Computational Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile
e.wout@uc.cl
Department of Mechanical Engineering, University College London, United Kingdom
r.haqshenas@ucl.ac.uk
Division of Surgery and Interventional Science, University College London, United Kingdom
p.gelat@ucl.ac.uk

**Summary.** Focused Ultrasound (FUS) is a non-invasive treatment technique where acoustic energy is transmitted into the human body. The high acoustic pressure in the focal region causes ablation of tissue. Computational simulations can aid in the design of ultrasound instruments and the patient-specific treatment planning, guiding sufficient energy towards to lesion while avoiding overheating of healthy tissue, organs and bone. The adoption of computational approaches hinges on their accuracy in modelling acoustic transmission at high frequencies through realistic geometries that model the targeted regions. The boundary element method (BEM) is a powerful algorithm to solve the Helmholtz equation for harmonic acoustic waves. However, standard approaches fail to efficiently model realistic FUS applications. This talk presents several algorithmic improvements, such as OSRC preconditioning [4], nested meshes for volume integrals [2], high-contrast formulations [5], FEM-BEM coupling [6], and nonconforming meshes [7]. Hundreds of boundary integral formulations were benchmarked to provide efficiency guidelines [3]. We used our fast and accurate BEM implementation to simulate FUS in the human body [1], which can be translated to important biomedical applications such as the non-invasive treatment of liver cancer and neuromodulation of the brain. We validated the methodology within the benchmarking exercise of the International Transcranial Ultrasonic Stimulation Safety and Standards (ITRUSST) consortium [8]. Finally, we implemented all functionality in our open-source Python library, OptimUS.

**Keywords**: Boundary Element Method, Integral Equations, Acoustics

**Mathematics Subject Classifications (2010)**: 65M38, 35J08

## References

1. S.R. Haqshenas, P. Gélat, E. van 't Wout, T. Betcke, and N. Saffari. A fast full-wave solver for calculating ultrasound propagation in the body. *Ultrasonics*, 110:106240, 2020.
2. S.P. Groth, P. Gélat, S.R. Haqshenas, N. Saffari, E. van 't Wout, T. Betcke, and G.N. Wells. Accelerating frequency-domain numerical methods for weakly nonlinear focused ultrasound using nested meshes. *Journal of the Acoustical Society of America*, 150(1):441-453, 2021.
3. E. van 't Wout, S.R. Haqshenas, P. Gélat, T. Betcke, and N. Saffari. Benchmarking preconditioned boundary integral formulations for acoustics. *Int. J. for Numerical Methods in Engineering*, 122(29):5873-5897, 2021.
4. E. van 't Wout, S.R. Haqshenas, P. Gélat, T. Betcke, and N. Saffari. Frequency-robust preconditioning of boundary integral equations for acoustic transmission. *Journal of Computational Physics*, 462:111229, 2022.
5. E. van 't Wout, S.R. Haqshenas, P. Gélat, T. Betcke, and N. Saffari. Boundary integral formulations for acoustic modelling of high-contrast media. *Computers and Mathematics with Applications*, 105:136-149, 2022.
6. E. van 't Wout. Stable and efficient FEM-BEM coupling with OSRC regularisation for acoustic wave transmission. *Journal of Computational Physics*, 450:110867, 2022.
7. E. van 't Wout. The Boundary Element Method for Acoustic Transmission with Nonconforming Grids. Preprint available on *arXiv*, 2206.00708, 2022.
8. J.-F. Aubry, O. Bates, C. Boehm, *et al.* Benchmark problems for transcranial ultrasound simulation: Intercomparison of compressional wave models. *JASA*, 152(2):1003-1019, 2022.

## MS4: Computational electromagnetism

# Existence and Uniqueness of Solution for a Family of Nonlinear Degenerate Mixed Parabolic Equations and its applications to Eddy Current Models

Ramiro Acevedo[1], Christian Gómez[2], and Juan David Samboní[3]

Universidad del Cauca, Popayán, Colombia
rmacevedo@unicauca.edu.co
Universidad de los Llanos, Villavicencio, Colombia
chgomez@unillanos.edu.co
Universidad del Cauca, Popayán, Colombia
jdsamboni@unicauca.edu.co

**Summary.** The aim of this talk is to show an abstract framework to analyze the solvability of a family of nonlinear degenerate mixed parabolic equations. More precisely, we joint the well-known Babuska-Brezzi theory for stationary mixed problems (see, for instance, [8, Section 1.5]) and the theory for nonlinear degenerate parabolic equations (see [10, Section III.6]), taking also inspiration from the hypothesis satisfied by the nonlinear operator in the three fields abstract framework presented by Gatica in [9, Section 2], to obtain sufficient conditions to guarantee the existence and uniqueness of solution.

Furthermore, we illustrate some applications of the abstract setting through particular problems that arise from a physical model that arises from the electromagnetism: nonlinear eddy current models in a general tridimensional bounded domain including conductors and dielectrics (see, for instance, [1, 2, 4]), and the case of an axisymmetrical domain (see [5, 6]).

We obtain in this work a generalization of the abstract framework proposed in 1985 by Bernardi & Raugel [7], since the problem proposed by the two authors considered a non-degenerate mixed linear parabolic equations and our abstract framework, on the other hand, is degenerate and nonlinear (see also [3]). Moreover, we show that the solutions of our problems have a desired regularity if we wish to approximate the solution by using, for instance, the finite element method.

**Keywords**: Well-posedness, parabolic degenerate equations, mixed problems, nonlinear problems, time-dependent Stokes problem, eddy current model.

**Mathematics Subject Classifications (2010)**: 35K55, 78A25.

## References

1. R. Acevedo, S. Meddahi, and R. Rodríguez. An **E**-based mixed formulation for a time-dependent eddy current problem. *Mathematics of Computation*, 78 (2009), 1929–1949.
2. R. Acevedo and S. Meddahi. An **E**-based mixed FEM and BEM coupling for a time-dependent eddy current problem. *IMA J. Numer. Anal.*, 31 (2011), pp. 667–697.
3. R. Acevedo, C. Gómez, and B. López-Rodríguez. Well-posedness for a family of degenerate parabolic mixed equations. *J. Math. Anal. Appl.*, 498 (2021).
4. A. Bermúdez, B. López-Rodríguez, R. Rodríguez and P. Salgado. An eddy current problem in terms of a time-primitive of the electric field with non-local source conditions. *ESAIM - Mathematical Modelling and Numerical Analysis*, 47 (2013), 875–902.
5. A. Bermúdez, C. Reales, R. Rodríguez and P. Salgado. Numerical analysis of a finite-element method for the axisymmetric eddy current model of an induction furnace. *IMA Journal of Numerical Analysis*, vol. 30, no. 3, pp. 654-676, July 2010, doi: 10.1093/imanum/drn063.
6. A. Bermúdez, C. Reales, R. Rodríguez and P. Salgado. Numerical analysis of a transient eddy current axisymmetric problem involving velocity terms. *Numerical Methods for Partial Differential Equations*, 2012; 28(3), 984-1012.
7. C. Bernardi and G. Raugel. A conforming finite element method for the time-dependent Navier-Stokes equations. *SIAM J. Numer. Anal.*, 22 (1985), pp.455–473.

8. D. Boffi, F Brezzi, L.F. Demkowicz, R.G. Durán, R.S. Falk and M. Fortin, *Mixed Finite Elements, Compatibility Conditions, and Applications*, Lecture Notes in Mathematics. Springer-Verlag Berlib Heidelberg. 2008.
9. G.N. Gatica, *Solvability and Galerkin Approximations of a Class of Nonlinear Operator Equations*, Zeitschrif fur Analysis und ihre Anwendungen, vol. 21, 3, pp. 761-781, 2002.
10. R. E. Showalter. Monotone Operators in Banach Space and Nonlinear Partial Differential Equations. *Math. Surveys Monogr.*, vol. 49, Amer. Math. Soc., Providence, RI, 1997.

1

2

# Reflectionless Discrete PMLs For High-Order Finite Difference Schemes and Finite Element Methods

Vicente A. Hojas[1], Carlos Pérez Arancibia[2], and Manuel A. Sánchez[3]

Pontificia Universidad Católica de Chile
vahojas@uc.cl
University of Twente, The Netherlands
c.a.perezarancibia@utwente.nl
Pontificia Universidad Católica de Chile
manuel.sanchez@ing.puc.cl

**Summary.** We introduce discrete-holomorphic Perfectly Matched Layers (PMLs) specifically designed for high-order finite difference (FD) and continuous, piecewise linear finite element discretizations of the scalar wave equation. In contrast to standard PDE-based PMLs, the proposed methods achieve the remarkable outcome of completely eliminating numerical reflections at the PML interface, in practice achieving reflection errors at the level of machine precision. Our approach builds upon the ideas put forth in a recent publication [1] expanding the scope from the standard second-order FD method to arbitrary high-order FD schemes [2] and the continuous, piecewise linear finite element method (FEM). Our RDPML-FEM method directly leverages the properties of the RDPML-FD method by combining standard FEM discretizations with Mass Lumping FEM [3] for the wave equation.

**Keywords**: Wave equation, Helmholtz equations, Perfectly Matched Layer, absorbing boundary condition, non-reflecting boundary condition, finite difference method, finite element method.

**Mathematics Subject Classifications (2010):** 65M60, 78A40, 76B15, 35L05.

## References

1. A. Chern. A reflectionless discrete perfectly matched layer. *Journal of Computational Physics*, 381 (2019): 91-109
2. V. A. Hojas, C. Pérez-Arancibia, and M. A. Sánchez. Reflectionless discrete perfectly matched layers for higher-order finite difference schemes. 2023.
3. G. Cohen, P. Joly, J. E. Roberts, and N. Tordjman. Higher Order Triangular Finite Elements with Mass Lumping for the Wave Equation. SIAM *Journal on Numerical Analysis*, 38(6):2047-2078, 2001.

*V.A. Hojas was supported by Beca ANID de Magíster Nacional N. 22230599.

†M.A. Sánchez was supported by FONDECYT Regular N. 1221189 and by Centro Nacional de Inteligencia Artificial CENIA, FB210017, Basal ANID Chile.

# Shape Uncertainty Quantification for Electromagnetic Wave Scattering via First-Order Sparse Boundary Element Approximation

Paul Escapil-Inchauspé[1] and Carlos Jerez-Hanckes[2]

Data Observatory Foundation
paul.escapil@dataobservatory.net
Facultad de Ingeniería y Ciencias, Universidad Adolfo Ibáñez
carlos.jerez@uai.cl

**Summary.** Quantifying the effects on electromagnetic waves scattered by objects of uncertain shape is key for robust design, particularly in high precision applications. Assuming small random perturbations departing from a nominal domain, the first-order sparse boundary element method (FOSB) has been proven to directly compute statistical moments with poly-logarithmic complexity for a prescribed accuracy [1, 2], without resorting to computationally intense Monte Carlo simulations. However, implementing the FOSB is not straightforward. To this end, we introduce an easy-to-use with open-source framework to directly apply the technique when dealing with complex objects. Exhaustive computational experiments confirm our claims and demonstrate the technique's applicability as well as provide pathways for further improvement.

**Keywords**: Electromagnetic Wave Scattering, Uncertainty Quantification, Shape Derivative, Combination Technique, Boundary Element Methods

**Mathematics Subject Classifications (2010)**: 47A40, 35J25, 49Q12

## References

1. C. Jerez-Hanckes, C. Schwab. Electromagnetic Wave Scattering by Random Surfaces: Uncertainty Quantification via Sparse Tensor Boundary Elements. *IMA Journal of Numerical Analysis*, 37(3):1175–1210, 2017.
2. P. Escapil-Inchauspé, C. Jerez-Hanckes. Helmholtz Scattering by Random Domains: First-Order Sparse Boundary Elements Approximation. *SIAM Journal of Scientific Computing*, 42(5):A2561–A2592, 2020.
3. P. Escapil-Inchauspé, C. Jerez-Hanckes. Fast Calderón Preconditioning for the Electric Field Integral Equation *IEEE Transactions on Antennas and Propagation*, 67(4):2555–2564, 2019.
4. A. Kleanthous, T. Betcke, D. Hewett, P. Escapil-Inchauspé, C. Jerez-Hanckes, A. Baran. Accelerated Calderón preconditioning for Maxwell transmission problems. *Journal of Computational Physics*, 458:111099, 2022.
5. P. Escapil-Inchauspé, C. Jerez-Hanckes. Bi-parametric Operator Preconditioning *Computers and Mathematics with Applications*, 102:220?232, 2021.

# Enhancing operation and design of alternate current-powered industrial furnaces: insights from mathematical modeling and simulation

Alfredo Bermúdez[1], Dolores Gómez[2], and David González[3]

Universidade de Santiago de Compostela and CITMAga
alfredo.bermudez@usc.es
Universidade de Santiago de Compostela and CITMAga
mdolores.gomez@usc.es
Universidade de Santiago de Compostela and CITMAga
david.gonzalez.penas@rai.usc.es

**Summary.** Electric furnaces play a key role in many industrial applications, providing precise control of heat generation and distribution. Research and development efforts in the field of industrial furnaces rely heavily on mathematical models and numerical simulations. These tools enable researchers to test hypotheses, explore new technologies and develop innovative solutions in a cost-effective and controlled manner. This presentation will examine a particular type of furnace and show how mathematical models and numerical simulations are used to improve its operation and efficiency. The furnace is a vacuum furnace used for the purification of silicon. A conductive molten mixture contained in a crucible is heated by a resistor connected to three-phase alternating current. This induces eddy currents that create an electromagnetic force within the melt. Stirring and heating cause impurities to evaporate and condense on a chamber wall. The whole problem is a multiphysics problem involving different mathematical models: electromagnetic, thermal, hydrodynamic, gas kinetic and thermodynamic. In this talk the main features of the different models are introduced. As the geometry of the furnace requires a 3D solution, a methodology combining distributed and lumped models is also presented to simulate the current distribution in the furnace and, in particular, to calculate the current to be supplied to obtain a desired power [1].

**Keywords**: Metallurgical furnaces, indirect resistance heating, numerical simulation, eddy current models

**Mathematics Subject Classifications (2010)**: 65N38, 65N30, 80M25, 78A55

## References

1. A. Bermúdez, D. Gómez, and D. González. Numerical simulation of resistance furnaces by using distributed and lumped models. Submitted, 2023.

# A five-field mixed formulation for stationary magnetohydrodynamic flows in porous media

Lady Angelo[1], Jessika Camaño[2], and Sergio Caucao[3]

GIANuC$^2$ and Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción, Concepción, Chile.
langelo@ucsc.cl
GIANuC$^2$ and Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción, Concepción, Chile and CI$^2$MA, Universidad de Concepción, Concepción, Chile.
jecamano@ucsc.cl
GIANuC$^2$ and Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción, Concepción, Chile.
scaucao@ucsc.cl

**Summary.** We introduce and analyze a new mixed variational formulation for a stationary magnetohydrodynamic flows in porous media problem, whose governing equations are given by the steady Brinkman–Forchheimer equations coupled with the Maxwell equations. Besides the velocity, magnetic field and a Lagrange multiplier asssociated to the divergence-free condition of the magnetic field, a convenient translation of the velocity gradient and the pseudostress tensor are introduced as further unknowns. As a consequence, we obtain a five-field Banach spaces-based mixed variational formulation, where the aforementioned variables are the main unknowns of the system. The resulting mixed scheme is then written equivalently as a fixed-point equation, so that the well-known Banach theorem, combined with classical results on nonlinear monotone operators and a sufficiently small data assumption, are applied to prove the unique solvability of the continuous and discrete systems. In particular, the analysis of the discrete scheme requires a quasi-uniformity assumption on mesh. The finite element discretization involves Raviart–Thomas elements of order $k \geq 0$ for the pseudostress tensor, discontinuous piecewise polynomial elements of degree $k$ for the velocity and the translation of the velocity gradient, Nédélec elements of degree $k$ for the magnetic field and Lagrange elements of degree $k+1$ for the associated Lagrange multiplier. Stability, convergence, and optimal *a priori* error estimates for the associated Galerkin scheme are obtained. Numerical tests illustrate the theoretical results.

**Keywords**: Brinkman–Forchheimer equations; Maxwell equations; Mixed finite element methods; Fixed point theory; A priori error analysis

**Mathematics Subject Classifications (2010)**: 65N30; 65N12; 65N15; 76M10.

## References

1. L. Angelo, J. Camaño, and S. Caucao, *A five-field mixed formulation for stationary magnetohydrodynamic flows in porous media*. Computer Methods in Applied Mechanics and Engineering, vol. 414, Art. Num. 116158, (2023).
2. Y. Amirat, L. Chupin, and R. Touzani, *Weak solutions to the equations of stationary magnetohydrodynamic flows in porous media*. Commun. Pure Appl. Anal. 13 (2014), no. 6, 2445–2464.
3. S. Caucao, G.N. Gatica, and J.P. Ortega, *A fully-mixed formulation in Banach spaces for the coupling of the steady Brinkman–Forchheimer and double-diffusion equations*. ESAIM Math. Model. Numer. Anal. 55 (2021), no. 6, 2725–2758.
4. D. Schötzau, *Mixed finite element methods for stationary incompressible magneto-hydrodynamics*. Numer. Math. 96 (2004), no. 4, 771–800.

# On time stepping schemes for the DG discretisation of Friedrichs Systems. Part 1.

Sebastien Impériale[1], Patrick Joly[2], and Jerónimo Rodríguez[3]

Inria, Université Paris-Saclay, France. LMS, Ecole Polytechnique, CNRS, Université Paris-Saclay, France
sebastien.imperiale@inria.fr
Inria, Université Paris-Saclay, France; and UMA, Ensta, CNRS, Université Paris- Saclay, France
patrick.joly@inria.fr
Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, Spain; CITMAGA, Universidade de Santiago de Compostela, Spain.
jeronimo.rodriguez@usc.es

**Summary.** Symmetric Friedrichs systems constitute a large class of linear hyperbolic systems that englobe most of mathematical models for linear wave propagation phenomena: acoustics, electromagnetics, elastodynamics but also copled phenomena such as piezo-electricity or aeroacoustics that include convection phenomena due to acoustics-hydrodynamics.

A privileged method for the space discretisation of these models is the Discontinuous Galerkin Method whose field of application is much larger than the one of Finite Element Methods for instance. This method also offers a lot of flexibility allowing local mesh refinement and the treatment of hanging nodes. The use of off-centered numerical fluxes permits to introduce some artificial dissipation, which appears useful, for instance to control the spurious oscillations observed with centred fluxes (the conservative case) when modelling convection phenomena.

For time dependent simulations, the time discretisation of the semi-discrete problem issued from the DG method in both conservative and dissipative cases is obviously a key issue. For large scale simulations such as those generally encountered for wave propagation problems, explicit schemes must be privileged, which naturally raises the question of their stability. Curiously, this theoretical question does not seem to have been addressed extensively in the literature.

In these two presentations, we shall present various results in this direction for two classes of schemes : Runge Kutta type schemes and leap-frog type schemes. For the numerical analysis, two different techniques will be used : the Von Neumann approach (that provides optimal results but remains limited to particular cases) and the energy method.

Our work is related to three previous contributions in the literature. Concerning Von Neumann analysis, our results are quite close to those of the following paper on ODEs [1]. Concerning energy methods, our work has to be seen in the continuation of the following two previous works [3, 2].

**Keywords**: Discontinuous Galerkin methods, Runge-Kutta integrator, Leap frog scheme, stability, Friedrichs systems, energy method, Von Neumann analysis.

**Mathematics Subject Classifications (2010)**: 65M12, 65N30, 65N55, 35L05.

## References

1. D. Ketcheson, L. Loczi. On the absolute stability regions corresponding to partial sums of the exponential function. *IMA Journal of Numerical Analysis*, 35: 1426–1455, 2015.
2. E. Burman, A. Ern, M. A. Fernández. Explicit Runge-Kutta schemes and finite elements with symmetric stabilization for first-order linear PDE systems. *SIAM Journal on Numerical Analysis*,48(6):2019–2042, 2010.
3. D. Levy, E. Tadmor From semi-discrete to fully discrete: Stability of Runge–Kutta schemes by the energy method, *SIAM Review*,40:40–73, 1998.

# On time stepping schemes for the DG discretisation of Friedrichs Systems. Part 2.

Sebastien Impériale[1], Patrick Joly[2], and Jerónimo Rodríguez[3]

Inria, Université Paris-Saclay, France. LMS, Ecole Polytechnique, CNRS, Université Paris-Saclay, France
sebastien.imperiale@inria.fr
Inria, Université Paris-Saclay, France; and UMA, Ensta, CNRS, Université Paris- Saclay, France
patrick.joly@inria.fr
Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, Spain; CITMAGA, Universidade de Santiago de Compostela, Spain.
jeronimo.rodriguez@usc.es

**Summary.** Symmetric Friedrichs systems constitute a large class of linear hyperbolic systems that englobe most of mathematical models for linear wave propagation phenomena: acoustics, electromagnetics, elastodynamics but also copled phenomena such as piezo-electricity or aeroacoustics that include convection phenomena due to acoustics-hydrodynamics.

A privileged method for the space discretisation of these models is the Discontinuous Galerkin Method whose field of application is much larger than the one of Finite Element Methods for instance. This method also offers a lot of flexibility allowing local mesh refinement and the treatment of hanging nodes. The use of off-centered numerical fluxes permits to introduce some artificial dissipation, which appears useful, for instance to control the spurious oscillations observed with centred fluxes (the conservative case) when modelling convection phenomena.

For time dependent simulations, the time discretisation of the semi-discrete problem issued from the DG method in both conservative and dissipative cases is obviously a key issue. For large scale simulations such as those generally encountered for wave propagation problems, explicit schemes must be privileged, which naturally raises the question of their stability. Curiously, this theoretical question does not seem to have been addressed extensively in the literature.

In these two presentations, we shall present various results in this direction for two classes of schemes : Runge Kutta type schemes and leap-frog type schemes. For the numerical analysis, two different techniques will be used : the Von Neumann approach (that provides optimal results but remains limited to particular cases) and the energy method.

Our work is related to three previous contributions in the literature. Concerning Von Neumann analysis, our results are quite close to those of the following paper on ODEs [1]. Concerning energy methods, our work has to be seen in the continuation of the following two previous works [3, 2].

**Keywords**: Discontinuous Galerkin methods, Runge-Kutta integrator, Leap frog scheme, stability, Friedrichs systems, energy method, Von Neumann analysis.

**Mathematics Subject Classifications (2010)**: 65M12, 65N30, 65N55, 35L05.

## References

1. D. Ketcheson, L. Loczi. On the absolute stability regions corresponding to partial sums of the exponential function. *IMA Journal of Numerical Analysis*, 35: 1426–1455, 2015.
2. E. Burman, A. Ern, M. A. Fernández. Explicit Runge-Kutta schemes and finite elements with symmetric stabilization for first-order linear PDE systems. *SIAM Journal on Numerical Analysis*,48(6):2019–2042, 2010.
3. D. Levy, E. Tadmor From semi-discrete to fully discrete: Stability of Runge–Kutta schemes by the energy method, *SIAM Review*,40:40–73, 1998.

# Solvability investigation on a nonlinear magneto-heat coupling axisymmetric problem

Tong Kang[1], Ran Wang[2], and Huai Zhang[3]

School of Data Science and Media Intelligence, Communication University of China, Beijing, 100024, P. R. China,
kangtong@cuc.edu.cn
School of Data Science and Media Intelligence, Communication University of China, Beijing, 100024, P. R. China,
ranwang@cuc.edu.cn
Key Laboratory of Computational Geodynamics, University of Chinese Academy of Sciences, Beijing, 100049, P. R. China,
hzhang@ucas.ac.cn

**Summary.** This paper aims to investigate a nonlinear magneto-heat coupling axisymmetric problem from induction heating models. The liquid metallic material satisfies a nonlinear constitutional relationship between the magnetic field and the magnetic induction and have the temperature-dependent electric conductivity. This material is allowed to move without changing its domain. Making full use of cylinder symmetry, we reduce the original three-dimensional problem to a two-dimensional one on a meridional section provided the current density has only azimuthal component in cylindrical coordinates. The variational formulation of a magnetic vector potential and a temperature variable in appropriate weighted Sobolev spaces is given. Employing Rothe's method and the theory of monotone operator, we prove the existence of a weak solution to this nonlinear coupling system. Finally we show some numerical simulation results to an approximate induction furnace model to support our conclusion.

**Keywords**: Magneto-heat coupling, Axisymmetric problem, Maxwell's equations, Heat convection-diffusion equation, Nonlinear, Solvability

**Mathematics Subject Classifications (2010)**: 35Q61, 35Q79, 65M12

## References

1. A. Bermúdez, C. Reales, R. Rodríguez and P. Salgado R. Bürger, K.H. Karlsen, and J.D. Towers. Numerical analysis of a transient eddy current axisymmetric problem involving velocity terms. *Numer. Methods Partial Differential Equations*, 28(3):984-1012, 2012.
2. J. Chovan, C. Geuzaine and M. Slodicka. A-$\phi$ formulation of a mathematical model for the induction hardening process with a nonlinear law for the magnetic field. *Computer Comput. Methods Appl. Mech. Engrg.*, 321:284-315, 2017.

# The Ultra Weak Variational Formulation of Maxwell's equations

Timo Lähivaara[1] and Peter Monk[2]

University of Eastern Finland, Kuopio, Finland
timo.lahivaara@uef.fi
University of Delaware, Newark, USA
monk@udel.edu

**Summary.** The Ultra Weak Variational Formulation (UWVF) is a special Trefftz discontinuous Galerkin method due to Cessenat and Déspres [1]. Here we are concerned with solving the time-harmonic Maxwell's equations. The method uses superpositions of plane waves to represent solutions element-wise on a finite element mesh. Following a study of the method [**?**], we implemented a parallel UWVF version of the code, called *ParMax*. This has undergone development for industrial applications [3]. In this talk, we emphasize high-order solutions in the presence of scatterers with piecewise smooth boundaries. We explain the incorporation of curved surface triangles into the UWVF, necessitating quadrature for system matrix assembly. We also show how to implement the transmission conditions across an interface to handle resistive sheets. We note also that a wide variety of element shapes can be used, that the elements can be very large compared to the wavelength of the radiation, and that a matrix-free version is easy to implement (although computationally costly). Our contributions are illustrated through numerical examples demonstrating the efficiency enhancement achieved by curved elements in the UWVF. The method accurately handles resistive screens, as well as perfect electric conductor and penetrable scatterers. By employing large curved elements and the matrix-free approach, we successfully simulated X-band frequency scattering from an aircraft. These innovations demonstrate the practicality of the UWVF for industrial applications.

**Keywords**: Maxwell equations, Trefftz method, Numerical analysis, Frequency domain analysis

**Mathematics Subject Classifications (2010)**: 65Z05, 65L60

## References

1. O. Cessenat and B. Després, Using plane waves as base functions for solving time harmonic equations with the Ultra Weak Variational Formulation, *J. Comput. Acoust.*, vol. 11, pp. 227-38, 2003.
2. ]T. Huttunen, M. Malinen, and P. Monk, Solving Maxwell's equations using the ultra weak variational formulation, *J. Comput. Phys.*, vol. 223, pp. 731-758, 2007.
3. Timo Lähivaara, William Hall, Matti Malinen, Dale Ota, Vijaya Shankar, Peter Monk, A High-Order Ultra-Weak Variational Formulation for Electromagnetic Waves Utilizing Curved Elements, Arxiv https://arxiv.org/abs/2309.02980 (2023).

# Strongly enforced waveguide port boundary condition and its application on the analysis of optical devices

Francisco T. Orlandini[1], Hugo E. Hernández-Figueroa[2], and Philippe R. B. Devloo[3]

Departamento de Comunicações, Faculdade de Engenharia Elétrica e de Computação,
UNICAMP, Av. Albert Einstein 400, CEP 13083-907 Campinas, SP, Brazil
francisco.orlandini@gmail.com
Departamento de Comunicações, Faculdade de Engenharia Elétrica e de Computação,
UNICAMP, Av. Albert Einstein 400, CEP 13083-907 Campinas, SP, Brazil
hugo@decom.fee.unicamp.br
Departamento de Estruturas, Faculdade de Engenharia Civil, Arquitetura e Urbanismo,
UNICAMP, Av. Albert Einstein, 951 CP 6021 CEP 13083-852 Campinas, SP, Brazil
phil@fec.unicamp.br

**Summary.** An implementation of the Waveguide Port Boundary Condition based on the restriction of the approximation space is presented in the context of a high precision scheme for the numerical analysis of optical devices. In the analysis and design of such devices, often is of interest to analyse the propagation of an electromagnetic field in a domain terminated, or partially terminated, by waveguide cross sections. Moreover, these domains are tipically characterized by curved geometries, subwavelength geometric features and reduced dimensions, which are aspects that, if not carefully treated, can significantly increase the computational cost of such analyses.

The Waveguide Port Boundary Condition[1] is based on the eigenfunction expansion method, in which the set of solutions for a homogeneous PDE, subject to given boundary conditions, is used as to represent the solution of the same PDE when subjected to an arbitrary source. In the current context, the eigenfunctions are chosen as a sufficiently large number of waveguide modes. In the present work, an implementation of such boundary condition based not only on the weak form but also on the restriction of the approximation space is presented. Such implementation results in significant decrease on the degrees of freedom at the boundary, as well as a simplified computational implementation. The efficiency on such boundary condition with respect to the chosen number of modes is also discussed.

The performance of the developed scheme, implemented in the NeoPZ framework (https://github.com/labmec/neopz), is analysed through numerical examples of increasing complexity, and it is shown that advanced Finite Element techniques present in this framework[2], such as *hp*-refinement, directional refinement and accurate representation of curved geometries, when allied with the aforementioned boundary condition, result in an efficient scheme for the analysis of optical devices.

**Keywords**: finite elements, high order elements, optical devices, waveguides.

**Mathematics Subject Classifications (2010)**: 78-10,78M10, 65N30, 78A50.

## References

1. J. M. Jin and S-W. Lee. Hybrid Finite-Element Analysis Of Scattering And Radiation By A Class Of Waveguide-Fed Structures WILEY *Microwave and Optical Technology Letters*, 7:798-803, 1994.
2. Jorge L. D. Calle, Philippe R. B. Devloo and Sônia M. Gomes. Implementation of continuous hp-adaptive finite element spaces without limitations on hanging sides and distribution of approximation orders. *Computers & Mathematics with Applications*, 70(5):1051–1069, 2015.

# Numerical simulation of wave propagation in a waveguide using Trefftz elements

Manuel Pena[1], Peter Monk[2], and Virginia Selgas[3]

Technical University of Madrid
manuel.pena@upm.es
University of Delaware
monk@udel.edu
University of Oviedo
selgasvirginia@uniovi.es

**Summary.** We investigate numerically the propagation of time-harmonic waves along an unbounded waveguide for medium and large piecewise constant wavenumbers. We do so based on a Trefftz Discontinuous Galerkin (TDG) formulation which we discretize with the superposition of travelling plane waves.

We first rewrite the problem on a bounded computational domain by using the Neumann-to-Dirichlet map on the artificial walls. This truncated problem is formulated variationally in a DG way, that is, the interelement continuity is imposed weakly within the variational formulation by introducing suitable numerical fluxes. We choose standard numerical fluxes for internal faces and some more exotic numerical fluxes for faces on the truncation boundary. We then get a consistent and coercive formulation which achieves quasi-optimal convergence when discretized with Trefftz elements. We also provide a priori error bounds for the discretization based on plane waves.

The behavior of the numerical solutions and their order of convergence is verified and illustrated in two dimensions with numerical experiments, including for the special case of the Ultra Weak Variational Formulation (UWVF). In particular, these experiments allow us to investigate the instability and ill-conditioning inherent in plane wave-based Trefftz methods, and if this issue can be overcome in practice with suitable regularization techniques.

**Keywords**: time-harmonic wave, waveguide, discontinuous Galerkin formulation, ultra weak variational formulation, Trefftz elements

**Mathematics Subject Classifications (2010)**: 35J05, 65N30, 65N15.

## References

1. S. Kapita, P. Monk, V. Selgas. A Trefftz Discontinuous Galerkin method for time-harmonic waves with a generalized impedance boundary condition, *Applicable Analysis*, 99(3):379-406, 2020.
2. T. Lähivaara, W. Hall, M. Malinen, D. Ota, V. Shankar, P. Monk. A High-Order Ultra-Weak Variational Formulation for Electromagnetic Waves Utilizing Curved Elements, *in press*, 2023.
3. A. Moiola, R. Hiptmair, I. Perugia. Plane wave approximation of homogeneous Helmholtz solutions, *Z. Angew. Math. Phys.*, 62(5):809-837, 2011.
4. P. Monk, D.Q. Wang. *A least-squares method for the Helmholtz equation*, *Computational Methods in Applied Mechanics and Engineering*, 175:121-136, 1999.

# MS5: Effective solvers for innovative discretizations of multiphysics phenomena

# Scalable preconditioned Newton–Krylov and quasi–Newton solvers for nonlinear cardiac models

Nicolás A. Barnafi[1], Ngoc Mai Monica Huynh[2], Luca F. Pavarino[3], and Simone Scacchi[4]

Centro de Modelamiento Matemático, Chile
nbarnafi@cmm.uchile.cl
Department of Mathematics, Università degli Studi di Pavia, Italy
ngocmaimonica.huynh@unipv.it
Department of Mathematics, Università degli Studi di Pavia, Italy
luca.pavarino@unipv.it
Department of Mathematics, Università degli Studi di Milano, Italy
simone.scacchi@unimi.it

**Summary.** This talk focuses on preconditioned Newton–Krylov and quasi-Newton solvers for the solution of the nonlinear cardiac models arising in electrophysiology and cardiac mechanics. The preconditioners that we consider belong to the classes of both Algebraic Multigrid Methods (AMG) and Dual-Primal Domain Decomposition, such as Balancing Domain Decomposition by Constraints (BDDC) and Dual-Primal Finite Element Tearing and Interconnecting (FETI-DP). We first study the performance of AMG and BDDC preconditioners in a Newton–Krylov solver for cardiac mechanics, varying the choice of BDDC local and coarse solvers, primal degrees of freedom, finite element degree and investigating the strong scalability of the solvers [1]. We also study alternative nonlinear solvers for cardiac mechanics where the classical Newton – Krylov method is replaced by inexact Newton–Krylov and quasi-Newton methods, varying the problem size, data magnitude and number of processors, showing in some cases a significant speed-up over the standard Newton–Krylov method [2]. BDDC and FETI-DP preconditioners with deluxe scaling can also be applied to Newton–Krylov solvers for the Bidomain model in cardiac electrophysiology where a polylogarithmic convergence rate bound can be proven and validated by parallel numerical tests, showing that the proposed parallel solvers are scalable and quasi-optimal [3]. Ongoing work is investigating the extension of Quasi-Newton solvers to implicit Bidomain discretizations [4].

**Keywords**: Newton–Krylov methods, Quasi-Newton, domain decomposition methods, algebraic multigrid, FETI-DP and BDDC preconditioners, nonlinear elasticity, bidomain system.

**Mathematics Subject Classifications (2010)**: 65N55, 65M55, 65F10, 92C30.

## References

1. Nicolás A. Barnafi, Luca F. Pavarino, and Simone Scacchi. A comparative study of scalable multilevel preconditioners for cardiac mechanics. Journal of Computational Physics 492 (2023): 112421.
2. Nicolás A. Barnafi, Luca F. Pavarino, and Simone Scacchi. Parallel inexact Newton–Krylov and quasi-Newton solvers for nonlinear elasticity. Computer Methods in Applied Mechanics and Engineering 400 (2022): 115557.
3. Huynh, Ngoc Mai Monica, Luca F. Pavarino, and Simone Scacchi. Parallel Newton–Krylov BDDC and FETI-DP Deluxe Solvers for Implicit Time discretizations of the Cardiac Bidomain Equations. SIAM Journal on Scientific Computing 44.2 (2022): B224-B249.
4. Nicolás A. Barnafi, Huynh, Ngoc Mai Monica, Luca F. Pavarino, and Simone Scacchi. Analysis and numerical validation of robust parallel nonlinear solvers for implicit time discretizations of the Bidomain equations. arXiv preprint arXiv:2209.05193 (2022).

# A parallel solver for fluid-structure interaction problems with Lagrange multiplier

Daniele Boffi[1], Fabio Credali[2], Lucia Gastaldi[3], and Simone Scacchi[4]

CEMSE Division, King Abdullah University of Science and Technology, Saudi Arabia; Dipartimento di Matematica "F. Casorati", Università degli Studi di Pavia, Italy
daniele.boffi@kaust.edu.sa
Dipartimento di Matematica "F. Casorati", Università degli Studi di Pavia, Italy; CEMSE Division, King Abdullah University of Science and Technology, Saudi Arabia
fabio.credali01@universitadipavia.it
DICATAM, Università degli Studi di Brescia, Italy
lucia.gastaldi@unibs.it
Dipartimento di Matematica "F. Enriques", Università degli Studi di Milano, Italy
simone.scacchi@unimi.it

**Summary.** 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 $\mathscr{Q}_2 - \mathscr{P}_1$ element, while the solid variables are approximated by $\mathscr{Q}_1$ 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 library [4] 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

**Mathematics Subject Classifications (2010)**: 65N30, 65N12, 74F10, 65F08.

## 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.

# Optimal block preconditioners for high-order discretizations of multiphysics problems in the de Rham complex

Pablo D. Brubeck[1] and Patrick E. Farrell[2]

Mathematical Institute, University of Oxford
brubeckmarti@maths.ox.ac.uk
Mathematical Institute, University of Oxford
patrick.farrell@maths.ox.ac.uk

**Summary.** The Riesz maps of the $L^2$ de Rham complex frequently arise as subproblems in the construction of fast preconditioners for multiphysics problems. In this work we present multigrid solvers for high-order finite element discretizations of these Riesz maps with the same time and space complexity as sum-factorized operator application, i.e., with optimal complexity in polynomial degree in the context of Krylov methods. The key idea of our approach is to build new finite elements for each space in the de Rham complex with orthogonality properties in both the $L^2$- and $H(\mathrm{d})$-inner products ($\mathrm{d} \in \{\mathrm{grad}, \mathrm{curl}, \mathrm{div}\}$) on the reference hexahedron. The resulting sparsity enables the fast solution of the patch problems arising in the Pavarino, Arnold–Falk–Winther, and Hiptmair space decompositions, in the separable case. In the non-separable case, the method can be applied to an auxiliary operator that is sparse by construction. With exact Cholesky factorizations of the sparse patch problems, the application complexity is optimal but the setup costs and storage are not. We overcome this with the finer Hiptmair space decomposition and the use of incomplete Cholesky factorizations imposing the sparsity pattern arising from static condensation, which applies whether static condensation is used for the solver or not. This yields multigrid relaxations with time and space complexity that are both optimal in the polynomial degree.

We illustrate our preconditioning approach by solving mixed formulations of a pseudostress-displacement formulation of linear elasticity and the vorticity-velocity-pressure formulation of Stokes flow, for which we observe robustness with respect to the mesh size, the polynomial degree, and the problem parameters.

**Keywords**: preconditioning, high-order, de Rham complex, additive Schwarz, multigrid

**Mathematics Subject Classifications (2010)**: 65F08, 65N35, 65N55

# Efficient Domain Decomposition Preconditioners for Time Stepping in EMI Models

Fatemeh Chegini[1] and Martin Weiser[2]

Zuse Institute Berlin
chegini@zib.de
Zuse Institute Berlin
weiser@zib.de

**Summary.** The cardiac extracellular-membrane-intracellular (EMI) model [1] enables the precise geometrical representation and resolution of aggregates of individual myocytes. Achieving efficient higher-order time stepping is imperative in this context due to large problem sizes. The locality of solution features in cardiac electrophysiology simulations calls for adaptive methods. Yet, traditional mesh refinement and coarsening approaches incur significant overheads. Firstly, this study investigates an efficient spatial adaptivity method that is based on nested subset selection for algebraic degrees of freedom in spectral deferred correction methods (SDC) [2] and realizes a multirate integration with minimal overhead. Consequently, shrinking effective support of SDC corrections allows for a reduction of the spatial domains on which Euler subproblems need to be solved, such that the smaller size of systems to solve translates directly into a significant reduction of simulation time compared to the baseline [3]. Since the first sweep is always performed on the whole domain, a second acceleration technique in the SDC computations is to consider coarser collocation grids on the first sweeps, called ladder method [4]. Due to the frequently changing linear equation systems to be solved, preconditioners with expensive setups cannot be used except for the very first SDC sweep. This study uses the Balancing Domain Decomposition by Constraints (BDDC) method [5] as a preconditioner in the SDC method. We propose a novel combination of BDDC and algebraic adaptivity where no updating of the preconditioner on system reduction is necessary. This is achieved by a subdomain-wise group selection of algebraic degrees of freedom. We assess the computational efficiency of BDDC and block Jacobi preconditioners at some numerical examples.

**Keywords**: EMI Model, high-order time integration, spectral deferred correction, algebraic adaptivity, multirate integration scheme, Ladder Method, BDDC method.

## References

1. Bécue, P. and Potse, M and Coudière, Y. Microscopic Simulation of the Cardiac Electrophysiology: A Study of the Influence of Different Gap Junctions Models. Computing in Cardiology Conference (CinC) (2018) pp. 1-4, doi: 10.22489/CinC.2018.057.
2. M. Weiser. Faster SDC convergence on non-equidistant grids by DIRK sweeps. BIT Numerical Mathematics, 55(4):1219–1241, 2015.
3. Chegini F, Steinke T, Weiser M. Efficient adaptivity for simulating cardiac electrophysiology with spectral deferred correction methods. In: Submitted; 2022.
4. M.L. Minion. Semi-implicit spectral deferred correction methods for ordinary differential equations. Comm. Math. Sci., 1(3):471–500, 2003.
5. N.M.M. Huynh, F. Chegini, L. F. Pavarino, M. Weiser, and S. Scacchi. Convergence analysis of BDDC preconditioners for hybrid DG discretizations of the cardiac cell-by-cell model, arXiv:2212.12295 2022.

# A polytopal discontinuous Galerkin method for the approximation of brain multiphysics flow dynamics

Ivan Fumagalli[1], Mattia Corti[2], Nicola Parolini[3], and Paola F. Antonietti[4]

MOX, Department of Mathematics, Politecnico di Milano
ivan.fumagalli@polimi.it
MOX, Department of Mathematics, Politecnico di Milano
mattia.corti@polimi.it
MOX, Department of Mathematics, Politecnico di Milano
nicola.parolini@polimi.it
MOX, Department of Mathematics, Politecnico di Milano
paola.antonietti@polimi.it

**Summary.** Several neurodegenerative diseases are associated with an impairment of the waste clearance mechanism carried out by the Cerebrospinal Fluid (CSF), which filtrates in the cerebral tissue and flows in brain ventricles to remove waste proteins. In this work, the CSF dynamics is modeled by a multiphysics model encompassing Multiple-Network Poroelasticity (MPE) equations for filtration and Stokes equations for the three-dimensional CSF flow in hollow regions [1]. The MPE equations also account for blood perfusion of the brain [2]: indeed, the production and washout function of CSF are significantly affected by blood pressure pulsatility [3]. To accurately represent the complex geometry of the brain and of the interface between the two physical domains, we introduce a discontinuous Galerkin method based on polytopal grids (PolyDG) for the spatial discretization of the model, for which we provide stability and convergence results [1]. We implemented this model in `lymph` [4], an open-source library developed at MOX for the solution of multiphysics problems with the PolyDG method. Simulations in patient-specific geometries reconstructed from magnetic resonance images show the suitability of the mathematical model and the effectiveness of the method.

**Acknowledgments**: IF, NP, and PFA acknowledge the funding by the Italian Research Center on High Performance Computing, Big Data and Quantum Computing (ICSC), under the NextGenerationEU project, and by MUR on the PRIN 2020 research grant n. 20204LN5N5. The authors are members of INdAM-GNCS and IF acknowledges the funding by the INdAM-GNCS Project CUP_E53C22001930001. We acknowledge CINECA for the availability of HPC resources under the ISCRA initiative. This work is part of the project Dipartimento di Eccellenza 2023-2027, Dipartimento di Matematica, Politecnico di Milano.

**Keywords**: Cerebrospinal fluid, Stokes' equation, Multiple-Network Poroelasticity Theory, Polygonal/polyhedral mesh, Multiphysics system

**Mathematics Subject Classifications (2010)**: 65N12, 65N22, 65N30, 76Z05.

## References

1. I. Fumagalli, M. Corti, N. Parolini, and P.F. Antonietti. Polytopal discontinuous Galerkin discretization of brain multiphysics flow dynamics. Submitted. Preprint: `https://arxiv.org/abs/2310.07651`.
2. M. Corti, P.F. Antonietti, L. Dede', and A. Quarteroni. Numerical modelling of the brain poromechanics by high-order discontinuous Galerkin methods. *Mathematical Models and Methods in Applied Sciences*, 33(8):1577-1609, 2023.
3. M. Causemann, V. Vinje, and M.E. Rognes. Human intracranial pulsatility during the cardiac cycle: a computational modelling framework. *Fluids Barriers CNS*, 19:84, 2022.
4. P.F. Antonietti, S. Bonetti, M. Botti, M. Corti, I. Fumagalli, and I. Mazzieri. lymph: an efficient high-order solver for differential problems with polytopal discontinuous Galerkin methods. Submitted.

# Efficient solvers in nonlinear poroelasticity

Nicolás A. Barnafi[1]

Centro de Modelamiento Matemático
nbarnafi@cmm.uchile.cl

**Summary.** Poroelasticity addresses the deformation of a porous medium, understood as a continuum with a complex interconnected structure through which fluid flows. This field has become attractive from a modeling perspective in biomedicine because soft tissue is naturally porous, as it contains both the circulatory and lymphatic systems. Its downside is that the equations describing such phenomena are much more involved than their elastic conterparts, which makes them more difficult to handle. A very successful strategy for solving the equations of poroelasticity, in the linear setting, has been that of alternating minimization methods, which applied to the original problem gives rise to the *undrained* scheme, whereas the dual formulation gives rise to the *fixed-stress* scheme. The connection of these methods to alternate minimization was possible after finding the mathematical structure of poroelasticity: Generalized Gradient Flows [1].

In this talk, we will study the mathematical structure of nonlinear poroelasticity, which has the main difficulty of presenting pressure as a function of porosity and not as a variable. This work extends previous works on linear and partially nonlinear poroelasticity [2, 3]. Its main objective of this study is that of developing robust iterative methods for poroelasticity, where an interesting feature of the model is that a primal formulation is *never* consistent, as it relies on second order derivatives that are not well-defined in the standard functional setting. We refer to this problem as *primal inconsistency*. Our formulation will allow for an iterative procedure that leverages the theory of alternating minimizations, and at the same time is robust against the primal inconsistency phenomenon. The resulting solvers are robust and optimal, as we will show through numerical tests for up to several millions of degrees of freedom. This guarantees that our methodology is transparently transferable to supercomputing infrastructures.

**Keywords**: Porous media, nonlinear poroelasticity, scalable solvers, alternate minimization

**Mathematics Subject Classifications (2010)**: 65F10, 74S05, 76S05

## References

1. Both JW, Kumar K, Nordbotten JM, Radu FA. The gradient flow structures of thermo-poro-visco-elastic processes in porous media. arXiv preprint, 2019.
2. Both JW, Barnafi NA, Radu FA, Zunino P, Quarteroni A. Iterative splitting schemes for a soft material poromechanics model. Computer Methods in Applied Mechanics and Engineering, 2022.
3. Barnafi Wittwer NA, Both JW. Iterative quasi-newton solvers for poromechanics applied to heart perfusion VI ECCOMAS Young Investigators Conference, 2022.

# MS6: From BEM to DPG: a minisymposium dedicated to the 60th birthday of prof. Norbert Heuer

# On the finite element least squares approximation of eigenvalue problems

Daniele Boffi[1]

King Abdullah University of Science and Technology (KAUST)
daniele.boffi@kaust.edu.sa

**Summary.** In this talk I will review our recent work on the numerical approximation of the spectrum associated with finite element least squares discretizations.

We started from the Poisson problem [3] and linear elasticity [4, 1, 2] and went through DPG formulations [6].

Finally, the application of our investigations to the Maxwell eigenvalue problem [5] leads to a new convergent and spurious modes free numerical scheme based on nodal finite elements.

**Keywords**: Least squares finite element method. Eigenvalue problems. Maxwell's equations.

**Mathematics Subject Classifications (2010)**: 65N25, 65N12, 65N15, 65N30.

## References

1. L. Alzaben, F. Bertrand, and D. Boffi. On the spectrum of an operator associated with least-squares finite elements for linear elasticity. *Comput. Methods Appl. Math.*, 22(3):511-528, 2022.
2. L. Alzaben, F. Bertrand, and D. Boffi. On the spectrum of the finite element approximation of a three field formulation for linear elasticity. *Examples and Counterexamples*, 2:100076, 2022.
3. F. Bertrand and D. Boffi. First order least-squares formulations for eigenvalue problems. IMA *Journal of Numerical Analysis*, drab005, 2021.
4. F. Bertrand and D. Boffi. Least-squares formulations for eigenvalue problems associated with linear elasticity. *Computers and Mathematics with Applications*, 95:19-27, 2021.
5. F. Bertrand, D. Boffi, and L. Gastaldi. Approximation of the Maxwell eigenvalue problem in a Least-Squares setting. *Computers & Mathematics with Applications*, to appear.
6. F. Bertrand, D. Boffi, and H. Schneider. Discontinuous Petrov-Galerkin approximation of eigenvalue problems. *Comput. Methods Appl. Math.*, 32(1):1-17, 2023.

# Pointwise and free boundary approximation of the obstacle problem for nonlocal operators

Juan Pablo Borthagaray[1], Ricardo H. Nochetto[2], Abner J. Salgado[3], and Céline Torres[4]

Instituto de Matemática y Estadística, Facultad de Ingeniería, Universidad de la República, Montevideo, Uruguay
jpborthagaray@fing.edu.uy
Department of Mathematics, University of Maryland, College Park, MD 20742, USA
rhn@umd.edu
Department of Mathematics, University of Tennessee, Knoxville, TN 37996, USA
asalgad1@utk.edu
Department of Mathematics, University of Maryland, College Park, MD 20742, USA
cetorres@umd.edu

**Summary.** We develop a monotone, two-scale discretization for a class of elliptic integrodifferential operators of order $2s$, like the integral fractional Laplacian of order $s \in (0,1)$. This discretization naturally leads to max-norm error estimates for linear problems. We extend these to the obstacle problem and indicate how, from these, free boundary estimates can be obtained, provided a nondegeneracy condition takes place. As an application of this result, we obtain convergent numerical approximations of a class of fully nonlinear, convex, integrodifferential operators.

**Keywords**: Integrodifferential operators; Monotonicity; Obstacle problems; Fully nonlinear nonlocal equations; Rate of convergence.

**Mathematics Subject Classifications (2010)**: 65N06, 65K15, 35R35, 35R09, 35S15, 49L25.

,

# Local minimum-residual a posteriori error estimates for a class of mixed finite element discretizations

Liliana Camargo[1], Ignacio Muga[2], Sergio Rojas[3], and Patrick Vega[4]

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile.
liliana.camargo@pucv.cl
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile.
ignacio.muga@pucv.cl
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile.
sergio.rojas.h@pucv.cl
Departamento de Matemática y Ciencia de la Computación, Universidad de Santiago de Chile, Chile.
patrick.vega@usach.cl

**Summary.** We introduce reliable and efficient a posteriori error estimates for a class of mixed formulations to solve partial differential equations involving a diffusion term. It combines a superconvergent postprocessing technique for the primal variable with an adaptive finite element method via residual minimization. Such a residual minimization procedure is performed on a local postprocessing scheme, commonly used in mixed finite element methods. Given the local nature of such an approach, the underlying saddle point problems associated with residual minimizations can be solved with minimal computational effort. We propose and study a posteriori error estimators based on an improvement of the built-in residual representative associated with residual minimization schemes, which adds, on the one hand, a residual term quantifying the mismatch between discrete fluxes and, on the other hand, the interelement jumps of the post-processed solution. We present several numerical experiments in two dimensions, including a standard mixed formulation for advection-diffusion problems using Brezzi–Douglas–Marini elements and a mixed Hybridizable Discontinuous Galerkin (HDG) formulation for the Helmholtz equation. The experiments perfectly fit our key theoretical findings and suggest that our estimates are sharp.

**Keywords**: residual minimization, postprocessing, superconvergence, a posteriori error analysis, adaptive mesh refinement.

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N22, 65N30, 65N50.

## References

1. L. Camargo, S. Rojas, and P. Vega. Minimum-residual a posteriori error estimates for a hybridizable discontinuous Galerkin discretization of the Helmholtz equation *arXiv preprint*, arXiv:2304.00418, 2023.
2. I. Muga, S. Rojas, and P. Vega. An adaptive superconvergent mixed finite element method based on local residual minimization *SIAM Journal on Numerical Analysis*, 61(5):2084-2105, 2023.

# Frictional contact with Nitsche method

Rodolfo Araya[1] and Franz Chouly[2]

CI[2]MA, Universidad de Concepción, Chile
rodolfo.araya@udec.cl
CI[2]MA, Universidad de Concepción, Chile
franz.chouly@math.cnrs.fr

**Summary.** We consider frictional contact problems in small strain elasticity discretized with finite elements and the Nitsche method [3]. Both bilateral and unilateral contact problems are taken into account, as well as both Tresca and Coulomb friction models [2, 5, 6]. We derive residual posteriori error estimates for each friction model following [4]. For the incomplete variant of Nitsche, we prove an upper bound for the dual norm of the residual, for Tresca and Coulomb friction, without any extra regularity and without a saturation assumption. We also prove local lower bounds. Numerical experiments in FEniCS allow to assess the accuracy of the estimates and their interest for adaptive meshing in different situations [1].

**Keywords**: frictional contact; finite elements; Nitsche method; stabilized methods; bilateral contact; unilateral contact; Tresca friction; Coulomb friction; a posteriori error estimates; adaptive meshing.

**Mathematics Subject Classifications (2010)**: 65N30.

## References

1. R. Araya and F. Chouly. Residual a posteriori error estimation for frictional contact with Nitsche method. *J. Sci. Comput.*, 96, Paper No. 87, 2023.
2. F. Chouly. An adaptation of Nitsche's method to the Tresca friction problem. *J. Math. Anal. Appl.*, 411:329–339, 2014.
3. F. Chouly, M. Fabre, P. Hild, , R. Mlika, J. Pousin and Y. Renard. An overview of recent results on Nitsche's method for contact problems. *Lect. Notes Comput. Sci. Eng.*, 121:93–141, 2017.
4. F. Chouly, M. Fabre, P. Hild, J. Pousin and Y. Renard. Residual-based *a posteriori* error estimation for contact problems approximated by Nitsche's method. *IMA J. Numer. Anal.*, 38:921–954, 2018.
5. F. Chouly, P. Hild, V. Lleras and Y. Renard. Nitsche method for contact with Coulomb friction: existence results for the static and dynamic finite element formulations. *J. Comput. Appl. Math.*, 416, Paper No. 114557, 2022.
6. F. Chouly, P. Hild and Y. Renard. Finite element approximation of contact and friction in elasticity. Advances in Mechanics and Mathematics (Advances in Continuum Mechanics), volume 48. Springer/Birkhäuser, 2023.

# From DPG to mixed FEM

Carsten Carstensen[1], Thomas Führer[2], and Norbert Heuer[3]

Humboldt–Universität zu Berlin, Germany
cc@math.hu-berlin.de
Pontificia Universidad Católica de Chile, Chile
tofuhrer@mat.uc.cl
Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna 4860, Santiago, Chile
nheuer@mat.uc.cl

**Summary.** Since its start more than a decade ago [2, 3], the discontinuous Petrov–Galerkin (DPG) method with optimal test functions has itself established as a well-understood and useful framework. As the name suggests, special test functions are used in a DG-setting; they aim at discrete stability. Essential for progress has been the systematic use of ultra-weak variational formulations. They transfer all appearing derivatives onto the test side, and generate trace terms by doing so, giving rise to independent trace variables [1].

Considering challenging problems, e.g., from the mechanics of thin structures, it becomes clear that corresponding trace spaces and operations are critical to design robust well-posed DPG schemes, see [5, 6]. On the other hand, trace operators are directly related with interface conditions and thus, characterize the conformity of corresponding fields. This is a relevant subject for the numerical analysis of PDE in general. In this talk we present some new results for mixed finite element methods that originate from DPG trace and discretization techniques, for plate bending [4] (collaboration with T. Führer) and linear elasticity (collaboration with C. Carstensen).

Financial support by ANID through Fondecyt project 1230013 is gratefully acknowledged.

**Keywords**: DPG method, mixed FEM, plate bending, linear elasticity

**Mathematics Subject Classifications (2010)**: 65N30, 35J35, 74G15, 74S05, 74K20

## References

1. Carlo L. Bottasso, Stefano Micheletti, and Riccardo Sacco. The discontinuous Petrov-Galerkin method for elliptic problems. *Comput. Methods Appl. Mech. Engrg.*, 191(31):3391–3409, 2002.
2. Leszek F. Demkowicz and Jay Gopalakrishnan. A class of discontinuous Petrov-Galerkin methods. Part I: the transport equation. *Comput. Methods Appl. Mech. Engrg.*, 199(23-24):1558–1572, 2010.
3. Leszek F. Demkowicz and Jay Gopalakrishnan. A class of discontinuous Petrov-Galerkin methods. Part II: Optimal test functions. *Numer. Methods Partial Differential Eq.*, 27:70–105, 2011.
4. Thomas Führer and Norbert Heuer. Mixed finite elements for Kirchhoff–Love plate bending. arXiv 2305.08693, 2023.
5. Thomas Führer, Norbert Heuer, and Antti H. Niemi. An ultraweak formulation of the Kirchhoff–Love plate bending model and DPG approximation. *Math. Comp.*, 88(318):1587–1619, 2019.
6. Thomas Führer, Norbert Heuer, and Antti H. Niemi. A DPG method for shallow shells. *Numer. Math.*, 152(1):76–99, 2022.

# Nonlinear twofold saddle point-based mixed finite element methods for granular flows

Sergio Caucao[1], Gabriel N. Gatica[2], Saulo Medrado[3], and Yuri D. Sobral[4]

Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción, Casilla 297, Concepción, Chile
scaucao@ucsc.cl
CI$^2$MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Casilla 160-C, Concepción, Chile
ggatica@ci2ma.udec.cl
Departamento de Matemática, Universidade de Brasília, Campus Universitário Darcy Ribeiro, 70910-900 Brasília, DF, Brazil
saulo.medrado@aluno.unb.br
Departamento de Matemática, Universidade de Brasília, Campus Universitário Darcy Ribeiro, 70910-900 Brasília, DF, Brazil
ydsobral@unb.br

**Summary.** We propose and analyze new mixed finite element methods for a regularized $\mu(I)$-rheology model of granular materials with an equivalent viscosity depending nonlinearly on the pressure and the euclidean norm of the symmetric part of the velocity gradient. To this end, and besides the velocity, the pressure and the aforementioned strain rate, we introduce the stress and the skew-symmetric vorticity as auxiliary tensor unknowns, thus yielding two related mixed variational formulations within a Banach spaces framework. The first one solves for the pressure through a iterative postprocess suggested by the incompressibility condition of the fluid, whereas the second one incorporates this variable as one more of the respective unknowns. Fixed-point strategies combined with a solvability result for a class of nonlinear twofold saddle point operator equations in Banach spaces, are employed to show, along with the classical Banach fixed-point theorem, the well-posedness of the continuous and discrete formulations. In particular, PEERS and AFW elements of order $\ell \geq 0$ for the stress, the velocity, and the skew-symmetric vorticity, and piecewise polynomials of degree $\leq \ell + n$ (resp. $\leq \ell + 1$) for the strain rate with PEERS (resp. with AFW), and of degree $\leq \ell$ for the pressure, yield stable Galerkin schemes. Optimal a priori error estimates are derived and associated rates of convergence are established. Finally, numerical results confirming the latter and illustrating the good performance of the methods, are reported.

**Keywords**: granular flows, nonlinear viscosity, twofold saddle point, mixed finite elements, fixed-point theory, a priori error analysis

**Mathematics Subject Classifications (2020)**: 65N30, 65N12, 65N15, 47H10, 47J26, 76D05, 76T25,

## References

1. T. Barker, D.G. Schaeffer, P. Bohorquez and J.M.N.T. Gray. Well-posed and ill-posed behaviour of the $\mu(I)$-rheology for granular flow. *J. Fluid Mech*. 779 (2015), 794–818.
2. I. Bermúdez, C.I. Correa, G.N. Gatica and J.P. Silva. A perturbed twofold saddle point-based mixed finite element method for the Navier-Stokes equations with variable viscosity. *Preprint* 2023-19, Centro de Investigación en Ingeniería Matemática, Universidad de Concepción, Chile, (2023).
3. J. Camaño, C. García and R. Oyarzúa. Analysis of a momentum conservative mixed-FEM for the stationary Navier-Stokes problem. *Numer. Methods Partial Differential Equations* 37 (2021), no. 5, 2895–2923.
4. S. Caucao, G.N. Gatica and F. Sandoval. A fully-mixed finite element method for the coupling of the Navier-Stokes and Darcy-Forchheimer equations. *Numer. Methods Partial Differential Equations* 37 (2021), no. 3, 2550–2587.
5. J. Chauchat and M. Médale. A three-dimensional numerical model for dense granular flows based on the $\mu(I)$ rheology. *J. Comput. Phys.* 256 (2014), 696–712.
6. G.N. Gatica and N. Heuer. A dual-dual formulation for the coupling of mixed-FEM and BEM in hyperelasticity. SIAM *J. Numer. Anal.* 38 (2000), no. 2, 380–400.

7. G.N. Gatica, N. Heuer and S. Meddahi. On the numerical analysis of nonlinear twofold saddle point problems. IMA *J. Numer. Anal.* 23 (2003), no. 2, 301–330.
8. G.N. Gatica, N. Núñez and R. Ruiz-Baier. New non-augmented mixed finite element methods for the Navier-Stokes-Brinkman equations using Banach spaces. *J. Numer. Math.*, https://doi.org/10.1515/jnma-2022-0073.
9. G.N. Gatica, R. Oyarzúa, R. Ruiz-Baier and Y.D. Sobral. Banach spaces-based analysis of a fully-mixed finite element method for the steady-state model of fluidized beds. *Comput. Math. Appl.* 84 (2021), 244–276.
10. G.N. Gatica and W.L. Wendland. Coupling of mixed finite elements and boundary elements for linear and nonlinear elliptic problems. *Appl. Anal.* 63 (1996), no. 1-2, 39–75.
11. GDR-MiDi. On dense granular flows. *European Journal of Physics* E 14 (2004), 341–365.
12. L. Jing, C.Y. Kwok, Y.F. Leung and Y.D. Sobral. Characterization of base roughness for granular chute flows. *Physical Review* E 94 (2016), 052901.

# Adaptive boundary element methods for regularized combined field integral equations

Théophile Chaumont-Frelet[1] and Gregor Gantner[2]

Inria Univ. Lille and Laboratoire Paul Painlevé, 59655 Villeneuve-d'Ascq, France
theophile.chaumont@inria.fr
Institute for Numerical Simulation, University of Bonn, Friedrich-Hirzebruch-Allee 7, 53115 Bonn, Germany
gregor.gantner@uni-bonn.de

**Summary.** While exterior boundary value problems for the Helmholtz equation are uniquely solvable, this is not the case for associated standard boundary integral equations if the wave number is related to interior resonances. On smooth boundaries, so-called combined field integral equations are not affected. In [1, 2], regularized versions of the latter, which are coercive on general Lipschitz domains, have been proposed.

In this talk, we present *a posteriori* computable residual error estimators for the boundary element discretization of these regularized combined field integral equations. If used to steer local refinement of the underlying meshes, we show that these estimators converge linearly at optimal algebraic rate.

**Keywords**: exterior Helmholtz problem, boundary element method, *a posteriori* error estimate, adaptive algorithm, optimal convergence

**Mathematics Subject Classifications (2010)**: 35J05, 65N12, 65N15, 65N38, 65N50

## References

1. A. Buffa and R. Hiptmair Regularized combined field integral equations. *Numerische Mathematik*, 100:1–19, 2005.
2. A. Buffa and S. Sauter On the acoustic single layer potential: stabilization and Fourier analysis. SIAM *Journal on Scientific Computing*, 28(5):1974–1999, 2006.

# Full Envelope DPG Approximation for Electromagnetic Waveguides. Stability and Convergence Analysis.

Leszek Demkowicz[1], Markus J. Melenk[2], Stefan Henneking[3], and Jacob Badger[4]

Oden Institute, University of Texas at Austin
leszek@oden.utexas.edu
Institut fuer Analysis und Scientific Computing,TU Wien,
melenk@tuwien.ac.at
Oden Institute, University of Texas at Austin
stefan@oden.utexas.edu
Oden Institute, University of Texas at Austin
badger@utexas.edu

**Summary.** The presented work started with a convergence and stability analysis for the so-called full envelope approximation used in analyzing optical amplifiers (lasers). The specific problem of interest was the simulation of Transverse Mode Instabilities [1]. The problem translates into the solution of a system of two nonlinear time-harmonic Maxwell equations coupled with a transient heat equation. Simulation of a 1 m long fiber involves the resolution of 10 M wavelenghts. A superefficient MPI/openMP hp FE code run on a supercomputer gets you to the range of ten thousand wavelenghts. The resolution of the additional thousand wavelenghths is done using an exponential ansatz $e^{ikz}$ in the $z$-coordinate. This results in a non-standard Maxwell problem. The stability and convergence analysis for the problem has been restricted to the linear case only [2, 3]. It turns out that the modified Maxwell problem is stable if and only if the original waveguide problem is stable and the boundedness below stability constants are identical. We have converged to the task of determining the boundedness below constant. The stability analysis started with an easier, acoustic waveguide problem. Separation of variables leads to an eigenproblem for a self-adjoint operator in the transverse plane (in $x,y$). Expansion of the solution in terms of the corresponding eigenvectors leads then to a decoupled system of ODEs, and a stability analysis for a two-point BVP for an ODE parametrized with the corresponding eigenvalues. The $L^2$-orthogonality of the eigenmodes and the stability result for a single mode, lead then to the final result: the boundedness below constant depends inversely linearly upon the length $L$ of the waveguide. The corresponding stability for the Maxwell waveguide turned out to be unexpectedly difficult. The equation is vector-valued so a direct separation of variables is out to begin with. An exponential ansatz in $z$ leads to a non-standard eigenproblem involving an operator that is nonself adjoint even for the easiest, homogeneous case. The answer to the problem came from a tricky analysis of the eigenproblem combined with the perturbation technique for perturbed self-adjoint operators. The use of perturbation theory requires an assumption on the smallness of perturbation of the dielectric constant (around a constant value) but with no additional assumptions on its differentiability (discontinuities are allowed). In the end, the final result is similar to that for the acoustic waveguide - the boundedness below constant depends inversely linearly on $L$.

**Keywords**: DPG, Full envelope, stability

**Mathematics Subject Classifications**: 78A50, 35Q61

## References

1. S. Henneking, J. Grosek, and L. Demkowicz. Parallel simulations of high-power optical fiber amplifiers. *Lect. Notes Comput. Sci. Eng.* , 2022. accepted.
2. L. Demkowicz, M.J. Melenk, J. Badger, and S. Henneking. Stability Analysis for Acoustic and Electromagnetic Waveguides. Part 2: Non-homogeneous Waveguides. *Oden Institute Report 2023/3*, submitted.
3. M.J. Melenk, L. Demkowicz, and S. Henneking. Stability Analysis for Acoustic and Electromagnetic Waveguides. Part 1: Acoustic and Homogeneous Electromagnetic Waveguides. *Oden Institute Report 2023/2*, submitted.

# Optimal mesh coarsening under constraints

Michael Feischl[1] and Hubert Hackl[2]

TU Wien - Institute of Analysis and Scientific Computing
michael.feischl@tuwien.ac.at
TU Wien - Institute of Analysis and Scientific Computing
hubert.hackl@tuwien.ac.at

**Summary.** In many non-stationary PDE problems, evolving singularities are a cause for inefficiency of finite element approximations. Without coarsening of the underlying triangulation after each time step, a moving singularity will lead to overrefinement and thus many unnecessary degrees of freedom. While coarsening of triangulations is well-understood for non-constrained problems since [1], we consider vector valued equations with non-convex constraints. Particularly, we are interested in problems where the solution is restricted pointwise to a given manifold. A relevant application is computational micro-magnetism, where the governing equation is the Landau-Lifshitz-Gilbert equation which enforces a pointwise length constraint on the solution vector field. Our main result shows that Binev's coarsening algorithm can be adapted to this setting and still delivers optimal coarsening while respecting the constraint. A by-product of the analysis in [2] shows that the coarsening algorithm can also be used to improve on the JPEG image compression algorithm.

**Keywords**: adaptive mesh-refinement, coarsening, quasi-optimal convergence

**Mathematics Subject Classifications (2010)**: 65N30, 65N50, 15A23

## References

1. P. Binev and R. DeVore. Fast computation in adaptive tree approximation. *Numer. Math.*, 97:193-217, 2004.
2. M. Feischl and H. Hackl. Adaptive Image Compression via Optimal Mesh Refinement. *arXiv E-print*, arXiv:2304.01640, 2023.

# A DPG method for linear quadratic optimal control problems

Thomas Führer[1] and Francisco Fuica[2]

Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna 4860, Santiago, Chile.
tofuhrer@mat.uc.cl
Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna 4860, Santiago, Chile.
francisco.fuica@mat.uc.cl

**Summary.** The DPG method with optimal test functions for solving linear quadratic optimal control problems with control constraints is studied. We prove existence of a unique optimal solution of the nonlinear discrete problem and characterize it through first order optimality conditions. Furthermore, we systematically develop a priori as well as a posteriori error estimates. Our proposed method can be applied to a wide range of constrained optimal control problems subject to, e.g., scalar second-order PDEs and the Stokes equations. Numerical experiments that illustrate our theoretical findings are presented.

**Keywords**: optimal control, discontinuous Petrov–Galerkin method, optimal test functions, finite elements, convergence, error estimates.

**Mathematics Subject Classifications (2010)**: 49J20, 49M25, 65N15, 65N30.

## References

1. C. Carstensen, L. Demkowicz, and J. Gopalakrishnan. Breaking spaces and forms for the DPG method and applications including Maxwell equations. *Computers & Mathematics with Applications*, 72(3):494-522, 2016.
2. L. Demkowicz, J. Gopalakrishnan, and B. Keith. The DPG-star method. *Computers & Mathematics with Applications*, 79(11):3092-3116, 2020.
3. F. Tröltzsch. *Optimal control of partial differential equations*, volume 112 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2010. Theory, methods and applications, Translated from the 2005 German original by Jürgen Sprekels.

# A DPG method for the quad-curl problem

Thomas Führer[1], Pablo Herrera[2], and Norbert Heuer[3]

Pontificia Universidad Católica de Chile
tofuhrer@mat.uc.cl
Facultad de Matematicas, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna ˜ 4860, Santiago, Chile
{tofuhrer,pcherrera,nheuer}@mat.uc.cl
Pontificia Universidad Católica de Chile
nheuer@mat.uc.cl

**Summary.** In this talk we present an ultra-weak formulation for the quad-curl problem in two and three dimensions. We provide a discontinuous Petrov–Galerkin (DPG) method [4] and prove its quasi-optimal convergence. The quad-curl problem is related with many applications of science and engineering. For example, we can find some applications in the fields of magneto-hydrodynamics, electromagnetic inverse scattering theory, and fluid dynamics. For instance, we show an application of the quad-curl problem for the Stokes problem in two dimensions. We eliminate the pressure variable involved in the Stokes equations, via the application operator, and apply the DPG techniques for the Kirchoff–Love plate bending problem [2, 3]. Also, we provide a fully discrete DPG method in two dimensions. We show an a priori error estimate which also improves past error estimation for effective shear forces using a less restrictive regularity assumption. Finally, we show numerical experiments that confirm our findings.

**Keywords**: DPG, quad-curl, Stokes, Kirchhoff–Love

**Mathematics Subject Classifications (2010)**: 35J35, 65N30, 74K20, 35J67

**Acknowledgment**: Support by ANID-Chile through FONDECYT projects 1190009 and 1210391 is gratefully acknowledged.

## References

1. T. Führer, P. Herrera and N. Heuer. A DPG method for the quad-curl problem. *Comput. Math. Appl.* (in press), 2023.
2. T. Führer, N. Heuer, and A. H. Niemi. An ultraweak formulation of the Kirchhoff–Love plate bending model and DPG approximation. *Math. Comp.*, 88:1587–1619, 2019.
3. T. Führer and N. Heuer. Fully discrete DPG methods for the Kirchhoff–Love plate bending model. *Comput. Methods Appl. Mech. Engrg.*, 343:550–571, 2019.
4. L. F. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov–Galerkin methods. Part ii. optimal test functions. *Numer. Methods Partial Differential Equations.*, 27 (1):70–105, 2011.

# Test spaces and Fortin operators for DPG

Thomas Führer[1] and Norbert Heuer[2]

Facultad de Matemáticas, Pontificia Universidad Católica de Chile
tofuhrer@mat.uc.cl
Facultad de Matemáticas, Pontificia Universidad Católica de Chile
nheuer@mat.uc.cl

**Summary.** At the fully discrete setting, stability of the discontinuous Petrov–Galerkin (DPG) method with optimal test functions requires local test spaces that ensure the existence of Fortin operators. We construct such operators for $H^1$ and $H(\mathrm{div})$ on simplices in any space dimension and arbitrary polynomial degree. The resulting test spaces are smaller than previously analyzed cases. For parameter-dependent norms, we achieve uniform boundedness by the inclusion of exponential layers. As an example, we consider a canonical DPG setting for reaction-dominated diffusion. Our test spaces guarantee uniform stability and quasi-optimal convergence of the scheme. We present numerical experiments that illustrate the loss of stability and error control by the residual for small diffusion coefficient when using standard polynomial test spaces, whereas we observe uniform stability and error control with our construction.

**Keywords**: Fortin operator, DPG method, singularly perturbed problem

**Mathematics Subject Classifications (2010)**: 65N30, 65N12

## References

1. T. Führer and N. Heuer (2023). *Robust DPG Fortin operators*. arXiv.org, 2301.13021.

# Space-time finite elements for the wave equation

Thomas Führer[1], Roberto González[2], and Michael Karkulik[3]

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

**Summary.** 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

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

**Keywords**: wave equation, space time discretizations, least squares methods

**Mathematics Subject Classifications (2010)**: 65N30

## References

1. T. Führer and M. Karkulik (2021). *Space-time least-squares finite elements for parabolic equations*. Comput. Math. Appl., volume 92.
2. G. Gantner and R. Stevenson (2020). *Further results on a space-time FOSLS formulation of parabolic PDEs*. ESAIM: M2AN Volume 55.

# A time-stepping DPG scheme for the Timoshenko beam model.

Carlos Garcia Vera[1]

Departamento de Ciencias Exactas, Universidad de Los Lagos, Osorno, Chile
carlos.garcia@ulagos.cl

**Summary.** We introduce and analyze a discontinuous Petrov-Galerkin method with optimal test functions for the Timoshenko beam bending model in its time-dependent version. The scheme is based on the backward Euler time stepping and uses an ultra-weak variational formulation at each time step. We consider various boundary conditions, combining clamped, simply supported, and free ends. Our scheme approximates the transverse deflection and bending moment. It converges quasi-optimally in $L^2$ and is locking free. Several numerical results illustrate the performance of our method.

**Keywords**: Beam Bending, Timoshenko Model, Discontinuous Petrov–Galerkin Method, Optimal Test Functions

**Mathematics Subject Classifications (2010)**: 74S05, 74K10, 65L11, 65L60.

## References

1. Führer, T., Heuer, N., and Sen Gupta, J. A Time-Stepping DPG Scheme for the Heat Equation. *Computational Methods in Applied Mathematics*, 17(2):237-252, 2017.
2. L. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov–Galerkin methods. Part II: Optimal test functions. *Numerical Methods for Partial Differential Equations*, 27:70-105, 2011.
3. A. Niemi, J. Bramwell, L. Demkowicz. Discontinuous Petrov–Galerkin method with optimal test functions for thin–body problems in solid mechanics. *Comput. Methods Appl. Mech. Engrg.*, 200:1291–1300, 2011.
4. Führer, T., Heuer, N., and García Carlos. A Locking–Free DPG Scheme for Timoshenko Beams. *Computational Methods in Applied Mathematics.*, 21(2):373-383, 2021.

# A Residual Minimization Method onto Bubble Enrichment

Jose G. Hasbani[1], Paulina Sepúlveda[2], Ignacio Muga[3], Victor M. Calo[4], and Sergio Rojas[5]

Vista Energy, Argentina
jose.hasbani@vistaenergy.com
Pontificia Universidad Católica de Valparaíso, Chile
paulina.sepulveda@pucv.cl
Pontificia Universidad Católica de Valparaíso, Chile
ignacio.muga@pucv.cl
Curtin University, Australia
Victor.Calo@curtin.edu.au
Pontificia Universidad Católica de Valparaíso, Chile
sergio.rojas.h@pucv.cl

**Summary.** The Adaptive Stabilized Finite Element method (AS-FEM) introduced in [1] combines the idea of the residual minimization method with the inf-sup stability offered by the discontinuous Galerkin (DG) frameworks. Consequently, the discretizations deliver stabilized conforming approximations and residual representative spaces that can drive automatic adaptivity. In this talk, we will present an extension of the AS-FEM by considering a residual minimization method on a stable Continuous Interior Penalty (CIP) formulation. This formulation, developed in [2], utilizes a $C^0$-conforming trial FEM space and a test space enriched with bubble functions derived from the trial space. Numerical experiments show that the test space choice significantly reduces the total degrees of freedom compared to the DG test spaces of [1], while recovering the expected convergence rate for the error in the corresponding trial space norm.

**Keywords**: adaptivity, stabilized finite element methods, residual minimization, Continuous Galerkin, Continuous Interior Penalty

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N22, 65N30, 65N50.

## References

1. V.M. Calo, A. Ern, I. Muga, and S. Rojas. An adaptive stabilized conforming finite element method via residual minimization on dual discontinuous Galerkin norms. *Computer Methods in Applied Mechanics and Engineering*, 363: 11289, 2020.
2. J.G. Hasbani, P. Sepúlveda, I. Muga, V.M. Calo, and S. Rojas. Adaptive stabilized finite elements via residual minimization onto bubble enrichments. *Computers & Mathematics with Applications*, 151: 1-11, 2023.

# Discontinuous Petrov-Galerkin method for Arch Structures

Norbert Heuer[1] and Antti H. Niemi[2]

Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Santiago, Chile
nheuer@mat.uc.cl
Civil Engineering Research Unit, University of Oulu, Finland
antti.niemi@oulu.fi

**Summary.** Develpoment of effective numerical methods for the analysis of curved arch structures is of interest in many application areas of architecture, civil engineering and mechanical engineering. In this work we study the circular arch problem taking into account transvere shear deformations. The starting point is a structural model where the kinematic assumptions of the classical Timoshenko beam model are imposed in the curved reference geometry. We analyze ultra-weak variational formulations with small parameter, proportional to the slenderness of the structure. We prove wellposedness of the formulation and consider discontinuous Petrov-Galerkin finite element approximation of the problem involving direct approximations of all stress and displacement variables. The method is shown to be stable in the assumed finite element spaces for different boundary conditions and the performance is demonstrated by numerical experiments.

**Keywords**: Arches; Structural analaysis; Numerical analysis; Finite element theory

**Mathematics Subject Classifications (2010)**: 65L60, 74S05

## References

1. A.F.D. Loula, L.P. Franca, T.J.R. Hughes and I. Miranda. Stability, convergence and accuracy of a new finite element method for the circular arch problem. *Computer Methods in Applied Mechanics and Engineering*, 63:281-303, 1987.
2. A.H. Niemi, J.A. Bramwell, and L.F. Demkowicz. Discontinuous Petrov–Galerkin method with optimal test functions for thin-body problems in solid mechanics. *Computer Methods in Applied Mechanics and Engineering*, 200:1291-1300, 2011.
3. T. Führer, C. García Vera and N. Heuer. A Locking-Free DPG Scheme for Timoshenko Beams. *Computational Methods in Applied Mathematics*, 21(2): 373-383, 2021

# Resolving singularities in parabolic initial-boundary value problems

Torsten Linß[1] and Brice Girol[2]

FernUniversität in Hagen
torsten.linss@fernuni-hagen.de
Affiliation of the third author
email@third.author.org

**Summary.** We consider a time-dependent reaction-diffusion equation with a singularity arising from incompatible initial and boundary conditions:

$$u_t - u_{xx} + b(x,t)u = f \qquad \text{in } (0,\ell)\times(0,T],$$

subject to boundary conditions

$$u(0,t) = \phi_0(t), \quad u(\ell,t) = \phi_\ell(t), \quad t \in (0,T],$$

and the initial condition

$$u(x,0) = 0, \qquad x \in (0,\ell),$$

with $\phi_0(0) \neq 0$.

The discrepancy between initial and boundary conditions causes the formation of a singularity in the vicinity of the corner $(0,0)$. This singularity $s$ can be characterised as the solution of

$$s_t - s_{xx} + b(0,0)s = 0 \qquad \text{in } (0,\infty)\times(0,T],$$

subject to the boundary condition

$$s(0,t) = \phi_0(0), \quad t \in (0,T],$$

and the initial condition

$$s(x,0) = 0, \qquad x \in (0,\infty).$$

This in turn can be given analytically using the error function.

Now, the interesting question is: How can the remainder $y = u - s$ be resolved numerically?

We derive bounds on the derivative of $y$ — under significantly less restrictive assumptions then previously assumed by other authors — and show how a numerical approximation can be obtained using an appropriately designed mesh.

**Keywords**: singularities, parabolic problems, adapted meshes

**Mathematics Subject Classifications (2020)**: 35K20, 65M06

# Adaptive projections in dual norms: An overview of the state of the art

Ignacio Muga[1], Sergio Rojas[2], Kristoffer G. van der Zee[3], and Patrick Vega[4]

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile
ignacio.muga@pucv.cl
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile
sergio.rojas.h@pucv.cl
School of Mathematical Sciences, University of Nottingham, UK
KG.vanderZee@nottingham.ac.uk
Departamento de Matemática y Ciencia de la Computación, Universidad de Santiago de Chile, Chile.
patrick.vega@usach.cl

**Summary.** In [1], we proposed an adaptive projection method in negative Sobolev spaces $W^{-m,p}(\Omega)$ to regularize continuous linear functionals acting on regular Sobolev spaces such as $W^{m,q}(\Omega)$, where $m \geq 1$; $p^{-1}+q^{-1}=1$; $1 < p < +\infty$; and $\Omega$ being a Lipschitz domain. In this context, regularization means to find an optimal piecewise polynomial function $\ell_H : \Omega \to \mathbb{R}$, such that the action of a functional $\ell$ over any test function $v$, can be approximated by $\langle \ell, v\rangle \approx \int_\Omega \ell_H v$. In this talk, we provide a state of the art of the method, including extensions/adaptations to nonconforming settings, new compatible pairs, projection of rougher linear functionals, duality-map localization features, and averaging operators, together with some numerical validations.

**Keywords**: Rough linear functionals, adaptive regularization, projection in dual norms, nonconforming discretizations.

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N22, 65N30, 65N50.

## References

1. F. Millar, I. Muga, S. Rojas, and K. G. van der Zee. Projection in negative norms and the regularization of rough linear functionals. *Numerische Mathematik*, 150, 1087-1121, 2022.
2. I. Muga, S. Rojas, K. G. van der Zee, and P. Vega. Source regularization through projection in dual norms for nonconforming finite element discretizations. *In preparation*, 2023.

# Numerical analysis of the Landau–Lifshitz–Baryakhtar equation in micromagnetics

Agus Soenjaya[1] and Thanh Tran[2]

The University of New South Wales
a.soenjaya@unsw.edu.au
The University of New South Wales
thanh.tran@unsw.edu.au

**Summary.** The Landau–Lifshitz equation is commonly used in micromagnetics to model the effects of a magnetic field on ferromagnetic materials [4]. An important feature of this equation is the conservation of magnitude of the magnetisation vector. It is known that this equation is essentially valid only at very low temperature, since it completely ignores contributions from high-frequency spin waves responsible for longitudinal magnetisation fluctuation [1]. To rectify this problem, the Landau–Lifshitz–Baryakhtar (LLBar) [2] and the Landau–Lifshitz–Bloch (LLBloch) [3] equations were proposed in the physics literature. These models take into account longitudinal relaxation and are valid at high temperatures, which are important for applications, for instance in heat-assisted magnetic recording and magnonic devices.

Existence and uniqueness of global weak and strong solutions to the LLBar equation were proven in [6], while existence of global weak solutions to the LLBloch equation were shown in [5]. We proposed some fully discrete numerical schemes to solve the LLBar equation, including a method based on $C^1$-conforming finite element [7] and another based on mixed formulation of the equation [8], in each case obtaining optimal order of convergence to the solution. As a by-product of our analysis, we showed the convergence of solution of the LLBar equation to the LLBloch equation (for high temperature but still below the Curie temperature) and the uniqueness of weak solution to the LLBloch equation.

**Keywords**: Landau–Lifshitz, Landau–Lifshitz–Baryakhtar, micromagnetics, finite element.

**Mathematics Subject Classifications (2010)**: 65M12, 65M60, 35K35, 35Q60.

## References

1. U. Atxitia, O. Chubykalo-Fesenko, N. Kazantseva, D. Hinzke, U. Nowak, and R.W. Chantrell. Micromagnetic modeling of laser-induced magnetization dynamics using the Landau-Lifshitz-Bloch equation. *Appl. Phys. Lett.* 91(23):232507, 2007.
2. V.G. Baryakhtar. Phenomenological description of relaxation processes in magnets. *Zh. Eksp. Teor. Fiz.* 87, 1501–1510, 1997.
3. D.A. Garanin. Fokker-Planck and Landau-Lifshitz-Bloch equations for classical ferromagnets. *Phys. Rev. B* 55(5), 3050, 1997.
4. D.L. Landau and E. Lifshitz. On the theory of the dispersion of magnetic permeability in ferromagnetic bodies. *Phys. Z. Sowjetunion* 8:153, 1935.
5. K.N. Le. Weak solutions of the Landau-Lifshitz-Bloch equation. *J. Differential Equations*, 261, 6699–6717, 2016.
6. A.L. Soenjaya and T. Tran. Global solutions of the Landau-Lifshitz-Baryakhtar equation. *J. Differential Equations*, 371, 191–230, 2023.
7. A.L. Soenjaya and T. Tran. Stable $C^1$-conforming finite element methods for the Landau-Lifshitz-Baryakhtar equation. *arXiv:2309.05530*, 2023.
8. A.L. Soenjaya. Energy-stable mixed finite element methods for the Landau-Lifshitz-Baryakhtar equation. *Preprint*.

## MS7: Full and reduced-order modeling of multiphysics problems

# A priori error estimates for a coseismic slip optimal control problem

Jorge Aguayo[1] and Rodolfo Araya[2]

Centro de Modelamiento Matemático, Universidad de Chile
jaguayo@dim.uchile.cl
CI$^2$MA and Departamento de Ingeniería Matemática, Universidad de Concepción
rodolfo.araya@udec.cl

**Summary.** This article presents an a priori error estimation for a finite element discretization applied to an optimal control problem governed by a mixed formulation for linear elasticity equations, where weak symmetry is imposed for the stress tensor. The optimal control is given by a discontinuity jump in displacements, representing the coseismic slip along a fault plane. This slip corresponds to the moment of an earthquake occurs, rendering this optimal control problem scientifically significant. We establish an a priori error estimate using appropriate finite element spaces for both control and states. Our theoretical convergence rates were validated through numerical experiments.

**Keywords**: finite elements, elasticity equations, inverse problems, optimal control

**Mathematics Subject Classifications (2010)**: 65N30, 65R32, 65Z05, 49J50, 74G75

## References

1. S. Puel, E. Khattatov, U. Villa, D. Liu, O. Ghattas and T. W. Becker. A mixed, unified forward/inverse framework for earthquake problems: fault implementation and coseismic slip estimate OUP *Geophysical Journal International*, 230(2):733–758, 2022.
2. Douglas N. Arnold, Richard S. Falk and Ragnar Winther, Mixed finite element methods for linear elasticity with weakly imposed symmetry *Mathematics of Computation*, 76(260):1699–1724, 2008.
3. Axel Kröner and Boris Vexler, A priori error estimates for elliptic optimal control problems with a bilinear state equation *Journal of Computational and Applied Mathematics*, 230(2):781—802, 2009

# A finite element method for the Navier-Stokes equation with free surface

Gabriel R. Barrenechea[1]

University of Strathclyde
gabriel.barrenechea@strath.ac.uk

**Summary.** in this talk I will present a new finite element method for the incompressible Navier-Stokes equations with free surface. The evolution of the free surface is driven by the kinematic boundary condition, and an Arbitrary Lagrangian Eulerian (ALE) approach is used to derive a (formal) weak formulation which involves three fields, namely, velocity, pressure, and the function describing the free surface. This formulation is discretised using finite elements in space and a time-advancing explicit finite difference scheme in time. In fact, the domain tracking algorithm is explicit: first, we solve the equation for the free surface, then move the mesh according to the sigma transform, and finally we compute the velocity and pressure in the updated domain. This explicit strategy is built in such a way that global conservation can be proven, which plays a pivotal role in the proof of stability of the discrete problem. In addition, in the first and third steps of this algorithms appropriate stabilisation terms are added in order to prove stability of the scheme. The well-posedness and stability results are independent of the viscosity of the fluid, but while the proof of stability for the velocity is valid for all time steps, and all geometries, the stability for the free surface requires a CFL condition. The performance of the current approach is presented via numerical results and comparisons with the characteristics finite element method.

The work presented in this talk has been done in collaboration with Emmanuel Audusse (Université Sorbonne Paris Nord), Astrid Decoene (Université de Bordeaux), and Pierrick Quemar (Université Sorbonne Paris Nord).

**Keywords**: incompressible Navier-Stokes equation; free surface flows; finite element method; explicit scheme.

1

# Numerical simulation of phase change problems by variational multiscale techniques

Roberto C. Cabrales[1], Ernesto Castillo[2], and Douglas R. Q. Pacheco[3]

Multidisciplinary Institute of Research and Postgraduate, University of La Serena, Chile
rcabrales@userena.cl
Department of Mechanical Engineering, University of Santiago, Chile
ernesto.castillode@usach.cl
Department of Mathematical Sciences, Norwegian University of Science and Technology, Trondheim, Norway
douglas.r.q.pacheco@ntnu.no

**Summary.** Phase change problems are processes that consists in the change of state of the matter from liquid to solid as a result of decreasing temperature. Its understanding is a critical step in applied engineering design in several industry areas such as the freezing of foods to preserve their quality and the solidification of pure metals and alloys to obtaing high quality products. The mathematical model for this kind of problems consist in a coupled non-linear system of partial differential equations including continuity, linear momentum and energy. More specifically, if $t_f > 0$ is a time horizon and $\Omega \subset \mathbb{R}^d, d = 2,3$ is a bounded domain with boundary $\partial\Omega$, we want to find the velocity $u$, pressure $p$, temperature $T$ and the phase change function $f_{pc}(T)$ such that:

$$\rho \frac{\partial u}{\partial t} + \rho u \cdot \nabla u - \nabla \cdot (2\mu \nabla^s u) + \mathscr{K}(f_{pc}(T))u + \nabla p = f(\rho, T), \qquad \text{in } (0,t_f) \times \Omega, \tag{1}$$

$$\nabla \cdot u = 0, \qquad \text{in } (0,t_f) \times \Omega, \tag{2}$$

$$\left[\rho C_p + L \frac{\partial f_{pc}(T)}{\partial T}\right] \left[\frac{\partial T}{\partial t} + u \cdot \nabla T\right] = \nabla \cdot (\kappa \nabla T), \qquad \text{in } (0,t_f) \times \Omega. \tag{3}$$

This system is complemented with suitable initial and boundary conditions. Additionally, $\nabla^s u := \frac{1}{2}(\nabla u + (\nabla u)^T)$ is the symmetric gradient of the velocity, $f(\rho, T)$ is the body force vector, $\mu$ is the viscosity, $\kappa$ is the thermal conductivity, $\rho$ is the density, $C_p$ is the apparent specific heat, $L$ is the latent heat, $\mathscr{K}(f_{pc}(T))$ is a function used to reduce the velocity in the solidifying zone [ref].

In this talk, we present a numerical algorithm to solve system (1)-(3) based on a variational multiscale finite element method introduced by Hughes [4]. The method extend the ideas presented by Castillo and Codina in [2] performing a stabilization term-by-term with dynamic subescales for the velocity, pressure and temperature. We perform numerical simulations of some problems involving water freezing [3] and alloy solidification [1], to show the robustness and the efficiency of the proposed numerical scheme.

**Keywords**: Phase change, Finite element method, Variational multiscale framework.

**Mathematics Subject Classifications (2020)**: 65N30, 76D05, 76M10.

## References

1. B.A.V. Bennet. Adaptive numerical modeling of natural convection, conduction, and solidification within mold cavities *Numerical Heat Transfer*, Part A, 51:313-342, 2007.
2. E. Castillo and R. Codina. Dynamic term-by-term stabilized finite element formulation using orthogonal subgrid-scales for the incompressible Navier–Stokes problem. *Computer Methods in Applied Mechanics and Engineering*, 349:701-721, 2019.
3. M.A. Ezan, and M. Kalfa. Numerical investigation of transient natural convection heat transfer of freezing water in a square cavity. *International Journal of Heat and Fluid Flow*, 61:438-448, 2016.

*This work was partially funded by the Chilean Council for Science and Technological Research through the projects FONDECYT 1230969 and FONDECYT 1210156.

4. T.J. Hughes, G.R. Feijóo, L. Mazzei and J.B. Quincy. The variational multiscale method-a paradigm for computational mechanics. *Computer Methods in Applied Mechanics and Engineering*, 166(1-2):3-24, 1998.

# Total Pressure-based Frequency-Domain Formulation and Convergence Analysis of Biot's Poroelasticity Equations with A New Finite Element Stabilization

Alfonso Caiazzo[1], Cristian Cárcamo[2], Felipe Galarce[3], and Joaquín Mura[4]

Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e.V. (WIAS), Berlin, Germany
alfonso.caiazzo@wias-berlin.de
Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e.V. (WIAS), Berlin, Germany
carcamo@wias-berlin.de
Escuela de Ingeniería Civil, Pontificia Universidad Católica de Valparaíso, Valparaíso, Chile
felipe.galarce@pucv.cl
Department of Mechanical Engineering, Universidad Técnica Federico Santa María, Santiago, Chile
joaquin.mura@usm.cll

**Summary.** In time-harmonic imaging elastography, we delve into complex-variable-based poroelastic problems, wherein coefficients such as permeability may exhibit sudden spatial variations [3]. We explore their theoretical foundations, assess their practical implications, and consider their prospective applications as inverse problems. Our approach begins with the application of the well-established Fredholm Alternative to prove the solvability of the continuous problem. To overcome the challenges posed by the discrete inf-sup condition, we introduce an innovative and robust stabilized numerical system, optimized for equal polynomial order, which enhances computational efficiency. Additionally, we conduct a numerical evaluation to assess the stability of solutions relative to the permeability constant and offer an a priori analysis of these solutions. To elucidate our insights, we augment our theoretical discourse with numerical examples. These illustrations furnish compelling evidence of the practical applicability and efficacy of the proposed numerical framework. By bridging the theoretical complexities of complex-variable-based poroelastic problems with feasible solutions, our research contributes valuable insights for applications in Imaging Elastography and related disciplines.

**Keywords**: Biot, poroelasticity, magnetic resonance elastography, stabilized finite element.

**Mathematics Subject Classifications (2010)** 65N30, 76S05, 74F10, 65N15.

## References

1. M. Biot. General theory of three-dimensional consolidation. *Journal of Applied Physics*, 12,155-164, 1941.
2. R. Oyarzúa, R. Ruiz-Baier Locking-free finite element methods for poroelastic SIAM *J. Numer. Anal.*, 54(5), 2951–2973, 2016.
3. F. Galarce, K. Tabelown, J. Polzehl, C. Panagiotis P., V. Vavourakis, L. Lilaj, I. Sack, A. Caiazzo. Displacement and pressure reconstruction from magnetic resonance elastography images: application to an in silico brain model, *Preprint, https://doi.org/10.48550/arXiv.2204.12445*. 2023.

# Reduced order modeling of time-dependent purely viscous non-Newtonian fluid flows

Ernesto Castillo[1], Ricardo Reyes[2], and Camilo Bayona[3]

Departamento de Ingeniería Mecánica, Universidad de Santiago de Chile
ernesto.castillode@usach.cl
École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
ricardo.reyes@epfl.edu
Pontificia Universidad Javeriana, Bogotá Colombia
ca_bayonar@javeriana.edu.co

**Summary.** This work numerically evaluates the accuracy and performance of a stabilized finite element Reduced Order Modelling (ROM) approach designed to simulate time-dependent generalized Newtonian fluid flows. The method estimates off-trained parametric scenarios not included in the training data set composing the ROM basis and can adopt arbitrary values from other specific fluid and flow conditions. Also, a mesh-based hyper-reduction technique is included [1].

The numerical testing includes approximating well- established benchmark solutions of shear-thinning and shear-thickening fluid flows to demonstrate the method's robustness. Furthermore, the application of the method in two engineering problems related to hemodynamic and conjugate thermally coupled flows is presented [2,3].

Numerical results evidence the method's capability, accuracy, and performance to approximate complex flow conditions of generalized Newtonian fluids.

**Acknowledgment**: This work is partially founded by ANID Chile through the project FONDECYT 1210156.

**Keywords**: Stabilized Finite Element Metods, Variational Multiscale Method, Non-Newtonian Fluids, Reducer Order Modelling.

## References

1. R. Reyes, O. Ruz, C. Bayona-Roa, E. Castillo and A. Tello. Reduced order modeling for parametrized generalized Newtonian fluid flows. *Journal of Computational Physics*, 484: 112086, 2023.
2. N. Espinoza, C. Bayona-Roa, E. Castillo, T. Gandara and N.O. Moraga. Hyperreduced-order modeling of thermally coupled flows. *Applied Mathematical Modeling*, 125(Part A): 59-81, 2024.
3. C Farías, C Bayona-Roa, E Castillo, RC Cabrales, R Reyes. Reduced order modeling of parametrized pulsatile blood flows: Hematocrit percentage and heart rate. *International Journal of Engineering Science*, 193: 103943, 2023.

# Variational strategies for inverse problems in biomechanics

Felipe Galarce[1]

School of Civil Engineering. Pontificia Universidad Católica de Valparaíso, Chile.
felipe.galarce@pucv.cl

**Summary.** In recent times, there has been an increased focus on developing data assimilation techniques for interpreting medical data. This surge is primarily driven by the growing demand for non-invasive methods in the prevention, diagnosis, and treatment of various diseases [**?**, **?**].

Variational strategies are among the more popular avenues to offer a solution for this sort of problems. In this framework, a parameter, or a state, is computed by means of both fundamental ingredients: models and measures. The former is typically assumed as a governing partial differential equation, while the later is normally some sensor information, or an image.

This work offers a small review of the state of the art of inverse problems for state estimation in biomechanics, while it builds on top some useful strategies for scenarios where the dynamics of the underlying state has a complex Kolmogorov n-width, or where the sensor information is particularly degraded by observation bias.

We show the capabilities of this improvements in realistic scenarios for two image modalities: Doppler ultrasound [**?**] and Magnetic resonance elastography [**?**].

**Keywords**: Inverse problems, Model order reduction, Hemodynamics.

# Model Order Reduction for Time-Dependent Problems Using the Laplace Transform

Fernando Henríquez[1] and Jan S. Hesthaven[2]

Chair of Computational Mathematics and Simulation Science, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland
fernando.henriquez@epfl.ch
Chair of Computational Mathematics and Simulation Science, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland
jan.hesthaven@epfl.ch

**Summary.** We propose a reduced basis method for solving time-dependent partial differential equations utilizing the Laplace transform. Unlike traditional approaches, we begin by applying the Laplace transform to the evolution problem. This transformation yields a time-independent boundary value problem that depends on the complex Laplace parameter.

In the offline stage, we systematically sample the Laplace parameter and solve the underlying set of problems using the Finite Element Method (FEM). Subsequently, we employ Proper Orthogonal Decomposition (POD) on this set of solutions to obtain a reduced basis of significantly lower dimension compared to the original FEM space. This reduced basis is then utilized to solve the evolution problem using an appropriate time-stepping method.

Numerical experiments validate our theoretical claims and demonstrate the advantages of our proposed method, both in terms of accuracy and speed, in comparison to existing approaches.

**Keywords**: Model Order Reduction; Reduced Basis Method; Laplace Transform.

**Mathematics Subject Classifications (2010)**: 65M6; 65M12; 65M32; 65N12

## References

1. J. S. Hesthaven, C. Pagliantini, C., G. Rozza. Reduced basis methods for time-dependent problems. *Acta Numerica*, 31, 265-345, 2002
2. W. Arendt, et al. Vector-valued Laplace transforms and Cauchy problems. *Israel Journal of Mathematics*, 59 (1987): 327-352.
3. D.B. Phuong Huynh, D. J. Knezevic, and A. T. Patera. A Laplace transform certified reduced basis method; application to the heat equation and wave equation. *Comptes Rendus. Mathématique*, 349.7-8 (2011): 401-405.
4. K. L. Kuhlman Review of inverse Laplace transform algorithms for Laplace-space numerical approaches. *Numerical Algorithms* 63 (2013): 339-355.

# MS8: Mathematical modelling in biomedicine with cardiac applications

# Parameter estimation in cardiac fluid–structure interaction from solid and fluid data

Reidmen Aróstica[1], David Nolte[2], and Cristobal Bertoglio[3]

University of Groningen, Bernoulli Institute – Computational and Numerical Mathematics
r.a.arostica.barrera@rug.nl
University of Groningen, Bernoulli Institute – Computational and Numerical Mathematics
d.j.nolte@rug.nl
University of Groningen, Bernoulli Institute – Computational and Numerical Mathematics
c.a.bertoglio@rug.nl

**Summary.** Parameter estimation in the heart has been carried out so far using measurement in the myocardium, typically using displacement surrogates obtained from magnetic resonance imaging (MRI) [1, 2]. Nevertheless, blood flow velocity measurements are routinely acquired in the clinical practice and can be directly compared with the computed flow velocities of fluid–solid interaction (FSI) models. To the best of the authors' knowledge, inverse problems in cardiac mechanics using "velocity images" of the blood flow have remained unexplored, especially since fully coupled 3D FSI models are challenging mathematically, algorithmically and computationally.

We propose a parameter estimation approach involving sequential data assimliation of a coupled fluid–solid model using both measurements of the solid and the fluid mechanics. The forward solver consists of a one-way coupling of the solid mechanics to the fluid mechanics, using for the fluid an unconditionally stable fractional-step method in ALE form [3], while the nonlinear solid mechanics is defined by a compressible hyperelastic material law. The reduced-order Unscented Kalman Filter [4] is used for the efficient solution of the inverse problem.

First results are presented of estimated constitutive and boundary condition parameters of the solid for an idealized, synthetic myocardium model. Our findings show that combining measurements of the solid displacements and the fluid velocity significantly improves the estimation of parameters of the solid model in comparison to solid- or fluid-only measurements.

**Keywords**: inverse problems, cardiac mechanics, blood flows, fluid-structure interaction

## References

1. Martin R Pfaller, Maria Cruz Varona, Johannes Lang, Cristóbal Bertoglio, and Wolfgang A Wall. Using parametric model order reduction for inverse analysis of large nonlinear cardiac simulations. *International journal for numerical methods in biomedical engineering*, 36(4):e3320, 2020.
2. Stéphanie Marchesseau, Hervé Delingette, Maxime Sermesant, and Nicholas Ayache. Fast parameter calibration of a cardiac electromechanical model from medical images based on the unscented transform. *Biomechanics and modeling in mechanobiology*, 12(4):815–831, 2013.
3. Reidmen Aróstica and Cristóbal Bertoglio. On monolithic and chorin–temam schemes for incompressible flows in moving domains. *Applied Mathematics Letters*, 112:106830, 2021.
4. Philippe Moireau and Dominique Chapelle. Reduced-order Unscented Kalman Filtering with application to parameter identification in large-dimensional systems. *ESAIM: Control, Optimization and Calculus of Variations*, 17(2):380–405, 2011.

# Cardiac Ablation as a multi-phase thermoporoelastic continuum under large deformation

Nicolás A. Barnafi[1], Argyrios Petras[2], and Luca Gerardo-Giorda[3]

Centro de Modelamiento Matemático
nbarnafi@cmm.uchile.cl
Johann Radon Institute for Computational and Applied Mathematics (RICAM)
argyrios.petras@ricam.oeaw.ac.at
Johann Radon Institute for Computational and Applied Mathematics (RICAM)
luca.gerardo-giorda@jku.at

**Summary.** Cardiac ablation is a way of treating pathological electric patterns in the heart by burning strategically chosen points with a catheter. The entire process is extremely complex, as it involves: the generation of heat through an electromagnetic field at the catheter's tip, the increase of heat of the heart because of the catheter, the dissipation of heat in the tissue because of both diffusion and blood circulation, the deformation of the tissue induced by the burn injury, the increase of blood pressure because of the swelling and temperature, the formation of oedema through leakage from the lymphatic system, and the cooling of the catheter because of the blood within the heart chamber. This is of course a list of only the main mechanistic elements of the treatment, but many other factors are involved.

This talk will address the mathematical modeling of this phenomenon through the theory of porous media. Our approach will be mainly that of mathematical generality and physical accuracy, by building upon a thermodynamically consistent model developed in [1] through large deformations thermoelasticity. Our extension leverages multi-compartment models for cardiac perfusion [2] with the theory of thermoporoelasticity [3], and uses an ad-hoc approach for modeling the Gibbs potential, which has not yet been characterized in soft tissues. One fundamental technical difficulty in this context is that of computing a reference configura- tion that is in mechanical equilibrium. To circumvent this, we propose an extension of the inverse elasticity model [4] into a quasi-static poroelastic model that extends other simplified approaches [5] to yield a general framework for computational models of porous soft tissue. All claims will be validated through numerical tests.

**Keywords**: Poroelastic media, Thermodynamics, Inverse elasticity, Computational mechanics

**Mathematics Subject Classifications (2010)**: 65F10, 74S05, 76S05

## References

1. L Molinari, L Gerardo-Giorda, A Gizzi. A transversely isotropic thermo-hyperelastic constitutive model of myocardial tissue with a three-state cell death dynamics for cardiac radiofrequency ablation. Journal of the Mechanics and Physics of Solids, 2022.
2. NA Barnafi Wittwer, S Di Gregorio, L Dede', P Zunino, C Vergara, AM Quarteroni. A Multiscale Poromechanics Model Integrating Myocardial Perfusion and the Epicardial Coronary Vessels. SIAM Journal on Applied Mathematics, 82(4), 2022.
3. O Coussy. Poromechanics. John Wiley & Sons, 2004
4. S Govindjee, PA Mihalic. Computational methods for inverse finite elastostatics. Computer Methods in Applied Mechanics and Engineering, 1996.
5. C Patte, M Genet, D Chapelle. A quasi-static poromechanical model of the lungs. Biomechanics and Modeling in Mechanobiology, 2022.

# CFD Simulations in Cardiovascular Systems

Elias Karabelas[1], Gundolf Haase[2], and Federica Caforio[3]

University of Graz
Elias.Karabelas@uni-graz.at
University of Graz, Heinrichstrasse 36, 8010 - Graz Austria
Gundolf.Haase@uni-graz.at
University of Graz
Federica.Caforio@uni-graz.at

**Summary.** Simulating the total heart function includes CFD blood flow models which serve as the hydrodynamic load imposed on cardiac mechanics. Heart valves play a pivotal role in filling and ejection of cardiac chambers such as the left ventricle (LV). Thus, their functional representation in CFD simulations of hemodynamics in the LV and the attached aorta is vital. Usually this task is achieved using fluid-structure-interaction (FSI) where valves are modeled as thin structures.

We investigate the suitability of an alternative approach: A fictitious domain method is realized by extending the Navier-Stokes equation with a linear permeability term, which results in the Navier-Stokes-Brinkman equation. In this setting the permeability parameter is used to model a valve as a fictitious solid domain. The (fast) opening and closing of the valve is realized by changing the permeability within the finite elements which are covered by the moving valve in its current configuration. The underlying mesh representing the blood pool remains unchanged but the equations contain a volume fraction parameter denoting the degree of partial coverage of finite elements in the blood pool by the valve. To deal with turbulence occurring at higher Reynolds numbers the residual based variational multiscale (RBVMS) turbulence model [1] was employed. The RBVMS formulation has the additional property of stabilizing our method, which allowed the use of lowest equal order finite elements reducing also the implementation work in the cardiac modeling framework *CARPentry*. In this talk we will present ongoing validation work [5, 4] and applications stemming from clinical datasets [3, 2]. **Keywords**: fluid dynamics, fictitious domain, scientific computing

**Mathematics Subject Classifications (2010)**: 92C10, 65N12, 76Z99

## References

1. Y. Bazilevs,V. Calo, J. Cottrell, T. Hughes, A. Reali and G. Scovazzi: Variational multiscale residual-based turbulence modeling for large eddy simulation of incompressible flows, Comput. Methods Appl. Mech. Eng., 197 (2007), 173-201 (2007).
2. J. Fuchsberger, P. Aigner, G. Haase, S. Niederer, H. Schima, G. Plank, E. Karabelas: "On the Incorporation of Obstacles in a Fluid Flow Problem Using a Navier-Stokes-Brinkman Penalization Approach", Journal of Computational Science, 57 (2022); doi: 10.1016/j.jocs.2021.101506; arXiv:2009.03113.
3. J. Fuchsberger, E. Karabelas, P. Aigner, H. Schirma, G. Haase and G. Plank: "Validation study of computational fluid dynamics models of hemodynamics in the human aorta", in J. Proceedings in Applied Mathematics and Mechanics, 19(1), pp. e201900472 (2019-09-04), doi: 10.1002/pamm.201900472, No 72
4. E. Karabelas, G. Haase, G. Plank and C. Augustin: "Versatile stabilized finite element formulations for nearly and fully incompressible solid mechanics", in J. Computational Mechanics (65), pp. 193-215 (2020), doi: 10.1007/s00466-019-01760-w
5. E. Karabelas, S. Longobardi, J. Fuchsberger, O. Razeghi, C. Rodero, M. Strocchi, R. Rajani, G. Haase, G. Plank, S. Niederer: "Global Sensitivity Analysis of Four Chamber Heart Hemodynamics Using Surrogate Models", IEEE transactions on bio-medical engineering, 69(10) pp. 3216-3223, 2022, doi: 10.1109/TBME.2022.3163428

# Modelling and numerical simulation of Veno-Venous Extra-Corporeal Membrane Oxygenation (VV-ECMO)

Massimiliano Leoni[1], Johannes Szasz[2], Jens Meier[3], and Luca Gerardo-Giorda[4]

Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria
Massimiliano.Leoni@oeaw.ac.at
Department of Anaesthesiology and Intensive Care, Kepler University Klinikum, Linz, Austria

Department of Anaesthesiology and Intensive Care, Kepler University Klinikum, Linz, Austria

Institute for Mathematical Methods in Medicine and Data Based Modeling, Johannes Kepler University, Linz, Austria
luca.gerardo-giorda@jku.at

**Summary.** Extra-Corporeal Membrane Oxygenation (ECMO) is a well-established procedure used in Intensive-Care Units (ICU) to treat patients with either pulmonary or heart failure. The blood of the patient is drawn via a cannula, oxygenated and injected via another cannula. The extraction cannula is normally located in the inferior vena cava. In the case of lung failure, but with a heart in good conditions, the injection cannula is placed in the superior vena cava (veno-venous, VV-ECMO). In the case of heart failure, the injection cannula is placed in the aorta (veno-arterial, VA-ECMO) to ensure that the blood is actually pumped across the arterial system. VV-ECMO is the standard procedure in the case of Severe Acute Respiratory Syndrome and is used, among others, for Covid-19 patients in ICU. A known clinical problem for VV-ECMO is recirculation, where a significant portion of the fully oxygenated blood appears to be recaptured by the extraction cannula in the inferior vena cava, instead of joining the normal circulation pathway. This results in a limited efficacy of the procedure: blood is inserted fully oxygenated but distal measurements show values as low as 80%.

In this talk we will present our work on patient-specific modelling and simulation of VV-ECMO, a surprisingly uncharted territory in the current scientific literature. We will describe the major modelling challenges that ECMO poses, with a particular focus on the proper description of the blood flow. The patient geometry is reconstructed from a CT scan, while blood flow and oxygen diffusion are approximated by the Finite Element Method. We will present numerical results showing how poorly the standard VV-ECMO actually performs and we will discuss possible optimisation procedures or best practices to improve its effectiveness.

**Keywords**:

**Mathematics Subject Classifications (2010)**:

## References

1. M. Leoni, J. Szasz, J. Meier, L. Gerardo-Giorda. *Blood flow but not cannula positioning influences the efficacy of Veno-Venous ECMO therapy*. Scientific Reports., 2022.
2. M. Broman, B. Frenckner, A. Bjällmark, and M. Broomé. Recirculation during veno-venous extra-corporeal membrane oxygenation–a simulation study. *The International journal of artificial organs*, 38(1):23-30, 2015.
3. C. B. Chapman, J.N. Fisher, B. J. Sproule. Behavior of stroke volume at rest and during exercise in human beings. *The Journal of Clinical Investigation*, 39(8):1208–1213, 1960.
4. O. Bond, S. Pozzebon, F. Franchi, F. Zama Cavicchi, J. Creteur, J.L. Vincent, F.S. Taccone, S. Scolletta, S. . Comparison of estimation of cardiac output using an uncalibrated pulse contour method and echocardiography during veno-venous extracorporeal membrane oxygenation. *Perfusion (United Kingdom)*, 35(5): 397–401, 2020.

# Accurate cardiac tissue description in computational modeling of radiofrequency ablation

Argyrios Petras[1], Massimiliano Leoni[2], Zoraida Moreno Weidmann[3], Jose M. Guerra[4], and Luca Gerardo-Giorda[5]

Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria
argyrios.petras@ricam.oeaw.ac.at
Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria
Massimiliano.Leoni@oeaw.ac.at
Department of Cardiology, Hospital de la Santa Creu i Sant Pau Barcelona, Spain
email@third.author.org
Department of Cardiology, Hospital de la Santa Creu i Sant Pau and CIBERCV, and Universidad Autonoma de Barcelona, Barcelona, Spain
email@third.author.org
Institute for Mathematical Methods in Medicine and Data Based Modeling, Johannes Kepler University, Linz, Austria.
eluca.gerardo-giorda@jku.at

**Summary.** Radiofrequency catheter ablation (RFA) is a common, minimally invasive procedure to treat cardiac arrhythmias. A catheter is advanced through the patient's groin onto a cardiac chamber where the arrhythmogenic tissue is destroyed via electrocautery. Although RFA modeling is a reasonably mature field and Penne's Bioheat equation [1] is the standard to describe the power delivery to the tissue, the level of uncertainty in predicting the outcome of a given protocol remains significant. The electrode footprint (namely the contact surface between the catheter tip and the cardiac wall) is a major determinant to the power actually dissipated in the tissue and depends (among others) on the tip shape, the catheter orientation, the applied contact force, and the tissue response to it.

In this talk we will present a model that combines an orthotropic, nearly-incompressible, hyperelastic description for the tissue that accounts for the cardiac fibers, a three-state cell death model that accounts for the potential recovery of the damaged cells, as well as an improved electrical model that accurately captures the electric field of an in-vitro experimental settings.

**Keywords**:

**Mathematics Subject Classifications (2010)**:

## References

1. A. Petras, M. Leoni, J.M. Guerra, J. Jansson, and L. Gerardo-Giorda. A computational model of open-irrigated radiofrequency catheter ablation accounting for mechanical properties of the cardiac tissue. *International Journal for Numerical Methods in Biomedical Engineering*, 35(11), p3232, 2019.
2. A. Petras, M. Leoni, J.M. Guerra, and L. Gerardo-Giorda. Calibration of a three-state cell death model for cardiomyocytes and its application in radiofrequency ablation. *Physiological Measurement*, 44, p.065003, 2023.
3. M. Leoni, A. Petras, Z. Moreno Weidmann, J.M. Guerra, and L. Gerardo-Giorda. Should I tilt or should I push? Effect of contact force and catheter inclination in cardiac radiofrequency ablation. *Computing in Cardiology* (CinC), in press, 2023.

# On the inducibility of ventricular tachycardia by means of different stimulation protocols: an electrophysiology simulation study.

Jesus Jairo Rodríguez Padilla[1], Buntheng Ly[2], Mihaela Pop[3], and Maxime Sermesant[4]

Centre Inria d'Université Côte d'Azur, Epione team, Sophia Antipolis, France
jesus-jairo.rodriguez-padilla@inria.fr
IHU-Liryc, Université de Bordeaux, Pessac, France
buntheng.ly@ihu-liryc.fr
Centre Inria d'Université Côte d'Azur, Epione team, Sophia Antipolis, France,
Sunnybrook Research Institute, Toronto, Canada
mihaela.pop@inria.fr
Centre Inria d'Université Côte d'Azur, Epione team, Sophia Antipolis, France
maxime.sermesant@inria.fr

**Summary.** To date, in the European Union alone, annual incidences of sudden cardiac death (SCD) and out-of-hospital cardiac arrest (OHCA) reach 250,000 and 344,000 cases, respectively [1]. In particular, SCD following myocardial infarction poses a significantly critical public health problem [2]. In this context, there is a need of developing new effective and non-invasive predictive tools for arrhythmia risk stratification. Thus, a comprehensive understanding of the impact that each arrhythmic substrate component has on the electrophysiological function is necessary for accurate outcome predictions.

Besides the clinical and experimental studies, computer modeling is a powerful, reliable and effective tool that can be used to predict the arrhythmia risk of post-infarction patients as well as the ablation targets, as proposed in recent modelling works [3, 4].

In this work we propose to leverage on computer simulations to study the inducibility of ventricular tachycardia (VT) by replicating the stimulation protocols typically employed in the clinics, but testing different locations of the stimulus site. This will allow us to gain insight into the effect of stimulus location on the electrophysiologic response in the presence of scar tissue.

To this effect, we use an improved equivalent formulation of the Mitchell-Schaeffer model as in Djabella et. al. [5]. This modified Mitchell-Schaeffer (mMS) model alleviates the so-called "pacemaker cell behaviour" problem present in the usual Mitchell-Shaeffer model.

To numerically solve the mMS model, we used FEniCSx (`https://fenicsproject.org/`), an open-source computing platform that implements the finite element method to solve partial differential equations in an automated manner.

Here we present the full pipeline used of the current study: (i) Mesh generation and labelling of zones of interest (healthy tissue, GZ and dense scar); (ii) Numerical methods (Crank-Nicolson and a modified Adam-Bashford schemes for time and space, respectively) and variational formulation of the modified Mitchell-Schaeffer model; (iii) exemplary results for VT inducibility for different stimulation locations.

**Keywords**: Finite element, reaction-diffusion systems, numerical methods, electrophysiology

**Mathematics Subject Classifications (2010)**: 65M60, 35K57, 92E99

## References

1. Empana, J. P., Lerner, I., Valentin, E., Folke, F., Boettiger, B., Gislason, G., ... & ESCAPE-NET Investigators. (2022). Incidence of sudden cardiac death in the European Union. Journal of the American College of Cardiology, 79(18), 1818-1827.
2. Fishman, G. I., Chugh, S. S., DiMarco, J. P., Albert, C. M., Anderson, M. E., Bonow, R. O., ... & Zheng, Z. J. (2010). Sudden cardiac death prediction and prevention: report from a National Heart, Lung, and Blood Institute and Heart Rhythm Society Workshop. Circulation, 122(22), 2335-2348.

3. Arevalo, H. J., Vadakkumpadan, F., Guallar, E., Jebb, A., Malamas, P., Wu, K. C., & Trayanova, N. A. (2016). Arrhythmia risk stratification of patients after myocardial infarction using personalized heart models. Nature communications, 7(1), 11437.
4. Campos, F. O., Orini, M., Arnold, R., Whitaker, J., O'Neill, M., Razavi, R., ... & Bishop, M. J. (2021). Assessing the ability of substrate mapping techniques to guide ventricular tachycardia ablation using computational modelling. Computers in Biology and Medicine, 130, 104214.
5. Djabella, K., Landau, M., Sorine, M. (2007, December). A two-variable model of cardiac action potential with controlled pacemaker activity and ionic current interpretation. In 2007 46th IEEE Conference on Decision and Control (pp.5186-5191). IEEE.

# Comprehensive Evaluation of a Pseudo-Spectral Method for Wall Shear Stress Estimation in Cardiovascular Flows Under Varying Conditions

Jimena Martín Tempestti[1], Saeyoung Kim[2], Brooks Lindsey[3], and Alessandro Veneziani[4]

Department of Mathematics, Emory University
jimena.martin@emory.edu
George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology
sykim@gatech.edu
George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology
brooks.lindsey@bme.gatech.edu
Department of Mathematics, Emory University
avenez2@emory.edu

**Summary.** Wall Shear Stress (WSS) is a critical quantity that influences the development and progression of cardiovascular diseases, particularly atherosclerosis. Understanding the relationship between WSS and disease progression is essential for improving risk assessment, diagnosis, and treatment strategies for these diseases. This calls for an accurate WSS quantification based on available data [1, 2] This paper focuses on the validation of a previously introduced Pseudo-Spectral Method for WSS quantification from 2D ultrasound vector Doppler measurements, aiming to assess its performance under various conditions following a comprehensive validation approach. The validation process begins with an initial assessment using laboratory data in a stenotic case [3], demonstrating its accuracy under controlled conditions. Subsequently, the method's performance is rigorously tested through Computational Fluid Dynamics (CFD) simulations. Three crucial aspects are systematically studied in these simulations: diameter stenosis, stenosis length, and curvature. Recognizing the challenges posed by real-world data, the study also assesses the method's robustness by introducing varying levels of noise into the data, simulating real data scenarios. The findings of this study provide valuable insights into the performance of the Pseudo-Spectral Method for WSS estimation in cardiovascular flows. The pseudo-spectral method seems versatile in accommodating different configurations and robustness in handling noisy data. This highlights its potential as a valuable tool for clinicians and, possibly, device manufacturers.

**Keywords**: Wall Shear Stress, Doppler imaging, Interpolation, Pseudo-spectral differentiation, Numerical differentiation, Computational Fluid Dynamics

**Mathematics Subject Classifications (2010)**: 76D05, 65Z05, 76M22

## Acknowledgments

The support of National Institutes of Health (NIH) R01EB031101 is gratefully acknowledged.

## References

1. Galarce, F., Lombardi, D. & Mula, O. Reconstructing haemodynamics quantities of interest from Doppler ultrasound imaging. *International Journal For Numerical Methods In Biomedical Engineering*. **37**, e3416 (2021)
2. Martin Tempestti, J., Kim, S., Lindsey, B. & Veneziani, A. A Pseudo-Spectral Method for Wall Shear Stress Estimation from Doppler Ultrasound Imaging in Coronary Arteries. (submitted,2023)
3. Kim, S., Martin Tempestti, J., Jing, B., Lane, B., Padala, M., Veneziani, A. & Lindsey, B. Dynamic coronary blood flow velocity and wall shear stress estimation using ultrasound in an ex vivo porcine heart. (submitted,2023)

## MS9: Neural networks for partial differential equations

# Solving the Poisson-Boltzmann Equation for Macromolecules in Polarizable Media using (XPINNs) Extended Physics Informed Neural Networks

Martín A. Achondo[1], Christopher D. Cooper[2], and Jehanzeb H. Chaudhry[3]

Universidad Técnica Federico Santa María
martin.achondo@sansano.usm.cl
Universidad Técnica Federico Santa María
christopher.cooper@usm.cl
University of New Mexico
jehanzeb@unm.edu

**Summary.** The Poisson-Boltzmann Equation (PBE) serves as a fundamental tool for modeling electrostatic interactions in macromolecular systems immersed in polarizable media, underpinning various biophysical and chemical processes. In this investigation, we leverage the power of Extended Physics Informed Neural Networks (XPINNs) to approximate the electrostatic potential in these scenarios.

Our computational framework employs two distinct Neural Networks—Fully Connected Neural Networks (FCNNs) or Residual Networks (ResNet)—dedicated to different domains: the solute and solvent regions. We also ensure continuity between the two networks through interface conditions on the molecular surface.

This study explores multiple dimensions of our computational approach. We investigate hyperparameter combinations to optimize the accuracy and performance of XPINNs. Additionally, we explore convergence by implementing a self-adapting weighting scheme for loss terms, and a preconditioner loss term, within our XPINN architecture.

While our current model demonstrates success with spherical molecules with a single point charge, our goal for this conference is to extend its applicability to realistic molecular geometries. This is challenging because of the complex interface between the solute and solvent, and the presence of multiple point charges. This progress represents a significant step towards aiding numerical simulations of the electrostatics of macromolecules with machine learning.

**Keywords**: XPINNs, Physics Informed Neural Networks, Poisson-Boltzmann Equation.

## References

1. Roux, B., & Simonson, T. (1999). Implicit solvent models. *Biophysical chemistry*, 78(1-2), 1-20.
2. Jagtap, A. D.; Karniadakis, G. E. Extended Physics-informed Neural Networks (XPINNs): A Generalized Space-Time Domain Decomposition based Deep Learning Framework for Nonlinear Partial Differential Equations. *AAAI Spring Symposium: MLPS*. 2021.
3. Wang, S., Sankaran, S., Wang, H., & Perdikaris, P. (2023). An Expert's Guide to Training Physics-informed Neural Networks. arXiv preprint arXiv:2308.08468.

# A general framework for active learning in regression, with applications to numerical PDEs

Ben Adcock[1], Juan M. Cardenas[2], and Nick Dexter[3]

Simon Fraser University
ben_adcock@sfu.ca
University of Colorado, Boulder
juan_manuel_cardenas@sfu.ca
Florida State University
nick.dexter@fsu.edu

**Summary.** Active learning is an important concept in machine learning, in which the learning algorithm is able to choose where to query the underlying ground truth to improve the accuracy of the learned model. As machine learning techniques come to be more commonly used in scientific computing problems, where data is often expensive to obtain, the use of active learning is expected to be particularly important in the design of efficient algorithms. In this work, we introduce a general framework for active learning in regression problems. Our framework extends the standard setup by allowing for general types of data, rather than merely pointwise samples of the target function. This generalization covers many cases of practical interest, such as data acquired in transform domains (e.g., Fourier data), vector-valued data (e.g., gradient-augmented data), data acquired along continuous curves, and, multimodal data (i.e., combinations of different types of measurements). Our framework considers random sampling according to a finite number of sampling measures and arbitrary nonlinear approximation spaces (model classes). We introduce the concept of generalized Christoffel functions and show how these can be used to optimize the sampling measures. We prove that this leads to near-optimal sample complexity in various important cases. This work focuses on applications in scientific computing, where, as noted, active learning is often desirable, since it is usually expensive to generate data. We demonstrate the use of these ideas on several different scientific computing problems, including learning the solution map of high-dimensional parametric PDEs and the numerical solution of PDEs via Physics-Informed Neural Networks (PINNs). For the latter, we show how active learning can be deployed in an adaptive manner to specifically target the sampling scheme to the behaviour of the unknown PDE solution.

**Keywords**: active learning, leverage scores, Christoffel functions, parametric PDEs, Physics-Informed Neural Networks (PINNs)

**Mathematics Subject Classifications (2010)**: 65D40, 65N50, 68T07, 68Q32

## References

1. B. Adcock, J. M. Cardenas and N. Dexter *CS4ML: A general framework for active learning with arbitrary data based on Christoffel functions. arXiv:2306.00945*, 2023.
2. B. Adcock, J. M. Cardenas and N. Dexter CAS4DL: Christoffel adaptive sampling for function approximation via deep learning. *Sampling Theory, Signal Processing, and Data Analysis*, 20:2(21), 2022.
3. B. Adcock and J. M. Cardenas Near-optimal sampling strategies for multivariate function approximation on general domains. *SIAM Journal on Mathematics of Data Science*, 2(3):607-630, 2020.

# An adaptive sampling strategy to approximate partial differential equations from noisy data

Ben Adcock[1], Juan M. Cardenas[2], and Alireza Doostan[3]

Department of Mathematics, Simon Fraser University, BC, Canada
ben_adcock@sfu.ca
Department of Aerospace Engineering Sciences, University of Colorado, Boulder, CO, USA
juca7891@colorado.edu
epartment of Aerospace Engineering Sciences, University of Colorado, Boulder, CO, USA
alireza.doostan@colorado.edu

**Summary.** Many problems in computational science, engineering, and uncertainty quantification (UQ) require the approximation of Partial Differential Equations (PDEs) from corrupted data, which is similar to approximating a high-dimensional function from noisy samples. In many applications, the data is costly to generate: for example, each sample may require a finite element method to solve PDEs. Therefore, it is imperative to develop highly sample-efficient models. Many methods are based on the fidelity data, high-fidelity models output data with high accuracy but it is expensive to compute. On the other hand, low-fidelity models output less accurate data but it is cheap to generate. Multi-fidelity models, which combine a high-fidelity model with several low-fidelity models, have shown accurate predictions using machine learning techniques. However, these proposed methods work with Monte Carlo sampling (MCS) or variations of MCS. Recently, Christoffel Sampling for Machine Learning (CS4ML) has shown accurate results approximating functions on arbitrary types of data, such as approximating the solution of a PDE using Physic-Informed Neural Networks, that consider the PDE, boundary, and initial condition in the loss function of the neural network. In this work, we propose an adaptive sampling strategy for Multi-fidelity UQ models. In particular, it integrates the multi-fidelity models and the sampling framework CS4ML to increase the sample efficiency of the model approximating the PDEs. Our novel approach is based on the Christoffel function on each latent space of the low-fidelity models to construct low-cost sample measures that will improve the approximation of the multi-fidelity model. We test our method on several problems related to PDEs such as 'Thermally-driven cavity fluid flow', which models the temperature-driven fluid flow in a cavity, and 'Composite Beam', which models the deformation of plane stress, and 'Burgers equation'. Our results demonstrate that our method often yields substantial savings in the number of samples required to achieve a given accuracy. These results therefore are a promising step towards fully adapting Multi-fidelity methods towards scientific computing applications.

**Keywords**: high-dimensional approximation, sampling strategies, Christoffel function, physic-informed neural networks, Burgers equation, finite element methods, uncertainty quantification.

**Mathematics Subject Classifications (2010)**: 65C20, 68U20, 65M70.

## References

1. Ben Adcock, Juan M. Cardenas, and Nick Dexter. CS4ML: A general framework for active learning with arbitrary data based on Christoffel functions. Arxiv *arXiv:2306.00945v1*, 1-46, 2023.
2. Ben Adcock, Juan M. Cardenas, and Nick Dexter. *CAS4DL: Christoffel adaptive sampling for function approximation via deep learning*, *Sampling Theory, Signal Processing, and Data Analysis*, 20(21), 2022.
3. Hillary R. Fairbanks, Lluís Jofre, Gianluca Geraci, Gianluca Iaccarino, and Alireza Doostan. Bi-fidelity approximation for uncertainty quantification and sensitivity analysis of irradiated particle-laden turbulence. *Journal of Computational Physics*, 402:108996, 2020.

# Multi-level Neural Networks for Accurate Solutions of Boundary-Value Problems

Ziad Aldirany[1], Régis Cottereau[2], Marc Laforest[3], and Serge Prudhomme[4]

Département de mathématiques et de génie industriel, Polytechnique Montréal, Montréal, Québec, Canada
ziad.aldirany@polymtl.ca
Aix-Marseille Université, CNRS, Centrale Marseille, LMA UMR 7031, Marseille, France
cottereau@lma.cnrs-mrs.fr
Département de mathématiques et de génie industriel, Polytechnique Montréal, Montréal, Québec, Canada
marc.laforest@polymtl.ca
Département de mathématiques et de génie industriel, Polytechnique Montréal, Montréal, Québec, Canada
serge.prudhomme@polymtl.ca

**Summary.** The solution to partial differential equations using deep learning approaches, such as the physics-informed neural networks (PINNs) [1], the deep Ritz method [2], or the weak adversarial networks [3], have shown in recent years promising results for several classes of initial and boundary-value problems. However, their ability to surpass, particularly in terms of accuracy, classical discretization methods such as the finite element methods, remains a significant challenge. One of the main obstacles of deep learning approaches lies in their inability to consistently reduce the relative error in the computed solution. To better control the error, we present a new methodology for deep learning methods. The main idea consists in computing an initial approximation to the problem using a simple neural network and in estimating, in an iterative manner, a correction by solving the problem for the residual error with a new network of increasing complexity. A similar approach has been suggested in [4] to control the error in the case of symmetric problems. This sequential reduction of the residual associated with the partial differential equation allows one to decrease the solution error, which, in some cases, can be reduced to machine precision. The underlying explanation is that the method is able to capture at each level smaller scales of the solution using a new network. Numerical examples in 1D and 2D are presented to demonstrate the effectiveness of the proposed approach using PINNs. It is noted that the approach can also be extended to other neural network solvers based on weak or strong formulations of the residual.

**Keywords**: Neural networks, Partial differential equations, Physics-informed neural networks, Numerical error, Convergence, Frequency analysis

**Mathematics Subject Classifications (2010)**: 65N12, 68T05

## References

1. M. Raissi, P. Perdikaris, and G.E. Karniadakis. 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, 2019.
2. W. E and B. Yu. The deep Ritz method: a deep learning-based numerical algorithm for solving variational problems. *Communications in Mathematics and Statistics*, 6(1): 1-12, 2018.
3. Y. Zang, G. Bao, X. Ye, and H. Zhou. Weak adversarial networks for high-dimensional partial differential equations. *Journal of Computational Physics*, 411: 109409, 2020.
4. M. Ainsworth and J. Dong. Galerkin neural networks: A framework for approximating variational equations with error control. SIAM *Journal on Scientific Computing*, 43(4): A2474-A2501, 2021.

# Deep Learning Methods for a Fluid Inverse Problem

Cristóbal Álvarez[1]

Departamento de Matemáticas, Universidad Técnica Federico Santa María, Chile
cristobal.alvarez@sansano.usm.cl

**Summary.** This work addresses the study of the inverse problem of obstacle recovery in the context of the Stokes system through a Deep Learning-based approach. A method was developed, which consists of a process in which binary images of obstacles are generated, and the corresponding solutions to the direct problem are computed. From these simulations, a dataset is constructed, enabling the inverse problem measurements for various obstacles in a region of interest on the outer boundary. Subsequently, various convolutional neural networks are employed in combination with hyperparameter estimation techniques based on Bayesian methods to obtain an accurate approximation of the inverse problem solution. This involves the reconstruction of the obstacle image from the measurements of the Cauchy tensor, achieving error levels that allow the recovery of geometries associated with a particular family of obstacles in the Stokes system.[1]

**Keywords**: Geometrical Inverse Problems, Deep Learning, Stokes System, Numerical Reconstruction

**Mathematics Subject Classifications (2010)**:

## References

1. C. Alvarez, C. Conca, R. Lecaros, and J. Ortega. *On the identification of a rigid body immersed in a fluid: A numerical approach. Engineering Analysis with Boundary Elements*, 2008
2. F. Calabró, S.Cuomo, F. Giampaolo, S. Izzo, C. Nitsch, F. Piccialli, and C. Trombetti. *Deep Learning for the aproximation of a shape functional.* arXiv, 2021

[1]Funded by ANID through the Centro Nacional de Inteligencia Artificial CENIA

# Adaptive Deep Fourier Residual method for solving PDEs on polygonal domains

Manuela Bastidas[1], Jamie M. Taylor[2], and David Pardo[3]

University of the Basque Country (UPH/EHU), Leioa, Spain.
manuela.bastidas@ehu.eus
CUNEF Universidad, Madrid, Spain.
jamie.taylor@cunef.edu
University of the Basque Country (UPH/EHU), Leioa, Spain.
Basque Centre for Applied Mathematics (BCAM), Bilbao, Spain.
Ikerbasque (Basque Foundation For Sciences), Bilbao, Spain.
david.pardo@ehu.eus

**Summary.** The Deep Fourier Residual (DFR) method is a specific case of Variational Physics- Informed Neural Networks (VPINN) [1] among a large range of strategies for solving PDEs using Neural Networks (NNs). The loss function in the DFR method is an approximation of the dual norm of the PDE's weak-residual, that is, $\mathscr{R} : H \to H^*$, where $H$ is a Hilbert space of test functions and $H^*$ its dual. For many well-posed problems, the dual norm of the weak-residual corresponds directly to the energy norm of the error, i.e., there exist constants $0 < \gamma < M$, such that

$$\frac{1}{M}\|\mathscr{R}(u)\|_{H^*} \leq \|u - u^*\|_H \leq \frac{1}{\gamma}\|\mathscr{R}(u)\|_{H^*},$$

where $u$ is an approximation to the solution $u^*$. Therefore, this loss function ensures that reducing the loss during the training of a NN corresponds to reducing the error in the solution at the same rate.

In [2, 3], the DFR method was proposed for solving problems in $H_0^1(\Omega)$ and $H(\text{curl}, \Omega)$. There, the calculation of the dual norm is based on a spectral representation of the dual norms of the test function space. This spectral representation is well-known on rectangles in 2D or rectangular cuboids in 3D, but constructing an appropriate orthonormal basis in more general domains is non-trivial.

This talk discusses an extension of the DFR method to the use of adaptive strategies on general polygonal domains. We decompose the PDE domain $\Omega$ into rectangular subdomains and the loss function is computed as the sum of local loss functions. We then employ a Döfler marking algorithm to adaptatively refine the initial subdomain decomposition of $\Omega$ and increase the accuracy of the approximated solution on relevant regions of the domain.

Our numerical results show the generation of quasi-optimal refined meshes on several 1D and 2D problems, including the singular L-shape problem.

**Keywords**: Deep Learning, Residual minimisation, Physics-informed machine learning, Adaptive numerical methods

**Mathematics Subject Classifications (2010)**: 68T05, 65N50

## References

1. E. Kharazmi, Z. Zhang, and GE. Karniadakis VPINNs: variational physics-informed neural networks for solving partial differential equations. arXiv preprint : arXiv:1912.0087, 2019.
2. J.M. Taylor, D. Pardo and I. Muga. A Deep Fourier Residual method for solving PDEs using Neural Networks. Computer Methods in Applied Mechanics and Engineering, vol. 405, p. 115850, 2023.
3. J.M. Taylor, M. Bastidas, D. Pardo and I. Muga Deep Fourier Residual method for solving time-harmonic Maxwell's equations. arXiv preprint : arXiv:2305.09578, 2023.

# The Deep Fourier Residual Method for PDEs: $H^1$ and $H(\text{curl})$ Test Spaces

Manuela Bastidas[1], Ignacio Muga[2], David Pardo[3], and Jamie M. Taylor[4]

University of the Basque Country (UPH/EHU), Leioa, Spain.
manuela.bastidas@ehu.eus
Pontificia Universidad Católica de Valparaíso, Chile
ignacio.muga@pucv.cl
University of the Basque Country (UPH/EHU), Leioa, Spain; Basque Centre for Applied Mathematics (BCAM), Bilbao, Spain; Ikerbasque (Basque Foundation For Sciences), Bilbao, Spain.
david.pardo@ehu.eus
CUNEF University, Madrid, Spain
jamie.taylor@cunef.edu

**Summary.** Solving PDEs with machine learning techniques has become a popular alternative to conventional methods. In this context, Neural networks (NNs) are among the most commonly used machine learning tools, and in those models, the choice of an appropriate loss function is critical. In general, the main goal is to guarantee that minimizing the loss during training translates to minimizing the error in the solution at the same rate. In multiple problems, this error norm coincides with the dual-norm of the residual; however, it is often difficult to accurately compute it. This work assumes rectangular domains and proposes the use of a Discrete Sine/Cosine Transform to accurately and efficiently compute those dual-norms. The resulting Deep Fourier-based Residual (DFR) method efficiently and accurately approximate solutions to PDEs. This is particularly useful when solutions lack from regularity and methods involving strong formulations of the PDE fail. We focus on the case of variational formulations having $H^1$ and $H(\text{curl})$ test spaces.

**Keywords**: Deep learning; Neural Networks; Numerical PDEs; Fourier methods.

**Mathematics Subject Classifications (2010)**: 68T07, 65M12, 65M70.

## References

1. J.M. Taylor, D. Pardo, and I. Muga. A Deep Fourier Residual method for solving PDEs using Neural Networks. *Computer Methods in Applied Mechanics and Engineering*, 405, 115850, 2023.
2. J.M. Taylor, M. Bastidas, D. Pardo, and I. Muga. Deep Fourier Residual method for solving time-harmonic Maxwell's equations. *arXiv:2305.09578, 2023*

# Ultra-PINNs: Exploiting ultraweak implementations to boost the performance of Variational PINNs

Manuela Bastidas[1], Carlos Uriarte[2], Jamie M. Taylor[3], Sergio Rojas[4], and David Pardo[5]

University of the Basque Country (UPH/EHU), Leioa, Spain.
manuela.bastidas@ehu.eus
Basque Centre for Applied Mathematics (BCAM), Bilbao, Spain.
University of the Basque Country (UPH/EHU), Leioa, Spain.
curiarte@bcamath.org
CUNEF Universidad, Madrid, Spain.
jamie.taylor@cunef.edu
Pontificia Universidad Católica de Valparaíso, Chile.
sergio.rojas.h@pucv.cl
University of the Basque Country (UPH/EHU), Leioa, Spain; Basque Centre for Applied Mathematics (BCAM), Bilbao, Spain; Ikerbasque (Basque Foundation For Sciences), Bilbao, Spain.
david.pardo@ehu.eus

**Summary.** We propose UltraPINNs, a method for solving PDEs using NNs that offers two approaches: one based on the ultraweak variational formulation of a PDE, and the other considering its strong or weak formulation. In the latter, we compute the loss function by transferring derivatives from the trial to the test space through repeated integration by parts and assuming suitable regularity in the user-selected test functions. Our characterization of this strategy as an "ultraweak implementation" rather than an "ultraweak formulation" reflects that we retain the consistency between the loss and the error in relevant norms, while eliminating the need for numerical differentiation of the trial function.

Our method showcases two main advantages: (i) Due to the increased regularity of the integrand, using classical quadrature rules yields higher precision without increasing the number of integration points. (ii) Despite the often suboptimal convergence rates of gradient-based optimization algorithms like Adam, it is possible to expedite the convergence by interpreting the neurons in the last hidden layer of the NN as basis functions within the trial space and employing a least-squares (LS) solver to calculate the last-layer weights [1]. However, if the construction of the LS matrix requires the calculation of the spatial derivatives of the trial function, then its computational cost becomes dominant and increases linearly with its size. In UltraPINNs, the cost of constructing the LS matrix is significantly lower than in weak-type implementations, resulting in enhanced performance speeds.

We demonstrate the performance of UltraPINNs equipped with a hybrid Adam/LS solver using numerical examples in 1D, 2D, and 3D. We observe meaningful improvements in both convergence rate and computational cost, surpassing the performance of Adam or Adam/LS with weak-type implementations, and improving the integration error.

**Keywords**: Deep Learning, Physics-informed machine learning, Enhanced optimization algorithms

**Mathematics Subject Classifications (2010)**: 68T05, 65N50

## References

1. E.C. Cyr, et al. *Robust training and initialization of deep neural networks: An adaptive basis viewpoint.* Mathematical and Scientific Machine Learning, pp. 512-536. PMLR, 2020.

# Variational Physics Informed Neural Networks: the Role of Quadratures and Test Functions and Boundary conditions

Stefano Berrone[1], Claudio Canuto[2], Moreno Pintore[3], and N. Sukumar[4]

Politecnico di Torino
stefano.berrone@polito.it
Politecnico di Torino
claudio.canuto@polito.it
Politecnico di Torino
moreno.pintore@polito.it
University of California
nsukumar@ucdavis.edu

**Summary.** In this presentation, we investigate the impact of different quadrature rules' precision and varying degrees of piecewise polynomial test functions on the convergence rate of Variational Physics Informed Neural Networks (VPINNs) when addressing elliptic boundary-value problems through mesh refinement. Employing a Petrov-Galerkin framework, we derive an a priori error estimate in the energy norm. The proposed interpolation operator is crucial to obtain an inf-sup stable method and to remove all spurious modes from the output of the neural network. Our findings may seem counterintuitive, suggesting that, for smooth solutions, the optimal approach for achieving a rapid error decay rate is to opt for test functions with the lowest polynomial degree while employing precision-oriented quadrature formulas.

We proceed introducing an "a posteriori" error estimator, comprising a residual component, a loss function term, and data oscillation terms. Our analysis demonstrates the reliability and efficiency of this estimator in controlling the energy norm error between the exact solution and the VPINN-derived solution.

Furthermore, a comprehensive exploration of four distinct approaches for enforcing Dirichlet boundary conditions in PINNs and VPINNs is performed. Traditionally, these conditions are enforced by introducing penalization terms in the loss function and carefully selecting corresponding scaling coefficients, a process that often demands resource-intensive tuning. Through a series of numerical tests, we establish that modifying the neural network's output to precisely align with the specified values yields more efficient and accurate solvers. Our most promising results emerge from the exact enforcement of Dirichlet boundary conditions, achieved by employing an approximate distance function. We also demonstrate that variational imposition of these conditions using Nitsche's method yields suboptimal solvers.

**Keywords**: VPINN, rates of convergence, Dirichlet boundary conditions

**Mathematics Subject Classifications (2010)**: 35B45 , 35J20 , 65K10 , 65N20 , 68T07

## References

1. S. Berrone, C. Canuto, and M. Pintore. Solving PDEs by variational physics-informed neural networks: an a posteriori error analysis. *Annali dell'Università di Ferrara*, 68:575–595, 2022.
2. S. Berrone, C. Canuto, and M. Pintore. Variational physics informed neural networks: the role of quadratures and test functions. *Journal of Scientific Computing*, 92(3):1–27, 2022.
3. S. Berrone, C. Canuto, M. Pintore, and N. Sukumar. Enforcing dirichlet boundary conditions in physics-informed neural networks and variational physics-informed neural networks. *Heliyon*, 9(8):e18820, 2023.

# A deep first-order system least squares methods for solving elliptic PDEs

Francisco Bersetche[1] and Juan Pablo Borthagaray[2]

Universidad Técnica Federico Santamaría
bersetche@gmail.com
Universidad de la República
jpb@cmat.edu.uy

**Summary.** We propose a First-Order System Least Squares (FOSLS) method based on deeplearning for numerically solving second-order elliptic PDEs. The method we propose is capable of dealing with either variational and non-variational problems, and because of its meshless nature, it can also deal with problems posed in high-dimensional domains. We prove the $\Gamma$-convergence of the neural network approximation towards the solution of the continuous problem, and extend the convergence proof to some well-known related methods. Finally, we present several numerical examples illustrating the performance of our discretization.

**Keywords**: Elliptic PDEs, Machine learning, Deep learning, High-dimensional PDEs

# Neural Control of Finite Element Methods: Quasi-optimal convergence of quasi-minimizing neural networks

Ignacio Brevis[1], Ignacio Muga[2], and Kristoffer G. van der Zee[3]

University of Nottingham, School of Mathematical Sciences
ignacio.brevis@nottingham.ac.uk
Pontificia Universidad Católica de Valparaíso, Instituto de Matemáticas
ignacio.muga@pucv.cl
University of Nottingham, School of Mathematical Sciences
kg.vanderzee@nottingham.ac.uk

**Summary.** There is tremendous potential in using neural networks to optimize numerical methods. In this talk, I will introduce and analyse a framework [1, 2, 3, 4] for the neural optimization of discrete weak formulations, suitable for finite element methods. The main idea of the framework is to include a neural-network function acting as a control variable in the weak form. Finding the neural control that (quasi-) minimizes a suitable cost (or loss) functional, then yields a numerical approximation with desirable attributes. In particular, the framework allows in a natural way the incorporation of known data of the exact solution, or the incorporation of stabilization mechanisms (e.g., to remove spurious oscillations).

I will present the analysis of well-posedness and convergence of the associated constrained-optimization problem, i.e., under certain conditions, discrete weak forms are stable, and quasi-minimizing neural controls exist, which converge quasi-optimally. The analysis results are specialized to Galerkin, least- squares and minimal-residual formulations, where the neural-network dependence appears in the form of suitable weights.

I will also consider the case of parametric PDEs, where we are motivated by the desire to find a method that is tailored to quantities of interest of solutions to the parametric PDE. The central component in our approach is an efficient neural-network-weighted Minimal-Residual formulation, which, after training, provides Galerkin-based approximations in standard discrete spaces that have accurate quantities of interest, regardless of the coarseness of the discrete space. Elementary numerical experiments support our findings and demonstrate the potential of the framework.

**Keywords**: Optimal neural control; Artificial neural networks; Data-driven discretization; Weighted finite element methods; Quasi-minimization; Quasi-optimal convergence

**Mathematics Subject Classifications (2010)**: 65N30, 49J20, 65N12

## References

1. Brevis, Muga, Van der Zee. *Neural Control of Discrete Weak Formulations: Galerkin, Least-Squares and Minimal-Residual Methods with Quasi-Optimal Weights*. Computer Methods in Applied Mechanics and Engineering, 402, (2022). arXiv:2206.07475
2. Brevis, Muga, Pardo, Rodríguez, Van der Zee. *Learning quantities of interest from parametric PDEs: An efficient neural-weighted Minimal Residual approach*, (2023). arXiv:2304.01722
3. Brevis, Muga, Van der Zee. *A machine-learning minimal-residual (ML-MRes) framework for goal-oriented finite element discretizations*. Computers and Mathematics with Applications. 95, 186-199, (2021). arXiv:2003.04485
4. Muga, Van der Zee. *Discretization of Linear Problems in Banach Spaces: Residual Minimization, Nonlinear Petrov-Galerkin, and Monotone Mixed Methods*. SIAM Journal in Numerical Analysis. 58(6), 3406-3426, (2020). arXiv:1511.04400

# A unified and constructive framework for the universality of neural networks

Tan Bui-Thanh[1]

The Oden Institute for Computational Engineering and Sciences
The University of Texas at Austin
tanbui@oden.utexas.edu

**Summary.** One of the reasons why many neural networks are capable of replicating complicated tasks or functions is their universal approximation property. Though the past few decades have seen tremendous advances in theories of neural networks, a single constructive and elementary framework for neural network universality remains unavailable. This paper is an effort to provide a unified and constructive framework for the universality of a large class of activation functions including most of the existing ones. At the heart of the framework is the concept of neural network approximate identity (nAI). The main result is: *any nAI activation function is universal in the space of continuous functions on compacta*. It turns out that most of the existing activation functions are nAI, and thus universal. The framework induces **several advantages** over the contemporary counterparts. First, it is constructive with elementary means from functional analysis, probability theory, and numerical analysis. Second, it is one of the first unified and constructive attempts that is valid for most of the existing activation functions. Third, it provides new proofs for most activation functions. Fourth, for a given activation and error tolerance, the framework provides precisely the architecture of the corresponding one-hidden neural network with a predetermined number of neurons and the values of weights/biases. Fifth, the framework allows us to abstractly present the first universal approximation with a favorable non-asymptotic rate. Sixth, our framework also provides insights into the developments, and hence providing constructive derivations, of some of the existing approaches.

**Keywords**: Universal approximation; neural networks; activation functions; non-asymptotic analysis

# Robust Adaptive Mesh Refinement and Energy-driven Deep Distribution Transformers

Difeng Cai[1]

Department of Mathematics, Southern Methodist University, Dallas, TX 75205, USA
ddcai@smu.edu

**Summary.** Generating a mesh (or a distribution of points) with a certain structure plays a vital role in scientific computing. In the context of partial differential equations (PDEs), adaptive mesh generation is necessary to resolve the singularity in the solution in order to achieve desired accuracy with as little computational overhead as possible. Of particular importance is the a posteriori error estimation technique. We will present theoretical and numerical results on *robust* a posteriori error estimation for PDEs with high-contrast coefficients (including diffusion and convection-reaction-diffusion equations) to demonstrate the robustness of the estimators with respect to the PDE coefficient. In the second part of the talk, we present a new deep neural network-based distribution transformer for generating structured distribution of points with applications to fast algorithms in machine learning.

**Keywords**: adaptive mesh refinement, a posteriori error estimation, convection-reaction-diffusion equations, deep neural network, quasi-Monte Carlo, machine learning

**Mathematics Subject Classifications (2010)**: 65N15, 65N30, 65N50, 15A23, 11K38, 68W25, 65D99

## References

1. D. Cai. Physics-informed distribution transformers via molecular dynamics and deep neural networks. *Journal of Computational Physics*. vol.468 (2022) 111511.
2. D. Cai and Z. Cai. Hybrid A Posteriori Error Estimators for Conforming Finite Element Approximations to Stationary Convection-Diffusion-Reaction equations. *arXiv preprint arXiv:2107.06341*.
3. D. Cai and Z. Cai. A hybrid a posteriori error estimator for conforming finite element approximations *Computer Methods in Applied Mechanics and Engineering*, 339 (2018) 320?340.
4. D. Cai, J. Nagy, and Y. Xi Fast deterministic approximation of symmetric indefinite kernel matrices with high dimensional datasets *SIAM Journal on Matrix Analysis and Applications*, (2022) 43:2, 1003-1028

# Physics informed Neural Network for quasistatic fault slip forward and inverse problems

Sebastián Cobaise[1], Axel Osses[2], Francisco Ortega-Culaciati[3], and Paul Escapil-Inchauspé[4]

Universidad de Chile, Santiago, Chile
scobaise@dim.uchile.cl
Center for Mathematical Modeling, Santiago, Chile
axosses@dim.uchile.cl
Departamento de Geofísica, FCFM, Universidad de Chile, Santiago, Chile
ortega.francisco@uchile.cl
Data Observatory Foundation, Santiago, Chile
paul.escapil@dataobservatory.net

**Summary.** We consider the two-dimensional quasistatic linear elasticity equation for domains with slits. We use such construct to represent a slipping fault (slit) embedded in the Earth's crust, and relate displacements measured at the surface of the Earth with fault slip through the elasticity equations. Typically, the forward relationship is obtained by solving the elasticity equations for simplified physical models such as an homogeneous elastic half space [1], an stratified elastic medium [2], or for more complex media using Finite Element or Finite Differences methods. The inverse problem is typically solved by optimization or Bayesian methods [3]. In this work, in order to provide a surrogate for the forward and inverse problems, we apply physics-informed neural networks [4], this approach being a method of choice when dealing with partial information, as it allows for the straightforward incorporation of sensor observations. We solve the problems using the open-source DeepXDE [5] library, for both the forward and inverse settings (specifically, unique continuation problems [6]), demonstrating competitive performance and generalization even in the presence of missing and noisy information. To conclude, we delineate further actions required for the development of real-world data-centric, physics-informed fault simulation solvers.

**Keywords**: Physics informed neural network, linear elasticity, inverse problem.

**Mathematics Subject Classifications (2010)**: 68T04, 35Q04, 86A08.

## References

1. Y. Okada. Internal Deformation Due to Shear and Tensile Faults in a Half-Space, *Bulletin of the Seismological Society of America*, 82:1018-1040, 1992.
2. L. Zhu & L. Rivera. A note on the dynamic and static displacements from a point source in multilayered media. *Geophysical Journal International*, , Volume 148, Issue 3, 619:627, 2002.
3. F. Ortega-Culaciati, M. Simons, J. Ruiz, L. Rivera, N. Diaz-Salazar An EPIC Tikhonov Regularization: Application to Quasi-Static Fault Slip Inversion. *Journal of Geophysical Research: Solid Earth*, , Volume 126, Issue 7, 1:20, 2021.
4. M. Raissi,P. Perdikaris and G. Karniadakis. 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, 2019.
5. L. Lu, X. Meng , Z. Mao, and G. E. Karniadakis. DeepXDE: A Deep Learning Library for Solving Differential Equations, *SIAM Review*, 63(1):208-228, 2021.
6. S. Mishra and R. Molinaro. Estimates on the generalization error of physics-informed neural networks for approximating a class of inverse problems for PDEs. *JIMA Journal of Numerical Analysis*, , Volume 42, Issue 2, 981:1022, 2021.

# An unfitted method ($\phi$-FEM) combined with deep learning: variable geometries and correction

Michel Duprez[1], Emmanuel Franck[2], Fréderique Lecourtier[3], Vanessa Lleras[4], Alexei Lozinski[5], Vincent Vigon[6], and Killian Vuillemot[7]

MIMESIS team, Inria Nancy - Grand Est, MLMS team, Université de Strasbourg, Strasbourg, France.
michel.duprez@inria.fr, frederique.lecourtier@inria.fr
TONUS team, Inria Nancy - Grand Est, Université de Strasbourg, Strasbourg, France.
emmanuel.franck@inria.fr
IMAG, Univ Montpellier, CNRS UMR 5149, Montpellier, France.
frederique.lecourtier@inria.fr
IMAG, Univ Montpellier, CNRS UMR 5149, Montpellier, France.
vanessa.lleras@umontpellier.fr, killian.vuillemot@umontpellier.fr
Université de Franche-Comté, Laboratoire de mathématiques de Besançon, UMR CNRS 6623, Besançon, France.
alexei.lozinski@univ-fcomte.fr
Institut de Recherche Mathématique Avancée, UMR 7501, Université de Strasbourg et CNRS, Tonus team, Strasbourg, France.
vincent.vigon@math.unistra.fr
IMAG, Univ Montpellier, CNRS UMR 5149, 499-554 Rue du Truel, 34090 Montpellier, France. MIMESIS team, Inria Nancy - Grand Est, MLMS team, Université de Strasbourg, 1 place de l'hôpital, 67000 Strasbourg, France.
killian.vuillemot@umontpellier.fr

**Summary.** $\phi$-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]. The method relies on the use of a level-set function $\phi$, defining the domain and its boundary. In this talk, we shall present a way to combine $\phi$-FEM with Fourier Neural Operators (FNO)[3]. FNO uses Fast Fourier Transform, so that the solution should be represented on a Cartesian grid. In this context, $\phi$-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.
In a second part, the predictions of the neural network will be fed back into a finite element solver to apply a correction to improve the accuracy of the solution. We will present some numerical results for different correction methods: correction by adding or by multiplying on an elevated problem.

**Keywords**:Fourier Neural operator, Unfitted finite element method, level set, varying geometry, correction.

**Mathematics Subject Classifications (2010)**: 68T07, 65N85

## References

1. M. Duprez and A. Lozinski. $\phi$-FEM: a finite element method on domains defined by level-sets. SIAM *Journal on Numerical Analysis*, 58(2):1008–1028, 2020.
2. M. Duprez, V. Lleras, and A. Lozinski. A new $\phi$-FEM approach for problems with natural boundary conditions. *Numer. Methods Partial Differential Equations*, 39(1):281–303, 2023.
*ESAIM: M2AN*, 57: 1111–1142, 2023.
3. Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, and A. Anandkumar. Fourier neural operator for parametric partial differential equations, *paper ICLR*, 2021.

# Wavenumber-Robust Deep ReLU Neural Network Emulation in Acoustic Wave Scattering

Fernando Henríquez[1] and Christoph Schwab[2]

Chair of Computational Mathematics and Simulation Science, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland.
fernando.henriquez@epfl.ch
Seminar for Applied Mathematics, ETH Zürich, 8092 Zürich, Switzerland.
schwab@math.ethz.ch

**Summary.** We present wavenumber-robust error bounds using deep neural networks to emulate the solution to the time-harmonic, sound-soft acoustic scattering problem in the exterior of a smooth, convex, two-dimensional obstacle.

The starting point of our analysis is the reduction of the scattering problem in the unbounded exterior region to its (bounded) boundary by means of the wavenumber-robust Combined Field Integral Equation (CFIE), yielding a second-kind boundary integral equation posed on the smooth surface $\Gamma$ of the scatterer. This BIE is well-posed in $L^2(\Gamma)$, with explicit bounds on the continuity and stability constants that depend explicitly on the (non-dimensional) wavenumber $\kappa$.

Utilizing well-known wavenumber-explicit asymptotics of the solution to this problem, as introduced in the work of Melrose and Taylor [1], we explore the numerical approximation of the BIE using fully connected, deep feed-forward neural networks (DNNs) with the Rectified Linear Unit (ReLU) as the chosen activation function [2]. It's worth noting that the results presented here can be straightforwardly extended to different activation functions such as the hyperbolic tangent or the Rectified Power Unit.

Through a constructive argument, we prove the existence of DNNs affording an $\varepsilon$-error in the $L^\infty(\Gamma)$-norm with a fixed and small width and a depth that increases *spectrally* with the accuracy $\varepsilon$ and polynomially with respect to $\log(\kappa)$. By *spectral accuracy*, we mean that there exists $\alpha > 0$ such that for each $n \in \mathbb{N}$, there exists a constant $C_n > 0$, such that for a prescribed accuracy $\varepsilon > 0$, the depth of the DNN is bounded by $C_n \varepsilon^{-\frac{\alpha}{n}}$. The nature of this bound is not an artifact of the proof but a limitation determined by how the regularity of the problem as derived in [1].

The DNNs constructed in our proofs do not require any analytic information about the scatterer's shape or even the wavenumber $\kappa$ and can efficiently approximate the various behaviors that make the numerical solution of this problem a challenge in computational mathematics [3, 4].

**Keywords**: High Wavenumber; Acoustic Scattering; Boundary Integral Equations; Deep Neural Networks.

**Mathematics Subject Classifications (2010)**: 65N15; 65M32; 65N15; 68T07.

## References

1. Richard B. Melrose, and Michael E. Taylor. Near peak scattering and the corrected Kirchhoff approximation for a convex obstacle. *Advances in Mathematics*, 55(3), 242-315, 1985.
2. Dennis Elbrächter et al. Deep neural network approximation theory. *IEEE Transactions on Information Theory*, 67(5), 2581-2623, 2021.
3. Víctor Domínguez, Ivan G. Graham, and Valery P. Smyshlyaev. A hybrid numerical-asymptotic boundary integral method for high-frequency acoustic scattering. *Numerische Mathematik* 106(3), 471-510, 2007
4. Fatih Ecevit, and Hasan Hüseyin Eruslu. A Galerkin BEM for high-frequency scattering problems based on frequency-dependent changes of variables. *IMA Journal of Numerical Analysis* 39(2), 893-923, 2019.

# Adaptive quadratures for nonlinear approximation of low-dimensional PDEs using smooth neural networks

Alexandre Magueresse[1] and Santiago Badia[2]

School of mathematics, Monash university, Clayton, Victoria 3800, Australia.
alexandre.magueresse@monash.edu
Centre Internacional de Mètodes Numèrics a l'Enginyeria, Campus Nord, 08034 Barcelona, Spain.
santiago.badia@monash.edu

**Summary.** Physics-informed neural networks (PINNs) and their variants have recently emerged as alternatives to traditional partial differential equation (PDE) solvers, but little literature has focused on devising accurate numerical integration methods for neural networks (NNs), which is essential for getting accurate solutions. In this work [1], we propose adaptive quadratures for the accurate integration of neural networks and apply them to loss functions appearing in low-dimensional PDE discretisations. We show that at opposite ends of the spectrum, continuous piecewise linear (CPWL) activation functions enable one to bound the integration error, while smooth activations ease the convergence of the optimisation problem. We strike a balance by considering a CPWL approximation of a smooth activation function. The CPWL activation is used to obtain an adaptive decomposition of the domain into regions where the network is almost linear, and we derive an adaptive global quadrature from this mesh. The loss function is then obtained by evaluating the smooth network (together with other quantities, e.g., the forcing term) at the quadrature points. We propose a method to approximate a class of smooth activations by CPWL functions and show that it has a quadratic convergence rate. We then derive an upper bound for the overall integration error of our proposed adaptive quadrature. The benefits of our quadrature are evaluated on a strong and weak formulation of the Poisson equation in dimensions one and two. Our numerical experiments suggest that compared to Monte-Carlo integration, our adaptive quadrature makes the convergence of NNs quicker and more robust to parameter initialisation while needing significantly fewer integration points and keeping similar training times.

**Keywords**: Adaptive Quadrature, Numerical Integration, PDE, Neural Networks, PINN.

**Mathematics Subject Classifications (2010)**: 65N30, 65N50.

## References

1. Alexandre Magueresse, and Santiago Badia. Adaptive quadratures for nonlinear approximation of low-dimensional PDEs using smooth neural networks. arXiv preprint arXiv:2303.11617 (under review), 2023.

# Modeling Global Surface Dust Deposition Using Physics-Informed Neural Networks

Constanza A. Molina Catricheo[1], Fabrice Lambert[2], Julien Salomon[3], and Elwin van 't Wout[4]

School of Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile

Geography Institute, Pontificia Universidad Católica de Chile, Santiago, Chile

INRIA Paris, ANGE Project-Team, Paris, France and CNRS, Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris, France

Institute for Mathematical and Computational Engineering, Pontificia Universidad Católica de Chile, Santiago, Chile
e.wout@uc.cl

**Summary.** Physics-Informed Neural Networks (PINNs) follow an innovative approach to data analysis and physical modeling through machine learning, as they incorporate physical principles into the data-driven learning process. They can numerically solve partial differential equations while fitting the approximated function to a dataset. While these algorithms have attracted a lot of attention recently, their predictive skill on empirical data is still uncertain. Here, we develop PINNs to reconstruct global maps of atmospheric dust surface deposition fluxes from measurement data in paleoclimatic archives.

Paleoclimatic measurements serve to understand geophysical processes and evaluate climate model performances. However, their spatial coverage is generally sparse and unevenly distributed across the globe. Statistical interpolation methods are the prevalent techniques to grid such data, but these purely data-driven approaches sometimes produce results that are incoherent with our knowledge of the physical world.

In this study, we design an advection-diffusion equation to consider dominant wind directions at various latitudes, which prevents dust particles from flowing upwind. PINN calculations are performed on empirical data for the Holocene and Last Glacial Maximum periods. The results show that our PINN improves on standard kriging interpolation by allowing variable asymmetry around data points. The reconstructions display realistic dust plumes from continental sources towards ocean basins following prevailing winds.

**Keywords**: Neural Networks, Fluid Dynamics, Geophysics

**Mathematics Subject Classifications (2010)**: 62M45, 86A32

# Near-optimal learning of Banach-valued, high-dimensional functions via deep neural networks for parametric PDEs

Sebastián Moraga[1], Ben Adcock[2], simone Brugiapaglia[3], and Nick Dexter[4]

Simon Fraser University
smoragas@sfu.ca
Simon Fraser University
ben_adcock@sfu.ca
Concordia University
simone.brugiapaglia@concordia.ca
Florida State University
nick.dexter@fsu.edu

**Summary.** This work establishes practical existence theorems for approximating high-dimensional parametric functions from limited samples using deep neural networks motivated by, but not limited to, parametrized partial differential equations. Over the last decade, deep learning has become one of the most studied techniques in scientific computing. However, the mathematical principles of deep learning in terms of stability, accuracy and sample complexity for such functions are still in development. On the one hand, the ever-expanding literature on approximation theory using deep neural networks suggests that they can approximate functions from relevant function classes. On the other hand, deep learning is becoming an ever more practical tool for recovering parametric maps of physical systems modelled as differential equations. Moreover, while standard PDEs are naturally posed in a weak form in Hilbert spaces, there has been an increasing interest in solving problems whose solution belongs to more general Banach space. Despite the substantial recent work, the theory typically does not address what sample complexity suffices to construct such networks. Here, we observe a gap between theory and practice. This work is motivated by the desire to close this gap. We provide theoretical arguments combining tools from deep learning, best $s$-term polynomial approximation theory, compressed sensing and convex optimization to compute near-optimal approximations to Banach-valued functions. These approximations are also robust to all key sources of error in the problem, including sampling, optimization, approximation and physical discretization errors. Furthermore, our method is non-intrusive and establishes efficient approximation to infinite-dimensional Banach-valued functions from limited data. We also provide preliminary numerical results illustrating the practical performance for problems arising as solutions to parametric PDEs.

**Keywords**: deep neural networks, high-dimensional approximation, parametric PDEs, uncertainty quantification, Banach spaces

**Mathematics Subject Classifications (2020)**: 65D40; 68T07; 68Q32

## References

1. B. Adcock, S. Brugiapaglia, N. Dexter, and **S. Moraga**. *Deep neural networks are effective at learning high-dimensional Hilbert-valued functions from limited data.* MSML *Proceedings of Machine Learning Research*, 145:1–36, 2021.
2. B. Adcock, S. Brugiapaglia, N. Dexter, and **S. Moraga**. *Near-optimal learning of Banach-valued, high-dimensional functions via deep neural networks arXiv:2211.12633*, 2022.
3. E. Colmenares, G. N. Gatica, and **S. Moraga**. *A Banach spaces-based analysis of a new fully-mixed finite element method for the Boussinesq problem*, ESAIM *Math. Model. Numer. Anal.* 54(5):1525– 1568, 2020.

# Robust Variational Physics-Informed Neural Networks

Sergio Rojas[1], Pawel Maczuga[2], Judit Muñoz-Matute[3], David Pardo[4], and Maciej Paszyński[5]

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile.
sergio.rojas.h@pucv.cl
Faculty of Computer Science, AGH University of Krakow, Poland.
pmaczuga97@gmail.com
Basque Center for Applied Mathematics (BCAM), Spain. Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, USA.
judith.munozmatute@gmail.com
University of the Basque Country (UPV/EHU), Spain. Basque Center for Applied Mathematics (BCAM), Spain. Ikerbasque, Spain.
dzubiaur@gmail.com
Faculty of Computer Science, AGH University of Krakow, Poland.
paszynsk@agh.edu.pl

**Summary.** This talk introduces a Robust version of the Variational Physics-Informed Neural Networks method (RVPINNs). As in VPINNs, we define the quadratic loss functional in terms of a Petrov-Galerkin-type variational formulation of the PDE problem: the trial space is a (Deep) Neural Network (DNN) manifold, while the test space is a finite-dimensional vector space. Whereas the VPINN's loss depends upon the selected basis functions of a given test space (see, e.g. [1, 2]), herein, we minimize a loss based on the discrete dual norm of the residual. The main advantage of such a loss definition is that it provides a reliable and efficient estimator of the true error in the energy norm under the assumption of the existence of a local Fortin operator. We test the performance and robustness of our algorithm in several advection-diffusion problems. These numerical results perfectly align with our theoretical findings, showing that our estimates are sharp.

**Keywords**: Variational Physics-Informed Neural Networks, Minimum Residual method, a posteriori error estimation, Riesz representation theorem.

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N22, 65N30, 65N50.

## References

1. E. Kharazmi, Z. Zhang, and G. E. Karniadakis. Variational physics-informed neural networks for solving partial differential equations *arXiv preprint*, arXiv:1912.00873, 2019.
2. E. Kharazmi, Z. Zhang, and G. E. Karniadakis. hp-VPINNs: Variational physics-informed neural networks with domain decomposition *Computer Methods in Applied Mechanics and Engineering*, 374, p. 113547, 2021.
3. S. Rojas, P. Maczuga, J. Muñoz-Matute, D. Pardo, and M. Paszyński. Robust Variational Physics-Informed Neural Networks *arXiv preprint*, arXiv:2308.16910, 2023.

# MS10: Nonlinear hyperbolic PDE: numerical techniques and related models

# Mathematical and numerical analysis of conservation laws with continuous and discontinuous nonlocal fluxes

Raimund Bürger[1], Felisia Angela Chiarello[2], Harold Deivi Contreras Contreras[3], and Luis Miguel Villada[4]

Department of Mathematical Engineering, University of Concepción, Chile. CI2MA, University of Concepción, Chile.
rburger@udec.cl
Department of Engineering, Information Sciences and Mathematics, Uniersity of L'aquila, Italy.
felisiaangela.chiarello@univaq.it
Department of Metallurgical Engineering, University of Concepción, Concepción, Chile.
hdcontrerasc24@gmail.com
GIMNAP-Department of Mathematics, Uniersity of Bío Bío, Chile. CI2MA, University of Concepción, Chile.
lvillada@ubiobio.cl

**Summary.** In this talk, we introduce two scalar conservation laws with continuous and discontinuous nonlocal fluxes, which are motivated by applications in sedimentation and vehicular traffic. We approximate the problems through an Hilliges-Weidlich (HW)-type numerical scheme and provide compactness estimates for the sequence of approximate solutions. Then, we prove the existence and the uniqueness of entropy weak solutions. Some numerical simulations illustrate the behaviour of solutions in sample cases and corroborate the theoretical results.

**Keywords**: Conservation law, nonlocal flux, continuous flux, discontinuous flux, Hilliges-Weidlich type scheme, entropy weak solution.

**Mathematics Subject Classifications (2010)**: 35L65, 65M12, 90B20.

## References

1. F. Betancourt, R. Bürger, K. H. Karlsen and E. M.Tory. On nonlocal conservation laws modelling sedimentation. *Nonlinearity*, 24 (2011), 855-885.
2. R. Bürger, H. Contreras, L.Villada. A Hilliges-Weidlich-type scheme for a one-dimensional scalar conservation law with nonlocal flux. *Networks and Heterogeneous Media*, 18(2) (2023), 664-693.
3. R. Bürger, A. García, K. Karlsen and J. Towers. A family of numerical schemes for kinematic flows with discontinuous flux. *Journal of Engineering Mathematics*, 60 (2008), 387-425.
4. F. Chiarello, H. Contreras and L. Villada. Existence of entropy weak solutions for 1D non-local traffic models with space-discontinuous flux. *Journal of Engineering Mathematics.*, (2023), https://doi.org/10.1007/s10665-023-10284-5
5. P. Goatin and E. Rossi. Well-posedness of IBVP for 1D scalar non-local conservation laws. *ZAMM Z. Angew. Math. Mech.*, 99 (2019), e201800318, 26.
6. M. Hilliges and W. Weidlich. A phenomenological model for dynamic traffic flow in networks. *Trasportation Research Part B: Methodological*,29 (1995), 407-431.
7. H. Karlsen, N. H. Risebro, and J. D. Towers. L1 stability for entropy solutions of nonlinear degenerate parabolic convection-diffusion equations with discontinuous coefficients. *Skr. K. Nor. Vidensk. Selsk.*, 3 (2003), pp. 1-49.

# A system of of Hamilton-Jacobi equations characterizing geodesic centroidal tessellations

Fabio Camilli[1] and Adriano Festa[2]

Sapienza Università di Roma
fabio.camilli@uniroma1.it
Politecnico di Torino
adriano.festa@polito.it

**Summary.** We introduce a class of systems of Hamilton-Jacobi equations characterizing geodesic centroidal tessellations, i.e. tessellations of domains with respect to geodesic distances where generators and centroids coincide. Typical examples are given by geodesic centroidal Voronoi tessellations and geodesic centroidal power diagrams. An appropriate version of the Fast Marching method on unstructured grids allows computing the solution of the Hamilton-Jacobi system and therefore the associated tessellations. We propose various numerical examples to illustrate the features of the technique.

**Keywords**: geodesic distance; Voronoi tessellation; K-means; power diagram; HamiltonJacobi equation; Mean Field Games; Fast Marching method.

**Mathematics Subject Classifications (2010)**: 65K10, 49M05, 65D99, 35F21, 49N70.

## References

1. L.Aquilanti, S.Cacace, F.Camilli and R.De Maio. A Mean Field Games approach to cluster analysis. *Appl. Math. Optim.*, 84 (2021), 299-323.
2. F.Camilli and A. Festa, A system of Hamilton-Jacobi equations characterizing geodesic centroidal tessellations, to appear on *Communications on Applied Mathematics and Computation*.

# Deep Backward and Galerkin Methods for Learning Finite State Master Equations

Asaf Cohen[1], Mathieu Lauriere[2], and Ethan Zell[3]

University of Michigan, Ann Arbor
asafc@umich.edu
New York University Shanghai
mathieu.lauriere@nyu.edu
University of Michigan, Ann Arbor
ezell@umich.edu

**Summary.** We study two methods designed to efficiently solve high-dimensional PDEs in the setting of mean field master equations. Such master equations are independently interesting because they fully characterize the value of a game with a large number of players and have a myriad of applications in economics, finance, epidemiology, and more. The first method we explore is the deep backward dynamic programming (DBDP) method-we derive BSDEs for the master equation along some exploratory process and use this structure to train neural networks to approximate the master equation solution. Then we revisit the deep Galerkin method (DGM) as applied to the master equation and compare the efficacy of the two methods. This is joint work with Asaf Cohen and Ethan Zell (University of Michigan, Ann Arbor).

**Keywords**: mean field games, master equation, deep learning, backward dynamic programming, deep Galerkin method

**Mathematics Subject Classifications (2010)**: 49N70, 91A13, 91A15, 65N12, 62M45

# Multi-class and multi-population traffic flow models on networks

Paola Goatin[1]

Université Côte d'Azur, Inria, CNRS, LJAD
paola.goatin@inria.fr

**Summary.** We present a general framework for the modeling and simulation of multi-class (i.e. different vehicle types [2]) and multi-population (i.e. different routes [1, 3, 4]) traffic flow on road networks. The models consist of system of conservation laws coupled in the speed component of the flux function, allowing for overtaking and creeping of different vehicle types. Suitable, class specific, coupling conditions at junctions allow to design Godunov type numerical schemes exploiting the supply-demand formulation. The simulation can then be coupled to routing strategies at road junctions to represent the choices of the different populations of drivers. Some numerical tests are presented to illustrate the model behaviours.

**Keywords**: Macroscopic traffic flow models; Hyperbolic systems of conservation laws; Finite volume schemes

**Mathematics Subject Classifications (2010)**: 35L65, 65M08, 90B20,

## References

1. A. Festa, P. Goatin, F. Vicini. Navigation system based routing strategies in traffic flows on networks. *Journal of Optimization Theory and Applications*, 2023, 198 (3), pp.930-957.
2. A. Joumaa, P. Goatin, G. de Nunzio. A Macroscopic Model for Multi-Modal Traffic Flow in Urban Networks. ITSC 2023 - 26th IEEE International Conference on Intelligent Transportation Systems, Sep 2023, Bilbao, Spain.
3. E. Siri, P. Goatin. Assessing the impact of non-compliant users response to System-Optimal Dynamic Traffic Assignment. CDC 2023 - 62nd IEEE Conference on Decision and Control, Dec 2023, Singapore.
4. E. Siri, P. Goatin. System-Optimal Dynamic Traffic Assignment with partial users control: an analysis of different strategies. ITSC 2023 - 26th IEEE International Conference on Intelligent Transportation Systems, Sep 2023, Bilbao, Spain.

# High-Order numerical schemes for nonlocal macroscopic models of multi-population pedestrian flows.

Paola Goatin[1], Luis Miguel Villada[2], and Daniel Inzunza[3]

Université Côte d'Azur, Inria, CNRS, LJAD, France,
2004, route des Lucioles - BP 93, 06902 Sophia Antipolis Cedex, France
paola.goatin@inria.fr
GIMNAP-Departamento de Matemáticas, Universidad del Bío-Bío, Concepción, Chile,
CI$^2$MA-Universidad de Concepción, Casilla 160-C, Concepción, Chile.
lvillada@ubiobio.cl
Université Côte d'Azur, Inria, CNRS, LJAD, France,
2004, route des Lucioles - BP 93, 06902 Sophia Antipolis Cedex, France
daniel-eduardo.inzunza-herrera@inria.fr

**Summary.** In [3] a nonlocal macroscopic pedestrian flow model for two populations with different destinations trying to avoid each other in a confined environment is proposed, where the nonlocal term accounts for anisotropic interactions, mimicking the effect of different cones of view, and the presence of walls or other obstacles in the domain. In particular, obstacles can be incorporated in the density variable, thus avoiding to include them in the vector field of preferred directions. In order to compute the solution, we propose a Finite Difference scheme that couples high-order WENO approximations for spatial discretization, a multi-step TVD method for temporal discretization, and a high-order numerical derivative formula to approximate the derivatives of nonlocal terms, and in this way avoid excessive calculations. Numerical tests confirm that each population manages to evade both the presence of the obstacles and the other population. The evacuation time problem is studied, in particular, the optimal position of the obstacles is obtained using a total travel time optimization processes.

**Keywords**: nonlocal conservation laws; macroscopic pedestrian flow models; anisotropic interactions; WENO numerical schemes; domain shape optimization

**Mathematics Subject Classifications (2010)**: 35L65, 65K10, 93C20

## References

1. R. Bürger, P. Goatin, D. Inzunza and L. M. Villada. A non-local pedestrian flow model accounting for anisotropic interactions and domain boundaries. *Mathematical biosciences and engineering*, 17(5), 5883-5906, 2020.
2. D. Inzunza, P. Goatin and L. M. Villada. Numerical comparison of nonlocal macroscopic models of multi-population pedestrian flows with anisotropic kernel . To appear *Proceedings of Hyperbolic Problems: Theory, Numerics and Applications.* 2023.
3. P. Goatin, D. Inzunza and L. M. Villada. Nonlocal macroscopic models os multi-population pedestrian flows for walking facilities optimization. submitted 2023.
4. R. M. Colombo and M. Lécureux-Mercier. Nonlocal crowd dynamics models for several populations. *Acta Mathematica Scientia*, 32(1), 177-196. 2012.
5. R. M. Colombo, R. M. and E. Rossi. Modelling crowd movements in domains with boundaries. *IMA Journal of Applied Mathematics*, 84(5), 833-853. 2019.

# Functional Analytic Insights into Mean Field Game Theory

Diogo A. Gomes[1]

King Abdullah University of Science and Technology
diogo.gomes@kaust.edu.sa

**Summary.** Monotonicity conditions are crucial in Mean Field Game (MFG) theory, highlighted by the uniqueness results of Larry and Lions. This talk introduces a functional analytic framework to understand MFGs that satisfy monotonicity conditions. By leveraging ideas introduced in Hessian-Riemannian flows from optimization, we propose regularized versions of MFGs and construct contracting flows that can be used for numerical approximation. Our findings present a consolidated view of our prior works, give a different perspective on this class of problems, and provide a systematic way to build approximation methods for MFGs.

**Keywords**: Mean-field games, monotone flows, numerical methods

**Mathematics Subject Classifications (2010)**: 49N70, 91A25, 35Q91, 65M12

# The ENO-ET spatial reconstruction scheme: advances in non-linear high-order numerical schemes

Gino I. Montecinos[1] and Eleuterio F. Toro[2]

Universidad de La Frontera
gino.montecinos@ufrontera.cl
University of Trento
eleuterio.toro@unitn.it

**Summary.** Non-linear spatial reconstruction is a successful procedure in circumventing Godunov's theorem and building high-order non-linear numerical methods for hyperbolic balance laws. The pioneering Essentially-Non-Oscillatory (ENO) method of Harten et al. [1, 2, 3] and the Weighted Essentially-Non-Oscillatory (WENO) method of Jiang and Shu [5] have been fundamental breakthroughs in providing the basis for constructing schemes that are both high-order accurate in smooth regions and essentially non-oscillatory at discontinuities.

Although the literature that shows prominent results is extensive, there is not yet a complete theory of convergence for these reconstruction schemes. Therefore procedures have to be analysed case by case. Problems of interest here, associated to ENO, include the difficulty to attain steady state solutions and the loss of accuracy in cases involving smooth solutions with steep gradients and abrupt stencil changes, [4].

In the present work we present a new method called ENO-ET, which is a variant of ENO. The scheme preserves the main advantages of ENO and successfully overcomes its well-known shortcomings. The method is assessed as a building block for high-order fully-discrete ADER numerical schemes [6, 7]. The accuracy is extended up to the tenth order, not only to demonstrate its high order but also to identify features that become visible beyond the fifth order, the Gibbs phenomenon is one of them, which appears during the propagation of discontinuous profiles.

Results are presented in one and two dimensions and are compared with those from existing methods. Salient features include: i) attainment of theoretically expected convergence rates for smooth solutions arising from demanding initial conditions, ii) computation of essentially non-oscillatory profiles for discontinuous solutions, and (iii) successfully attainment of steady-steady state solutions through time marching.

**Keywords**: ENO reconstruction, WENO reconstruction, finite volume ADER schemes

## References

1. Harten, A. and Engquist, B. and Osher, S. and Chakravarthy, S. R. Some results on high-order accurate essentially non-oscillatory schemes *Applied Numerical Mathematics* , 2:347–377, 1986
2. Harten, A. and Osher, S. Uniformly High Order Accurate Essentially Non-oscillatory Schemes, I *SIAM Journal on Numerical Analysis*, 24(2):279–309, 1987
3. Harten, A. and Engquist, B. and Osher, S. and Chakravarthy, S. R. Uniformly High Order Accurate Essentially Non-oscillatory Schemes, III *Journal of Computational Physics*, 71:231–303, 1987
4. Chi-Wang Shu, Numerical experiments on the accuracy of ENO and modified ENO schemes, *Journal of Scientific Computing*, 5:127-149, 1990.
5. Jiang, G. S. and Shu, C. W. Efficient Implementation of Weighted ENO Schemes. *Journal of Computational Physics*, 126:202–228, 1996.
6. G.I. Montecinos, and E.F. Toro. ENO-ET: a reconstruction scheme based on extended ENO stencil and truncated highest-order term. *Applied Mathematics and Computation*, 442:127742, 2023.
7. G.I. Montecinos, and E.F. Toro. Extension of the ENO-ET Reconstruction Scheme to Two Space Dimensions on Cartesian Meshes in Conjunction with the ADER Approach. *East Asian Journal on Applied Mathematics*, 13:759-790, 2023.

# Well-posedness and numerical analysis of an elapsed time model with strongly coupled neural networks

Mauricio Sepúlveda[1], Nicolas Torres[2], and Luis Miguel Villada[3]

CI$^2$MA and DIM, Universidad de Concepción, Concepción-Chile
maursepu@udec.cl
Departamento de Matemática Aplicada, Universidad de Granada-España
torres@ugr.es
GIMNAP-Departamento de Matemática, Universidad del Bío-Bío and CI$^2$MA-Universidad de Concepción, Concepción-Chile
lvillada@ubiobio.cl

**Summary.** The elapsed time equation is an age-structured model that describes dynamics of interconnected spiking neurons through the elapsed time since the last discharge, leading to many interesting questions on the evolution of the system from a mathematical and biological point of view. In this work, we first deal with the case when transmission after a spike is instantaneous and the case when there exists a distributed delay that depends on previous history of the system, which is a more realistic assumption. Then we study the well-posedness and the numerical analysis of the elapsed time models. For existence and uniqueness we improve the previous works by relaxing some hypothesis on the non-linearity, including the strongly excitatory case, while for the numerical analysis we prove that the approximation given by the explicit upwind scheme converges to the solution of the non-linear problem. We also show some numerical simulations to compare the behavior of the system in the case of instantaneous transmission with the case of distributed delay under different parameters, leading to solutions with different asymptotic profiles.

**Keywords**: Structured equations; Mathematical neuroscience; Delay differential equations, Well-posedness, Numerical analysis; Periodic solutions.

**Mathematics Subject Classifications (2010)**: 35A35, 35F20, 35R09, 65M06.

## References

1. Pakdaman K, Perthame B, Salort D. Dynamics of a structured neuron population. *Nonlinearity*. 2009;23(1):55
2. Torres N, Cáceres MJ, Perthame B, Salort D. An elapsed time model for strongly coupled inhibitory and excitatory neural networks. *Physica D: Nonlinear Phenomena.* 2021:132977

*This work has been supported by ANID project ECOS200018. MS and LMV was partially supported by ANID-Chile through Centro de Modelamiento Matemático (FB210005) and INRIA Associated team ANACONDA. MS was supported by Fondecyt-ANID project 1220869, and Jean d'Alembert fellowship program, Université de Paris-Saclay. NT was supported by the grant Juan de la Cierva FJC2021-046894-I funded by MCIN/AEI and the European Union NextGenerationEU/PRTR.

# On the convergence of a second-order scheme for non-local conservation laws

G.D. Veerappa Gowda[1], Nikhil Manoj[2], and Sudarshan Kumar K.[3]

Centre for Applicable Mathematics, Tata Institute of Fundamental Research,Bangalore – 560065, India
gowda@tifrbng.res.in
School of Mathematics, Indian Institute of Science Education and Research, Trivandrum –695551, Inida
nikhilmanoj2020@iisertvm.ac.in
School of Mathematics, Indian Institute of Science Education and Research, Trivandrum –695551, India
sudarshan@iisertvm.ac.in

**Summary.** In this talk, we discuss the convergence analysis of a second-order numerical scheme for traffic flow models that incorporate non-local conservation laws. In the field of computational fluid dynamics, first-order methods are generally considered robust and reliable, and they aid in establishing well-posedness of problems. However, second- or high-order methods offer the advantage of considerably more accurate solutions with the same computing cost, particularly for two- or three-dimensional problems. As a result, there has been a surge of research activities aimed at improving these high-order methods. Those studies suggest that high-order schemes offer better solutions than the low-order schemes. In our work, we combine a MUSCL-type spatial reconstruction with strong stability preserving Runge-Kutta time-stepping to devise a fully discrete second-order scheme. The resulting scheme is shown to converge to a weak solution by establishing the maximum principle, bounded variation estimates and $L^1$ Lipschitz continuity in time. Further, using a space-step dependent slope limiter, we prove its convergence to the entropy solution. We also propose a MUSCL-Hancock type second-order scheme which requires only one intermediate stage unlike the Runge-Kutta schemes and is easier to implement. The performance of the proposed second-order schemes in comparison to a first-order scheme is demonstrated through several numerical experiments.

**Keywords**:Non-local conservation laws, MUSCL method, Second-order scheme, MUSCL-Hancock scheme, Convergence analysis, Entropy solution.

**Mathematics Subject Classifications (2010)**: 35L65, 76A30, 65M08, 65M12

## References

1. S. Blandin and P. Goatin. Well-posedness of a conservation law with non-local flux arising in traffic flow modeling. *Numer. Math.*, 132(2):217–241, 2016.
2. R. Bürger, P. Goatin, D. Inzunza, and L. M. Villada. A non-local pedestrian flow model accounting for anisotropic interactions and domain boundaries. *Math. Biosci. Eng.*, 17(5):5883–5906, 2020.
3. R. Bürger, H. D. Contreras, and L. M. Villada. A hilliges-weidlich-type scheme for a one-dimensional scalar conservation law with nonlocal flux. *Netw. Heterog. Media*, 18(2):664–693, 2023.
4. C. Chalons, P. Goatin, and L. M. Villada. High-order numerical schemes for one-dimensional nonlocal conservation laws. *SIAM J. Sci. Comput.*, 40(1):A288–A305, 2018.
5. F. Berthelin and P. Goatin. Regularity results for the solutions of a non-local model of traffic flow. *Discrete Contin. Dyn. Syst.*, 39(6):3197–3213, 2019
6. J. Friedrich and O. Kolb. Maximum principle satisfying CWENO schemes for nonlocal conservation laws. SIAM J. Sci. Comput., 41(2):A973–A988, 2019
7. F. A. Chiarello, P. Goatin, and L. M. Villada. Lagrangian-antidiffusive remap schemes for non-local multi-class traffic flow models. Comput. Appl. Math., 39(2):Paper No. 60, 22, 2020.
8. P. Amorim, R. M. Colombo, and A. Teixeira. On the numerical integration of scalar nonlocal conservation laws. *ESAIM Math. Model. Numer. Anal.*, 49(1):19–37, 2015

# MS11: Numerical approximation of eigenvalue problems of PDEs

# Characterization of singular flows of zeroth-order pseudo-differential operators via elliptic eigenfunctions

Javier Almonacid[1] and Nilima Nigam[2]

Department of Mathematics, Simon Fraser University
javiera@sfu.ca
Department of Mathematics, Simon Fraser University
nigam@math.sfu.ca

**Summary.** The propagation of internal gravity waves in stratified media (such as those found in ocean basins and lakes) leads to the development of geometrical patterns called "attractors". These structures accumulate much of the wave energy and make the fluid flow highly singular. In analytical terms, recent results have confirmed the long-time-believed fact that these attractors develop because of the presence of a continuous spectrum in a class of zeroth-order pseudo-differential operators.

In this talk, we discuss recent progress in the study of this phenomenon from a numerical perspective. First, we propose a high-order pseudo-spectral method to solve the evolution problem, whose long-term behavior is known to be non-square-integrable. Then, we use similar tools to discretize the corresponding eigenvalue problem. Since the eigenvalues are embedded in a continuous spectrum, their computation is based on viscous approximations. Finally, we explore the effect that the embedded eigenmodes have on the long-term evolution of the system.

**Keywords**: spectral methods, pseudo-differential operators, singular solutions, embedded eigenvalues, internal wave attractors.

**Mathematics Subject Classifications (2010)**: 35S10, 65M70, 65F15, 76B15.

## References

1. J.A. Almonacid and N. Nigam. Characterization of singular flows of zeroth-order pseudo-differential operators via elliptic eigenfunctions: a numerical study. *Journal of Applied and Computational Mathematics* 438:115510, 2024.
2. Y. Colin de Vèrdiere and L. Saint-Raymond. Attractors for two dimensional waves with homogeneous Hamiltonians of degree 0. *Communications in Pure and Applied Analysis* 2:421–462, 2020.
3. J. Galkowski and M. Zworski. Viscosity limits for zeroth-order pseudodifferential operators. *Communications on Pure and Applied Mathematics* 75:1798–1869, 2022.

# A virtual element method for the elasticity spectral problem allowing for small edges

Danilo Amigo[1], Felipe Lepe[2], and Gonzalo Rivera[3]

GIMNAP-Departamento de Matemática, Universidad del Bío-Bío
danilo.amigo2101@alumnos.ubiobio.cl
GIMNAP-Departamento de Matemática, Universidad del Bío-Bío
flepe@ubiobio.cl
Departamento de Ciencias Exactas, Universidad de Los Lagos
gonzalo.rivera@ulagos.cl

**Summary.** In this talk we present a virtual element method for the two dimensional elasticity spectral problem, where the polygonal meshes allow for the presence of small edges. Under this approach and with the aid of the theory of compact operators, we prove convergence for the proposed VEM and error estimates. We report a series of numerical tests in order to assess the performance of the method where we analyze the effects of the Poisson ratio on the computation of the order of convergence, together with the effects of the stabilization term on the arising of spurious eigenvalues.

**Keywords**: Elasticity equations, eigenvalue problems, error estimates, virtual element method.

**Mathematics Subject Classifications (2020)** : 35J25, 65N15, 65N25, 65N30, 65N12, 74B05.

## References

1. Amigo, D., Lepe, F. and Rivera, G., A virtual element method for the elasticity problem allowing small edges. *Calcolo. A Quarterly on Numerical Analysis and Theory of Computation*, 60 (2023), Paper No. 28.
2. Brenner, S.C., and Sung, L.-Y., Virtual element methods on meshes with small edges or faces. *Math. Models Methods Appl. Sci.*, 28 (2018), pp. 1291–1336.
3. Babuška, I. and Osborn, J., *Handbook of numerical analysis, Vol. II*, *North-Holland, Amsterdam*. (1991), pp. 641–787.
4. Beirão da Veiga, L., Lovadina, C. and Russo,A., Stability analysis for the virtual element method. *Math. Models Methods Appl. Sci.*, 27 (2017), pp. 2557–2594.

# Least-Squares Finite Element Methods for eigenvalue problems

Fleurianne Bertrand[1]

TU Chemnitz
fleurianne.bertrand@math.tu-chemnitz.de

**Summary.** Accurate flux approximations are of interest in many applications and this is particularly true for fluid-structure interaction problems. Considering the corresponding spectral problem, the Least-Squares method involves the flux and the stress as independent variables approximated in a suitable $H$ (div)-conforming finite element spaces. This talk will discuss the applicability of the Least-Squares method for the determination of the corresponding elastoacoustic vibrations, and show that the resulting scheme provides a correct spectral approximation. Quasi-optimal error estimates and numerical experiments to confirm those will be provided.

**Keywords**: LSFEM, eigenvalue problems, mixed FEM

**Mathematics Subject Classifications (2020)** : 65N30

## References

1. L. Alzaben, FB, and D. Boffi. Computation of eigenvalues in linear elasticity with least-squares finite elements: Dealing with the mixed system, 14th WCCM-ECCOMAS Congress, 2021.
2. FB. and D. Boffi. Least-squares formulations for eigenvalue problems associated with linear elasticity. *Computers and Mathematics with Applications*, 2021.
3. FB. and Daniele Boffi. First order least-squares formulations for eigenvalue problems. *IMA Journal of Numerical Analysis*, 42 (2), 2022.

# The Partition of Unity Finite Element Method for the Schrödinger Equation

Daniele Boffi[1], Francesca Gardini[2], and Gianmarco Manzini[3]

Computer, Electrical and Mathematical Science and Engineering Division, King Abdullah University of Science and Technology, Saudi Arabia
daniele.boffi@kaust.edu.sa
Dipartimento di Matematica "F. Casorati", Università di Pavia, Italy
francesca.gardini@unipv.it
IMATI, Consiglio Nazionale delle Ricerche, Pavia, Italy
gianmarco.manzini@cnr.it

**Summary.** A Schrödinger equation for the system's wavefunctions in a parallelepiped unit cell subject to Bloch-periodic boundary conditions must be solved repeatedly in quantum mechanical computations to derive the materials' properties. Recent studies have demonstrated how enriched finite element type Galerkin methods can substantially lower the number of degrees of freedom necessary to produce accurate solutions with respect to the standard plane-waves method. In particular, the flat-top partition of unity finite element method enriched with the radial eigenfunctions of the one-dimensional Schrödinger equation offers a very effective way of solving the three-dimensional Schrödinger eigenvalue problem. We investigate the theoretical properties of this approximation method, its well-posedness and stability, we prove its convergence and derive suitable bound for the $h$- and $p$-refinement in the $L^2$ and energy norm for both the eigenvalues and the eigenfunctions. Finally, we confirm these theoretical results by applying this method to the eigenvalue problem of the one-electron Schrödinger equation with the harmonic potential, for which the exact solution is known.

**Keywords**: Schrödinger eigenvalue problem, enriched partition of unity finite element method

**Mathematics Subject Classifications (2010)**: 65N25, 65N30.

## References

1. D. Boffi, O. Certik, F. Gardini, and G. Manzini The Partition of Unity Finite Element Method for the Schrödinger Equation (Submitted).

# Model order reduction for parametric eigenvalue problems

Daniele Boffi[1]

King Abdullah University of Science and Technology (KAUST)
daniele.boffi@kaust.edu.sa

**Summary.** Reduced order modeling is a consolidated and popular research area in the numerical approximation of parametric PDEs.

A naif generalization to elliptic and symmetric eigenvalue problems is working well only for the approximation of the fundamental mode, isolated from the rest of the spectrum [6], or to the simultaneous approximation of a number of eigenvalues in the lowest part of the spectrum and separated from the other ones [7].

We will discuss some of the difficulties arising in particular when eigenvalues intersect for various values of the parameters and we report on some new results obtained in this fascinating field [3, 5, 1, 4, 2].

**Keywords**: Model order reduction. Numerical approximation of eigenvalue problems. Finite elements. Eigenvalue tracking.

**Mathematics Subject Classifications (2010)**: 65N25, 65C30, 65-04.

## References

1. M. Alghamdi, F. Bertrand, D. Boffi, and A. Halim. A data-driven method for parametric PDE Eigenvalue Problems using Gaussian Process with different covariance functions. arXiv:2303.18064 [math.NA].
2. M. Alghamdi, D. Boffi, and F. Bonizzoni. A greedy MOR method for the tracking of eigensolutions to parametric elliptic PDEs. arXiv:2208.14054 [math.NA].
3. F. Bertrand, D. Boffi, and A. Halim. A reduced order model for the finite element approximation of eigenvalue problems. *Computer Methods in Applied Mechanics and Engineering*, 404:115696, 2023.
4. F. Bertrand, D. Boffi, and A. Halim ata-driven reduced order modeling for parametric PDE eigenvalue problems using Gaussian process regression. *Journal of Computational Physics*, to appear.
5. D. Boffi, A. Halim, and G. Priyadarshi. Reduced basis approximation of parametric eigenvalue problems in presence of clusters and intersections. arXiv:2302.00898 [math.NA].
6. I. Fumagalli, A. Manzoni, N. Parolini, and M. Verani. Reduced basis approximation and a posteriori error estimates for parametrized elliptic eigenvalue problems. ESAIM *Math. Model. Numer. Anal.*, 50(6):1857-1885, 2016.
7. T. Horger, B. Wohlmuth, T. Dickopf. Simultaneous reduced basis approximation of parameterized elliptic eigenvalue problems. ESAIM *Math. Model. Numer. Anal.*, 51(2):443-465, 2017.

# Adaptive FEM for Stokes eigenvalue problems

Daniele Boffi[1] and Arbaz Khan[2]

Computer, electrical and mathematical sciences and engineering division, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia
daniele.boffi@kaust.edu.sa
Department of Mathematics, IIT Roorkee, India
arbaz@ma.iitr.ac.in

**Summary.** Over the last few decades, the numerical analysis of the finite element method for eigenvalue problems has been of increasing interest because of various practical applications. Specifically, the a posteriori error analysis of eigenvalue problems using finite element approximations has been well developed. However, most results are for the Laplace eigenvalue problem and only a few papers consider the a posteriori error analysis for the Stokes eigenvalue problem. It is the aim of this talk to present the Adaptive FEM for Stokes Eigenvalue problems. Specifically, we will discuss the optimal convergence of a standard adaptive scheme.

**Keywords**: Adaptive FEM, Stokes eigenvalue problems, a posteriori error estimates.

**Mathematics Subject Classifications (2010)**: 65N30, 65N15,65N25, 65N30

## References

1. D. Boffi, D. Gallistl, F. Gardini, and L. Gastaldi. Optimal convergence of adaptive fem for eigenvalue clusters in mixed form. *Mathematics of Computation*, 86: 2213-2237, 2018.
2. C. Lovadina, M. Lyly, and R. Stenberg. A posteriori estimates for the stokes eigenvalue problem. *Numerical Methods for Partial Differential Equations: An International Journal*, 25, 244-257, 2009.
3. J. Gedicke and A. Khan. Arnold–winther mixed finite elements for sSokes eigenvalue problems. SIAM *Journal on Scientific Computing*, 40, A3449-A3469, 2018.
4. J. Gedicke and A. Khan. Divergence-conforming discontinuous Galerkin finite elements for stokes eigenvalue problems. *Numerische Mathematik*, 144, 585-614, 2020.
5. M. Feischl. Optimality of a standard adaptive finite element method for the stokes problem. SIAM *Journal on Numerical Analysis*, 57 1124-1157, 2019.
6. M. Feischl. Inf-sup stability implies quasi-orthogonality. *Mathematics of Computation*, 91, 2059-2094, 2022.
7. F. Lepe and D. Mora. Symmetric and nonsymmetric discontinuous Galerkin methods for a pseudostress formulation of the Stokes spectral problem. SIAM *Journal on Scientific Computing*, 42, A698–A722, 2020.

# An a priori error analysis for a Steklov eigenvalue problem using a Hybrid High-Order method

Rommel Bustinza[1], Matteo Cicuttin[2], and Ariel L. Lombardi[3]

Universidad de Concepción, Chile
rbustinza@udec.cl
Politecnico di Torino, Italy
matteo.cicuttin@polito.it
Universidad Nacional de Rosario, Argentina
ariel@fceia.unr.edu.ar

**Summary.** In this talk we discuss the approximation of the spectrum of the Steklov eigenvalue problem, when using the well known Hybrid High-Order (HHO) method. The analysis developed here, adapt ideas described in a previous HHO work, that deals with the classical Laplacian eigenvalue problem. As expected, we are able to eliminate the volume unknowns, by introducing a suitable discrete operator. This allows us to numerically solve on the skeleton of the mesh, reducing the computational cost. The a priori error analysis lets us to prove optimal convergence rates for the eigenvalues and the eigenfunctions, when the latter are smooth enough. Numerical examples, with smooth and non-smooth eigenfunctions, verify our theoretical findings.

**Keywords**: Steklov eigenvalue problem, Hybrid High-Order method, a priori error analysis, polytopal meshes.

**Mathematics Subject Classifications (2010)**: 62N25, 65N30, 74S99

**Acknowlegdments:** First author has been partially support by ANID (Chile) through FONDECYT Project No. 1200051.

## References

1. I. Babuška, and J. Osborn. *Eigenvalue problems, Handbook of Numerical Analysis*, volume II of *Handb. Numer. Anal.* North-Holland, Amsterdam, 1991, pp. 641-787.
2. V. Calo, M. Cicuttin, Q. Deng, and A. Ern. Spectral approximation of elliptic operators by the Hybrid High-Order method. *Mathematics of Computation*, 88(318):1559-1586, 2019.
3. P. Monk, and Y. Zhang. An HDG method for the Steklov eigenvalue problem. IMA *Journal of Numerical Analysis*, 42(3):1929-1962, 2022.

# Computation of Interior Eigenvalues from the Scattering Data

Fioralba Cakoni[1]

DeRutgers University, New Brunswick, USA
fc292@math.rutgers.edu

**Summary.** In the recent years new spectral imaging methods have been introduced for solving the inverse scattering problem [3]. These methods make use interior eigenvalue problems defined on the support of the scatterer, which arise from the study of injectivity of the relative scattering operator. In the case of the scattering by an impenetrable obstacle with Dirichlet or Robin boundary condition this is merely the Dirichlet or Robin eigenvalue problem for a symmetric elliptic operator [1]. A more intriguing situation arises in the scattering by an inhomogeneous medium, where a non-selfadjoint eigenvalue problems arises, known as the transmission eigenvalue problem [2]. The interior eigenvalues contain information about the geometry and/or constitutive material properties of the scatterer that can be used in the imaging. In this presentation we show how to determine the interior eigenvalues associated with a particular scattering problem from measured scattering data. The numerical algorithm is based on the lack of injectivity of the relative scattering operator at an interior eigenvalues, which in the literature is often referred to as inside-outside duality in scattering theory.

**Keywords**: scattering operator, inverse scattering theory, inside outside duality, transmission eigenvalues, interior eigenvalues

**Mathematics Subject Classifications (2010)**: 35R30; 35J25; 35P25; 35P05

## References

1. F. Cakoni, D. Colton, and H. Haddar. On the determination of Dirichlet or transmission eigenvalues from far field data *C. R. Math. Acad. Sci. Paris*, 348: 379-383, 2010.
2. F. Cakoni, D. Colton, and H. Haddar. Transmission Eigenvalues *AMS Notices*, 68 no 9:1499-1510, 2008.
3. F. Cakoni, D. Colton, and H. Haddar. *Inverse Scattering Theory and Transmission Eigenvalues*, volume 98 *CBMS-NSF*. SIAM Publications, 2023.

# Sum-of-squares Polynomial Optimization to Study the Stability of Shear Flows

Elizabeth Carlson[1], Federico Fuentes[2], and David Goluskin[3]

California Institute of Technology
elizcar@caltech.edu
Pontificia Universidad Católica de Chile
federico.fuentes@uc.cl
University of Victoria
goluskin@uvic.ca

**Summary.** The stability of steady states for complex dynamical systems are notoriously difficult problems, even for the seemingly simplest cases. For example, it is expected that the standard steady state shear profile for 2D Couette flow is globally stable for all Reynolds numbers, however the state-of-the-art analysis using standard energy method approaches (including potentially background method techniques as well) is decades old and only proves the stability for relatively low Reynolds numbers. In recent years, a promising computational approach uses polynomial sum-of-squares optimization to find Lyapunov functions based on low-mode projections onto an orthogonal basis. The choice of this basis can technically be arbitrary, but the natural basis comes from solving a numerical eigenvalue problem uncovered by solving a calculus of variations problem. One can solve this numerical eigenvalue problem (and similar eigenvalue problems) exploiting the inherent geometry. The solutions to these eigenvalue problems moreover yield heuristic insight into the difficulty of this problem and the sensitivity of this approach for determining global stability for Reynolds numbers greater than the current state-of-the-art critical value given by analysis.

**Keywords**: sum of squares, stability, eigenvalue problems, Chebyshev collocation

**Mathematics Subject Classifications (2010)**: 65, 76, 35, 49

## References

1. C. R. Doering and P. Constantin Energy dissipation in shear driven turbulence *Physics Review Letters* 69, 1648, (1992).
2. P. G. Drazin and W. H. Reid. *Hydrodynamic Stabilty*, Cambridge University Press; 2nd edition, 2004.
3. F. Fuentes, D. Goluskin, and S. Chernyshenko. Global Stability of Fluid Flows Despite Transient Growth of Energy. *Phys. Rev. Lett.*, 128(20):204502, 2022.
4. D. Huang , S. Chernyshenko , P. Goulart , D. Lasagna , O. Tutty and F. Fuentes. Sum-of-squares of polynomials approach to nonlinear stability of fluid flows: an example of application *Proceedings of the Royal Society A* 471: 20150622 (2015).
5. P.J. Goulart and S. Chernyshenko. Global stability analysis of fluid flows using sum-of-squares. *Physica D: Nonlinear Phenomena*, 241(6):692-704, 2012.
6. A. Mironchenko and F. Wirth. A non-coercive Lyapunov framework for stability of distributed parameter systems. 2017 IEEE 56th Annual Conference on Decision and Control (CDC), Melbourne, VIC, Australia, 1900-1905, (2017).

# Finite element solution of the Reynolds-Orr energy eigenvalue problem

Federico Fuentes[1] and Wilmar Imbachí[2]

Pontificia Universidad Católica de Chile, Institute for Mathematical and Computational Engineering (IMC), Santiago, Chile.
federico.fuentes@uc.cl
Pontificia Universidad Católica de Chile, Faculty of Mathematics, Santiago, Chile.
waimbachi@mat.uc.cl

**Summary.** We introduce a convergence analysis of the finite element method applied to the Reynolds-Orr eigenvalue problem in wall-bounded shear-driven incompressible flows with arbitrary cross-section. The Reynolds-Orr eigenproblem can be written as a mixed formulation similar to Stokes flow, but including an extra term involving the strain rate tensor of the underlying laminar flow. The analysis of the resulting discrete eigenproblem must be adapted to the standard spectral approximation framework, since one of the bilinear forms which is coercive in the Stokes equations is no longer coercive. We demonstrate that the proposed approach delivers accurate estimates of errors associated with both eigenvalues and eigenfunctions. We carry out various numerical tests to showcase how well the method performs and to confirm the accuracy of our theoretical results.

**Keywords**: Reynolds-Orr eigenvalue problem; Stokes eigenvalue problem; Spectral problems; Error estimates.

**Mathematics Subject Classifications (2010)**: 65N12, 65N15,65N25, 65N30; 76D07, 35Q35.

## References

1. Reynolds, O. (1895). IV. On the dynamical theory of incompressible viscous fluids and the determination of the criterion. *Philosophical Transactions of the Royal Society of London*.(a.), (186), 123-164.
2. Orr, W. M. F. (1907, January). The stability or instability of the steady motions of a perfect liquid and of a viscous liquid. Part II: A viscous liquid. In *Proceedings of the Royal Irish Academy. Section A: Mathematical and Physical Sciences* (Vol. 27, pp. 69-138). Royal Irish Academy.
3. Drazin, P. G., & Reid, W. H. (2004). *Hydrodynamic stability*. Cambridge University Press.
4. Doering, C. R., & Gibbon, J. D. (1995). *Applied analysis of the Navier-Stokes equations* (No. 12). Cambridge University Press.
5. Serrin, J. (1959). On the stability of viscous fluid motions. *Archive for Rational Mechanics and Analysis*, 3, 1-13.
6. Fuentes, F., Goluskin, D., & Chernyshenko, S. (2022). Global stability of fluid flows despite transient growth of energy. *Physical Review Letters*, 128(20), 204502.
7. Boffi, D. (2010). Finite element approximation of eigenvalue problems. *Acta Numerica*, 19, 1-120.
8. Boffi, D., Brezzi, F., & Gastaldi, L. (1997). On the convergence of eigenvalues for mixed formulations. *Annali della Scuola Normale Superiore di Pisa-Classe di Scienze*, 25(1-2), 131-154.
9. Joseph, D. D., & Carmi, S. (1969). Stability of Poiseuille flow in pipes, annuli, and channels. *Quarterly of Applied Mathematics*, 26(4), 575-599.
10. Goulart, P. J., & Chernyshenko, S. (2012). Global stability analysis of fluid flows using sum-of-squares. *Physica D: Nonlinear Phenomena*, 241(6), 692-704.
11. Joseph, D. D. (2013). *Stability of fluid motions I* (Vol. 27). Springer Science & Business Media.

# Spectrally accurate eigen solvers for elliptic eigenvalue problems

Himanshu Garg[1], N. Kishore Kumar[2], and Subhashree Mohapatra[3]

IIIT Delhi
himanshug@iiitd.ac.in
BITS Pilani Hyderabad Campus
naraparaju@hyderabad.bits-pilani.ac.in
IIIT Delhi
subhashree@iiitd.ac.in

**Summary.** In this work, we present high order eigen solvers for various partial differential equations related eigen value problems. A least squares based spectral element formulation alongwith power method has been used to obtain the first eigenvalue. The eigen value problems related to non self-adjoint elliptic differential operators and Stokes eigenvalue problems have been investigated with this approach. Exponential converegence of eigenvalues and eigenfunctions have been established. Numerical results on various domains alongwith different boundary conditions confirm the proposed theoretical claims.

**Keywords**:

**Mathematics Subject Classifications (2020)** :

## References

1. Felipe Lepe, Gonzalo Rivera, A virtual element approximation for the pseudostress formulation of the Stokes eigenvalue problem, Comput. Methods Appl. Mech. Engrg. 379 (2021) 113753.
2. Felipe Lepe, Gonzalo Rivera, Felipe Lepe, Gonzalo Rivera, VEM discretization allowing small edges for the reaction-convection-diffusion equation : source and spectral problems, Comput. Methods Appl. Mech. Engrg. 379 (2021) 113753.
3. Lokendra K. Balyan, Pravir K. Dutt, R.K.S. Rathore, Least squares h-p spectral element method for elliptic eigenvalue problems, Appl. Math. Comput., 218 (2012) 9596–9613.
4. Önder Türk, Ramon Codina, Chebyshev spectral collocation method approximations of the Stokes eigenvalue problem based on penalty techniques, Appl. Numer. Math., 145 (2019) 188–200.

# Virtual element schemes for an acoustic vibration problem

Lucia Gastaldi[1]

Università di Brescia, Italy
lucia.gastaldi@unibs.it

**Summary.** In this paper we study and analyze a virtual element method (VEM) introduced in [1] for the approximation of an acoustic vibration problem. An important feature of VEM is that suitable stabilizing forms, depending on appropriate parameters, have to be introduced in order to guarantee consistency and stability of the approximation. This is due to the virtual nature of the basis functions corresponding to the degrees of freedom at the interior of elements. In the case of the approximation of eigenvalue problems by means of virtual elements it has been observed recently in [2] that the choice of the optimal parameters for the computation of the eigenvalues might not be an easy task. Here I present some new results on the approximation of the eigenvalue for the acoustic vibration problem showing that in some cases there is no need of using any stabilization for the stiffness and mass matrix. These results have been obtained, in collaboration with Daniele Boffi, Linda N. Alzaben and Andreas S. Dedner.

**Keywords**: Eigenvalue problem; Virtual element method; Stabilization free VEM; Acoustic problem; Discrete compactness property.

**Mathematics Subject Classifications (2010)**: 65N25, 65N30, 70J30, 76M10.

## References

1. L. Beirão da Veiga, D. Mora, G. Rivera, and R. Rodríguez. A virtual element method for the acoustic vibration problem *Numerische Mathematik*, 136(3):725-763, 2017.
2. D. Boffi, F. Gardini, and L. Gastaldi. Approximation of PDE eigenvalue problems involving parameter dependent matrices *Calcolo*, 57(4):Paper No. 41, 21, 2020.

# A posteriori virtual element method for the acoustic vibration problem

Felipe Lepe[1], David Mora[2], Gonzalo Rivera[3], and Iván Velásquez[4]

Universidad del Bío-Bío
flepe@ubiobio.cl
Universidad del Bío-Bío
dmora@ubiobio.cl
Universidad de Los Lagos
gonzalo.rivera@ulagos.cl
Universidad del Sinú Elías Bechara Zainúm, Montería, Colombia.
ivanvelasquez@unisinu.edu.co

**Summary.** In this talk, we present a two dimensional analyze of an a posteriori error estimator for the acoustic spectral problem based on the virtual element method in $\mathrm{H}(\div;\Omega)$. Introducing an auxiliary unknown using the fact that the primal formulation of the acoustic problem is equivalent to a mixed formulation, in order to prove a superconvergence result, necessary to despise high order terms. Under the virtual element approach, we prove that our local indicator is reliable and globally efficient in the $\mathrm{L}^2$-norm. We provide numerical results to evaluate the performance of the proposed error estimator.

**Keywords**: virtual element method, acoustic vibration problem, polygonal meshes, a posteriori error estimates.

**Mathematics Subject Classifications (2010)**: 65N30, 65N25, 70J30, 76M25.

## References

1. Beirão da Veiga L., Mora D., Rivera G. and Rodríguez R., A virtual element method for the acoustic vibration problem, *Numer. Math.,* **136**, (2017), pp. 725–763.
2. Boffi D., Gastaldi L., Rodríguez R. and Šebestová I., Residual-based *a posteriori* error estimation for the Maxwell's eigenvalue problem, *IMA J. Numer. Anal.,* **37**, (2017), pp. 1710–1732.
3. Lepe F. and Rivera G., A priori error analysis for a mixed VEM discretization of the spectral problem for the Laplacian operator, *Calcolo,* **58**, (2021), pp. 30.
4. Lin Q. and Xie H., A superconvergence result for mixed finite element approximations of the eigenvalue problem, *ESAIM Math. Model. Numer. Anal.*, **46**, (2012), pp. 797–812.

# VEM allowing small edges for the reaction-convection-diffusion equation: source and eigenvalue problems

Felipe Lepe[1] and Gonzalo Rivera[2]

Universidad del Bío-Bío
flepe@ubiobio.cl
Universidad de Los Lagos
gonzalo.rivera@ulagos.cl

**Summary.** In this talk we present a lowest order virtual element method for the classic load reaction-convection-diffusion problem and the convection-diffusion spectral problem, where the assumptions on the polygonal meshes allow to consider small edges for the polygons. Under well defined seminorms depending on a suitable stabilization for this geometrical approach, we derive the well posedness of the numerical scheme and error estimates for the load problem, whereas for the spectral problem we derive convergence and error estimates fo the eigenvalues and eigenfunctions. We report numerical tests to asses the performance of the method. **Keywords**: Virtual element methods a priori error estimates, small edges.

**Mathematics Subject Classifications (2010)**: 49K20, 49M25, 65N12, 65N15, 65N25, 65N30.

## References

1. L. Beirão da Veiga, C. Lovadina, and A. Russo, Stability analysis for the virtual element method. *Math. Models Methods Appl. Sci.*, 27, pp. 2557–2594, 2017.
2. D. Boffi, Finite element approximation of eigenvalue problems *Acta Numerica*, 19, pp. 1–120, 2010.
3. F. Gardini and G. Vacca, Virtual element method for second-order elliptic eigenvalue problems, *IMA J. Numer. Anal.*, 38, pp. 2026–2054, 2018.

# Finite element analysis of the Oseen eigenvalue problem

Felipe Lepe[1], Gonzalo Rivera[2], and Jesus Vellojin[3]

GIMNAP-Departamento de Matemática, Universidad del Bío - Bío, Casilla 5-C, Concepción, Chile
flepe@ubiobio.cl
Departamento de Ciencias Exactas, Universidad de Los Lagos, Casilla 933, Osorno, Chile.
gonzalo.rivera@ulagos.cl
GIMNAP-Departamento de Matemática, Universidad del Bío - Bío, Casilla 5-C, Concepción, Chile
jvellojin@ubiobio.cl

**Summary.** The aim of this talk is to present a finite element method for the Oseen eigenvalue problem. This problem is an extension of the Stokes eigenvalue problem, where the presence of the convective term leads to a non-symmetric problem and hence, to complex eigenvalues and eigenfunctions. With the aid of the compact operators theory, we prove that for inf-sup stable finite elements the convergence holds and hence, error estimates for the eigenvalues and eigenfunctions are derived. We also propose an a posteriori error estimator which results to be reliable and efficient. We report a series of numerical tests in two and three dimension in order to assess the performance of the method and the proposed estimator.

**Keywords**: Oseen equations, Eigenvalue Problems, A posteriori error analysis

**Mathematics Subject Classifications (2010)**: 35Q35, 65N15, 65N25, 65N30, 65N50.

## References

1. J. Volker. *Finite element methods for incompressible flow problems.* Springer *Springer Series in Computational Mathematics*,Cham, 51, 2014.
2. C. Carstensen and J. Gedicke. *Robust residual-based a posteriori Arnold-Winther mixed finite element analysis in elasticity Comput. Methods Appl. Mech. Engrg.*, 300, 245–264, 2016.
3. F. Lepe and G. Rivera. *VEM discretization allowing small edges for the reaction–convection–diffusion equation: source and spectral problems.* ESAIM *Math. Model. Numer. Anal,* 57, 3139–3164, 2023.
4. D. Mora and I. Velásquez *A C*1 – *C*0 *conforming virtual element discretization for the transmission eigenvalue problem. Res. Math. Sci,* 8, Paper No. 56, 21, 2021.

# Approximation of a Laplace-Steklov eigenvalue problem by finite and boundary element methods

Önder Türk[1]

Middle East Technical University, Ankara, Turkey
onder.turk@yandex.com

**Summary.** The discrete formulations based on finite and boundary element methods to approximate the solution of a Laplace-Steklov eigenvalue problem are investigated. The problem is defined in a way that the eigenvalue is involved in both the differential equation and boundary conditions. Therefore, it can be obtained by originally generalizing the Laplace and Steklov eigenvalue problems. Such generalized problems arise for instance as the auxiliary eigenproblems when a parabolic initial-boundary value problem with dynamic/Wentzell type boundary condition is spectrally analyzed. The study aims primarily to provide several characteristics related to the application of finite and boundary element approaches to approximate the novel eigenproblem. A comparative analysis of the results obtained from these two methods will be presented. The characteristic properties of the components in the spaces obtained from the discretization of this problem on appropriately defined domains will also be studied along with the mathematical properties of functions existing in these solution spaces.

**Keywords**: Laplace-Steklov eigenvalue problems, finite element methods, boundary element methods.

# MS12: Numerical methods for fluid-membrane interaction

# A divergence-free finite element method for flow-transport coupling with osmotic effects

Arbaz Khan[1], David Mora[2], Ricardo Ruiz-Baier[3], and Jesus Vellojin[4]

Department of Mathematics, Indian Institute of Technology Roorkee, Roorkee 247667, India.
arbaz@ma.iitr.ac.in
GIMNAP-Departamento de Matemática, Universidad del Bío - Bío, Casilla 5-C, Concepción, Chile
dmora@ubiobio.cl
School of Mathematics, Monash University, 9 Rainforest Walk, Melbourne, Victoria 3800, Australia; and Universidad Adventista de Chile, Casilla 7–D Chillan, Chile.
ricardo.ruizbaier@monash.edu
GIMNAP-Departamento de Matemática, Universidad del Bío - Bío, Casilla 5-C, Concepción, Chile
jvellojin@ubiobio.cl

**Summary.** The aim of this talk is to propose a model for the coupling of flow and transport equations with porous membrane-type conditions on part of the boundary. The governing equations consist of the incompressible Navier–Stokes equations coupled with an advection-diffusion equation, and we employ a Lagrange multiplier to enforce the coupling between penetration velocity and transport on the membrane while mixed boundary conditions are considered in the remainder of the boundary. Existence and uniqueness of the continuous problem using a fixed-point argument is proved. By means of a new H(div)-conforming finite element formulation, we address the model approximation, together with its a priori error analysis. We showcase a set of numerical examples validating the theory and illustrating the use of the new methods in the simulation of reverse osmosis processes.

**Keywords**: Navier–Stokes equations coupled with transport, Lagrange multipliers, Reverse osmosis, Divergence-conforming finite element methods.

**Mathematics Subject Classifications (2010)**: 35Q30, 65N22, 65N30, 76D07.

## References

1. R. Oyarzúa, T. Qin, and D. Schötzau. *An exactly divergence-free finite element method for a generalized Boussinesq problem.* IMA *journal of numerical analysis*, 34(3), 1104–1135, 2014.
2. N. Carro, D. Mora, and J. Vellojin. *A finite element model for concentration polarization and osmotic effects in a membrane channel.* arXiv preprint 2212.08140, 2022.
3. R. Verfürth. *Finite element approximation on incompressible Navier-Stokes equations with slip boundary condition. Numerische Mathematik,* 50, 697–721. 1986.
4. W. Layton. *Weak imposition of "no-slip" conditions in finite element methods. Mathematics with Applications,* 38(5-6), 129–142. 1999.
5. G. Zhou, T. Kashiwabara, and I. Oikawa. *Penalty method for the stationary Navier–Stokes problems under the slip boundary condition. Journal of Scientific Computing,* 68, 339–374. 2016.
6. B. Bernales, P. Haldenwang, P. Guichardon, and N. Ibaseta *Prandtl model for concentration polarization and osmotic counter-effects in a 2-d membrane channel. Desalination,* 404, 341–359. 2017.

# A Mixed Finite Element Method for a Reverse Osmosis Model

Víctor Burgos[1], Ricardo Oyarzúa[2], and Manuel Solano[3]

Center for Research in Mathematical Engineering CI$^2$MA, Universidad de Concepción,Concepción, Chile
vicburgos@udec.cl
GIMNAP-Departamento de Matemática, Universidad del Bío Bío, Concepción, Chile
royarzua@ubiobio.cl
Department of Mathematical Engineering and Center for Research in Mathematical Engineering CI$^2$MA, Universidad de Concepción, Concepción, Chile
msolano@ing-mat.udec.cl

**Summary.** We develop and analyze a numerical method to approximate the solution to a partial differential equation arising from a phenomenological model of water desalination through reverse osmosis within a channel module. The problem involves a coupled nonlinear system, which considers the steady state of mass transport phenomena through a convection-diffusion equation and linear momentum balance via the Navier-Stokes equation. To address this problem, we introduce a mixed variational formulation for both phenomena, utilizing suitable Lebesgue spaces to define nonlinear terms, and introducing a Lagrange multiplier that couples both phenomena at the boundary. We establish existence and uniqueness of the solution under smallness assumptions on the physical parameters. We consider conforming subspaces, show well-posedness of the discrete formulation, and the respective *a priori* error estimates. Finally, we compare our results against benchmarks available in the literature to assess the proper functioning of the numerical method.

**Keywords**: desalinitaion process, mixed finite element method, *a priori* error analysis, reverse osmosis.

**Mathematics Subject Classifications (2010)**: 65N30, 65N12, 65N15

## References

1. I. Babuška, and G. Gatica. On the mixed finite element method with Lagrange multipliers. *Numerical Methods for Partial Differential Equations*, 19(2):135-270, 2003.
2. R. Oyarzúa and M. Serón. A Divergence-Conforming DG-Mixed Finite Element Method for the Stationary Boussinesq Problem *Journal of Scientific Computing*, 85(14):1-36, 2020.
3. J. Camaño, C. García and R. Oyarzúa. Analysis Of A Momentum Conservative Mixed-Fem For The Stationary Navier-Stokes Problem. *Numerical Methods for Partial Differential Equations*, 37(5):2895-2923, 2021.
4. C. Correa and G. Gatica. On the continuous and discrete well-posedness of perturbed saddle-point formulations in Banach spaces. *Computers & Mathematics with Applications*, 117: 14-23, 2022.

# Numerical approximation of a fluid flow in a deformable tube with slip boundary condition of friction type on the interface

Leonardo Baffico[1]

Laboratoire de Mathématiques N. Oresme, LMNO Normandie Univ, UNICAEN, CNRS
leonardo.baffico@unicaen.fr

**Summary.** We are interested in the numerical resolution of an unsteady fluid–structure interaction problem with a slip boundary condition. In this problem, an incompressible Newtonian viscous fluid flows in a deformable tube. The fluid and structure behavior are governed by the incompressible Navier–Stokes equation and a generalized membrane equation (see [3]), respectively. On the fluid–structure interface, instead of the usual no-slip boundary condition for the fluid, we impose a slip boundary condition of friction type (see [4]). This condition allows the fluid to slip on the interface if the fluid shear stress reaches a threshold value. The threshold value could be either a known function or it could depend on the fluid state. The problem is completed with an impermeability condition and with a stress continuity condition (based on the action-reaction principle) between the fluid and the solid.

First, we show that the energy system presents an additional dissipative term due to the slip boundary condition. Next, we present a numerical scheme for the fluid problem based on the Characteristic-ALE method (see, e.g., [2]) for the time discretization and on a finite element four-field mixed variational formulation for the space discretization. In this formulation two Lagrange multipliers are introduced in order to release the impermeability condition and the slip boundary condition (see [1]). The structure problem is discretized using a Newmark scheme in time and a finite element approximation in space. Finally, the implicit coupling conditions between the fluid and structure, at each time step, are ensured using an iterative scheme. After that, we study the discrete energy balance for the semi-discretized variational problem. Finally, we will present some numerical simulations.

**Keywords**: Fluid-structure interaction problem, Friction type slip boundary condition, Mixed variational formulation.

**Mathematics Subject Classifications (2010)**: 65M50, 65N30, 76M10, 74F10, 76D07.

## References

1. M. Ayadi, H. Ayed, L. Baffico, and T. Sassi. Stokes problem with slip boundary conditions of friction type: error analysis of a four-field mixed variational formulation. *Journal of Scientific Computing*, 81(1):312–341, 2019.
2. A. Decoene, and B. Maury. Moving meshes with freefem++. *Journal of Numerical Mathematics*, 20(3-4):195–214, 2012.
3. L. Formaggia, J. F. Gerbeau, F. Nobile, and A. Quarteroni. On the coupling of 3D and 1D Navier-Stokes equations for flow problems in compliant vessels. *Computer Methods in Applied Mechanics and Engineering*, 191(6-7):561–582, 2001.
4. H. Fujita. A coherent analysis of Stokes flows under boundary conditions of friction type, *Journal of Computational and Applied Mathematics*, 149(1):57–69, 2002.

# A nonconforming finite element method for a nonisothermal fluid-membrane interaction

Jessika Camaño[1], Ricardo Oyarzúa[2], Miguel Serón[3], and Manuel Solano[4]

Universidad Católica de la Santísima Concepción
jecamano@ucsc.cl
Universidad del Bío-Bío
royarzua@ubiobio.cl
Universidad del Bío-Bío
mseron@ubiobio.cl
Universidad de Concepción
msolano@ing-mat.udec.cl

**Summary.** We propose and analyze an $H(div)$-conforming and mass conservative finite element method for a nonisothermal fluid-membrane interaction problem. The problem consists of a Navier-Stokes/heat system, commonly known as the Boussinesq system, in the free-fluid region, and a Darcy-heat coupled system in the membrane. These systems are coupled through buoyancy terms and a set of transmission conditions on the fluid-membrane interface, including mass conservation, balance of normal forces, the Beavers-Joseph-Saffman law, and continuity of heat flux and fluid temperature. We consider the well-known velocity-pressure-temperature variational scheme for the Boussinesq system in the free-fluid region whereas in the membrane region we consider a dual-mixed formulation for the Darcy system coupled with a primal equation for the temperature model. In this way, the unknowns of the resulting formulation are given by the velocity, the pressure, and the temperature in both domains. For the associated Galerkin scheme, we combine an $\mathbf{H}(\mathrm{div})$-conforming scheme for the fluid variables and a conforming Galerkin discretization for the heat equation. Therefore, the resulting numerical scheme yields exactly divergence–free velocities. We prove well-posedness by means of a fixed–point strategy and derive the corresponding convergence. Finally, we present some numerical examples to illustrate the performance of the method.

**Keywords**: nonisothermal fluid-membrane, Navier–Stokes equation, Darcy equation, heat equation, discontinuous Galerkin methods.

**Mathematics Subject Classifications (2010)**: 65N15, 65N30, 35K05, 76D05, 76S05, 74K15, 76R05, 76B03.

## References

1. Camaño, J., Oyarzúa R., Serón, M., & Solano M.E. A conforming finite element method for a nonisothermal fluid-membrane interaction. Preprint 2023-14, Centro de Investigación en Ingeniería Matemática (CI$^2$MA), UdeC, (2023).
2. Cockburn, B., Kanschat, G., & Schötzau, D. A note on discontinuous Galerkin divergence-free solutions of the Navier-Stokes equations. J. Sci. Comput., vol. 31, no. 1-2, pp. 61–73, (2007).
3. Colmenares, E., & Neilan, M. Dual-mixed finite element methods for the stationary Boussinesq problem. Comput. Math. Appl., vol. 72, no. 7, pp. 1828–1850, (2016).
4. Kanschat, G., & Riviére, B. A strongly conservative finite element method for the coupling of Stokes and Darcy flow. J. Comput. Phys., vol. 229, no. 17, pp. 5933–5943, (2010).
5. McCurdy, M., Moore, N., & Wang, X. Convection in a coupled free flow-porous media system. SIAM J. Appl. Math., vol. 79, no. 6, pp. 2313–2339, (2019).

# Banach space-based analysis of a fully mixed formulation for the Navier–Stokes/Darcy equations

Sergio Caucao[1], Ricardo Oyarzúa[2], and Segundo Villa-Fuentes[3]

Universidad Católica de la Santísima Concepción, Chile
scaucao@ucsc.cl
Universidad del Bío-Bío, Chile
royarzua@ubiobio.cl
Monash University, Australia
segundo.villafuentes@monash.edu

**Summary.** We propose and analyze a fully-mixed formulation to couple fluid flow with porous media flow, governed by the Navier–Stokes and Darcy equations, respectively. The transmission conditions consist of mass conservation, balance of normal forces, and the Beavers-Joseph-Saffman law. Our approach involves introducing a modified pseudostress tensor dependent on pressure, the diffusive and convective terms of the fluid Navier–Stokes equations, while employing the standard dual-mixed formulation for the Darcy model. The method results in a mixed variational formulation based on Banach spaces and a twofold saddle point structure. The key unknowns for the Navier-Stokes fluid are the pseudostress tensor, vorticity, and velocity, whereas the porous medium has velocity and pressure as its corresponding unknowns. We establish the well-posedness of both continuous and discrete formulations using a fixed-point strategy and the Banach–Nečas–Babuška and Banach's fixed point theorems. These results apply to arbitrary finite element subspaces under suitable stability assumptions. Additionally, we identify specific finite element subspaces that satisfy the necessary conditions and provide convergence analysis, demonstrating the method's optimal rate of convergence. Finally, we present several numerical results to illustrate the performance of the proposed method.

**Keywords**: Navier–Stokes, Darcy, momentum conservativity, mixed finite element method, Banach spaces, Arnold–Falk–Winther elements, Raviart–Thomas elements

**Mathematics Subject Classifications (2010)**: 65N15, 65N30, 76D05, 76M10

## References

1. J. Camaño, C. García, and R. Oyarzúa. Analysis of a momentum conservative mixed-FEM for the stationary Navier–Stokes problem. *Numerical Methods for Partial Differential Equations*, 37 (5): 2895–2923, 2021.
2. J. Camaño, G.N. Gatica, R. Oyarzúa, R. Ruiz-Baier, and P. Venegas. New fully-mixed finite element methods for the Stokes-Darcy coupling. *Computer Methods in Applied Mechanics and Engineering*, 295: 362–395, 2015.
3. G.N. Gatica, N. Heuer, and S. Meddahi. On the numerical analysis of nonlinear twofold saddle point problems. *IMA Journal of Numerical Analysis* 23(2): 301–330, 2003.
4. G.N. Gatica, R. Oyarzúa, and F. Sayas. Analysis of fully-mixed finite element methods for the Stokes–Darcy coupled problem. *Mathematics of Computation*, 80(276): 1911-1948, 2011.

# A stabilized finite element method for the Stokes–Temperature coupled problem

Rodolfo Araya[1], Cristian Cárcamo[2], and Abner H. Poza[3]

Departamento de Ingeniería Matemática & CI$^2$MA, Universidad de Concepción, Concepción, Chile.
rodolfo.araya@udec.cl
Weierstrass Institute, Germany.
email@second.author.org
Departamento de Matemática y Física Aplicadas and Grupo de Investigación en Análisis Numérico y Cálculo Científico, GIANuC$^2$ Universidad Católica de la Santísima Concepción, Concepción, Chile.
apoza@ucsc.cl

**Summary.** In this talk, we introduce and analyze a new stabilized finite element scheme for the Stokes–Temperature coupled problem. This new scheme allows equal order of interpolation to approximate the quantities of interest, i.e. velocity, pressure, temperature, and stress. We analyze an equivalent variational formulation of the coupled problem inspired by the ideas proposed in [2]. The existence of the discrete solution is proved, decoupling the proposed stabilized scheme and using the help of continuous dependence results and Brouwer's theorem under the standard assumption of sufficiently small data. Optimal convergence is proved under classic regularity assumptions of the solution. Finally, we present some numerical examples to show the quality of our scheme, in particular, we compare our results with those coming from a standard reference in geosciences described in [5].

**Keywords**: Coupled Stokes–Temperature problem, Stabilized finite element method, A priori error analysis.

**Mathematics Subject Classifications (2010)**: 65L60.

## References

1. R. Araya, C. Cárcamo and C. A. H. Poza, *An adaptive stabilized finite element method for the Darcy's equations with pressure dependent viscosities*, Comput. methods Appl. Mech. Engrg. **387**, (2021). 114100.
2. M. Alvarez, G. N. Gatica and R. Ruiz–Baier, *An augmented mixed-primal finite element method for a coupled flow-transport problem*, ESAIM: M2AN **5**, (2015). 1399-1427.
3. L. P. Franca, S. L. Frey and T.J. R. Hughes, *Stabilized finite element methods. I. Application to the advective-diffusive model*, Comput. methods Appl. Mech. Engrg. **95**, (1992). 253-276.
4. L.P. Franca and R. Stenberg, *Error analysis of Galerkin least squares methods for the elasticity equations*, SIAM J. Numer. Anal. **28**, (1991). 1680-1697.
5. P. E. van Keken, C. Currie, S. D. King, M. D. Behn, A. Cagnioncle, J. He, R. F. Katz, SC. Lin, E. M. Parmentier, M. Spiegelman and K. Wang, *A community benchmark for subduction zone modeling*, Phys. Earth Planet. Inter. **171**, (2008). 187-197.

# Banach spaces-based fully mixed FEMs for the Boussinesq problem with temperature-dependent parameters

Gabriel N. Gatica[1], Zeinab Gharibi[2], and Ricardo Oyarzúa[3]

CI$^2$MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Casilla 160-C, Concepción, Chile, ggatica@ci2ma.udec.cl
CI$^2$MA and GIMNAP-Departamento de Matemática, Universidad del Bío-Bío, Casilla 5-C, Concepción, Chile zgharibi@ubiobio.cl
CI$^2$MA and GIMNAP-Departamento de Matemática, Universidad del Bío-Bío, Casilla 5-C, Concepción, Chile royarzua@ubiobio.cl

**Summary.** In this talk, we develop a family of Banach spaces-based approach yielding a fully-mixed finite element method to numerically solve the heat-driven flows with temperature- dependent viscosity modeled by the stationary Boussinesq equations. The momentum and energy conservation equations are formulated in terms of velocity and the tensors of strain rate, vorticity and stress, pseudoheat, temperature and its gradient; and the incompressibility constraint is used to eliminate the pressure, which is computed afterwards by a postprocessing formula depending on the stress and the velocity. The unique solvability of the continuous problem is addressed by invoking a global inf-sup property in an adequate abstract setting for perturbed saddle-point problems in Banach spaces and two assumptions further regularities on the solutions of the problem. Adopting an analogue approach for the associated Galerkin scheme, and under suitable hypotheses on arbitrary finite element subspaces employed, we show existence and then uniqueness of the discrete solution. In addition, the error analysis is conducted under appropriate assumptions on data and applying the first Strang lemma for the discrete solution as well as for the post-processed pressure. Finally, we report several numerical experiments.

**Keywords**: Boussinesq problem, temperature-dependent parameters, Banach spaces, fully mixed FEM, a priori error analysis.

**Mathematics Subject Classifications (2010)**: 65M12, 65M15, 65M60

## References

1. J.A. Almonacid, G. N. Gatica, R. Oyarzúa and R. Ruiz-Baier. A new mixed finite element method for the n-dimensional Boussinesq problem with temperature-dependent viscosity. *Netw. Heterog. Media.*, 15 (2):215–245, 2020.
2. G. N. Gatica and Z. Gharibi. A Banach spaces-based fully mixed virtual element method for the stationary two-dimensional Boussinesq equations. *Preprint 2023-17, Centro de Investigación en Ingeniería Matemática (CI$^2$MA), Universidad de Concepción(2023).*
3. R. Oyarzúa, T. Qin and D. Schötzau. *An exactly divergence-free finite element method for a generalized Boussinesq problem*, *IMA J. Numer. Anal.*, 34 (3):1104–1135, (2014).

# A mixed FEM for the coupled Brinkman–Forchheimer/Darcy problem

Sergio Caucao[1] and Marco Discacciati[2]

Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción, Casilla 297, Concepción, Chile, and Grupo de Investigación en Análisis Numérico y Cálculo Científico, GIANuC$^2$, Concepción, Chile
scaucao@ucsc.cl
Department of Mathematical Sciences, Loughborough University, Epinal Way, Loughborough LE11 3TU, UK
m.discacciati@lboro.ac.uk

**Summary.** This work develops the *a priori* analysis of a mixed finite element method for the filtration of an incompressible fluid through a non-deformable saturated porous medium with heterogeneous permeability. Flows are governed by the Brinkman–Forchheimer and Darcy equations in the more and less permeable regions, respectively, and the corresponding transmission conditions are given by mass conservation and continuity of momentum. We consider the standard mixed formulation in the Brinkman–Forchheimer domain and the dual-mixed one in the Darcy region, and we impose the continuity of the normal velocities by introducing suitable Lagrange multiplier. The finite element discretization involves Bernardi–Raugel and Raviart–Thomas elements for the velocities, piecewise constants for the pressures, and continuous piecewise linear elements for the Lagrange multiplier. Stability, convergence, and *a priori* error estimates for the associated Galerkin scheme are obtained. Numerical tests illustrate the theoretical results.

**Keywords**: Brinkman–Forchheimer problem, Darcy problem, pressure-velocity formulation, mixed finite element methods, *a priori* error analysis

**Mathematics Subject Classifications (2020)**: 65N30, 65N12, 65N15, 74F10, 76D05, 76S05.

## References

1. S. Caucao and M. Discacciati. A mixed FEM for the coupled Brinkman–Forchheimer/Darcy problem. *Applied Numerical Mathematics*, 190, 138–154, 2023.
2. S. Caucao, G.N. Gatica, and J.P. Ortega. A fully-mixed formulation in Banach spaces for the coupling of the steady Brinkman–Forchheimer and double-diffusion equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, 55, no. 6, 2725–2758, 2021.
3. M. Discacciati and R. Oyarzúa. A conforming mixed finite element method for the Navier–Stokes/Darcy coupled problem. *Numerische Mathematik*, 135, no. 2, 571–606, 2017.
4. C.A. Dumitrache and A. Petrache. Interface condition for the coupling of a fluid and porous media. *Acta Technica Napocensis, Series: Applied Mathematics and Mechanics*, 55, no. II, 2012.
5. M. Ehrhardt. Theory and Practice of Finite Elements. In *Coupled Fluid Flow in Energy, Biology and Environmental Research*, vol. 2. Bentham Books, pp. 3–12, 2012.
6. G.N. Gatica, S. Meddahi, and R. Oyarzúa. A conforming mixed finite-element method for the coupling of fluid flow with porous media flow. *IMA Journal of Numerical Analysis*, 29, no. 1, 86–108, 2009.
7. Y. Li, X. Chen, and J. Shi. Structural stability in resonant penetrative convection in a Brinkman–Forchheimer fluid interfacing with a Darcy fluid. *Applied Mathematics & Optimization*, 84, suppl. 1, S979–S999, 2021.

# Fully mixed methods for the coupled poroelasticity and Poisson−Nernst–Planck equations

Gabriel N. Gatica[1], Cristian Inzunza[2], and Ricardo Ruiz-Baier[3]

CI[2]MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Casilla 160-C, Concepción, Chile.
ggatica@ci2ma.udec.cl
CI[2]MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Casilla 160-C, Concepción, Chile.
crinzunza@udec.cl
School of Mathematics, Monash University, 9 Rainforest Walk, Melbourne VIC 3800, Australia.
ricardo.ruizbaier@monash.edu

**Summary.** We introduce and analyze a Banach space-based approach yielding a fully-mixed finite element method for numerically solving the Biot poroelasticity and Poisson–Nernst–Planck equations. For the poroelasticity we consider a four-field formulation, whose primary variables are the solid displacement, the fluid pressure, the fluid flux, and the total pressure. In turn, besides the electrostatic potential and the concentration of ionized particles, we introduce as new unknowns its gradients and the total ionic fluxes. The resulting continuous formulation, posed in suitable Banach spaces, consists of a coupled system of two saddle point-type problems, for the poroelasticity and Poisson equations, and a twofold saddle-point problem for the ionized particles concentration equations. The well-posedness of it is then analyzed by applying the classical Banach fixed point theorem, along with a smallness assumption on the data, the Babuška–Brezzi theory in Banach spaces, and a slight variant of a recently obtained solvability result for perturbed saddle point formulations in Banach spaces as well. The associated Galerkin schemes are addressed similarly, and the Brouwer theorem yields the existence of discrete solutions. A priori error estimates are derived for both approaches, and rates of convergence for specific finite element subspaces satisfying the required discrete inf-sup conditions, are established in 2D. Finally, several numerical examples illustrating the performance of the two methods and confirming the theoretical findings, are reported.

**Keywords**: Biot problem; Poisson–Nernst–Planck problem; Mixed finite elements; Fixed point.

**Mathematics Subject Classifications (2020)**: 35J66, 65N30, 65N12, 76S05.

## References

1. C.I. Correa, G.N. Gatica, R. Ruiz-Baier, *New mixed finite element methods for the coupled Stokes and Poisson-Nernst-Planck equations in Banach spaces.* ESAIM Math. Model. Numer. Anal. 57 (2023), 1511-1551.
2. S. Kumar, R. Oyarzúa, R. Ruiz-Baier, R. Sandilya *Conservative discontinuous finite volume and mixed schemes for a new four-field formulation in poroelasticity,* ESAIM Math. Model. Numer. Anal. 54 (2020), no. 1, 273-299.

# Robust finite element methods and solvers for the Biot-Brinkman Equations in vorticity form

Ruben Caraballo[1], Chansophea Wathanak In[2], Alberto F. Martín[3], and Ricardo Ruiz-Baier[4]

GIMNAP, Departamento de Matemática, Universidad del Bío-Bío, Concepción, Chile
ruben.caraballo1801@alumnos.ubiobio.cl
School of Mathematics, Monash University, 9 Rainforest Walk, Melbourne, Victoria 3800, Australia
cwin18@student.monash.edu
School of Computing, Australian National University, Acton ACT 2601, Australia
alberto.f.martin@anu.edu.au
School of Mathematics, Monash University, 9 Rainforest Walk, Melbourne, Victoria 3800, Australia; and Universidad Adventista de Chile, Casilla 7-D, Chillán, Chile
ricardo.ruizbaier@monash.edu

**Summary.** This presentation discusses a novel approach and a finite element technique tailored for the stable coupling of viscous fluid flow within deformable porous materials using divergence-conforming filtration fluxes. The suggested method relies on utilizing spaces weighted by parameters, enabling a more precise and resilient examination of both continuous and discrete problems. Additionally, we perform an analysis of the method's solvability and establish optimal error estimates within suitable norms. These error estimates are demonstrated to remain reliable even when dealing with high Lamé parameters and low permeability and storativity coefficients. To showcase the effectiveness of this approach, we offer several illustrative numerical instances, including verification of convergence, simulation of poroelastic channel flow, and an assessment of the resilience of block-diagonal preconditioners concerning model parameters.

**Keywords**: Biot-Brinkman coupled problem; deformable porous media; vorticity-based formulation; mixed finite element methods.

**Mathematics Subject Classifications (2010)**: 65N30, 65N15, 76S05, 35Q74.

## References

1. M. Amara, E. Chacón Vera, and D. Trujillo, *Vorticity–velocity–pressure formulation for Stokes problem*. Math. Comp., **73**(248) (2004) 1673–1697.
2. V. Anaya, M. Bendahmane, D. Mora, and R. Ruiz-Baier, *On a vorticity-based formulation for reaction-diffusion-Brinkman systems*. Netw. Heterog. Media, **13**(1) (2018) 69–94.
3. S. Badia, A. F. Martín, and R. Planas, *Block recursive LU preconditioners for the thermally coupled incompressible inductionless MHD problem*. J. Comput. Phys., **274** (2014), 562–591.
4. S. Badia and F. Verdugo, *Gridap: An extensible finite element toolbox in julia*. J. Open Source Softw., **5** (2020), 2520.
5. S. Badia, A. F. Martín, and F. Verdugo, *GridapDistributed: a massively parallel finite element toolbox in Julia*, J. Open Source Softw., **7**(74) (2022), 4157.
6. T. Bærland, M. Kuchta, K.-A. Mardal, and T. Thompson, *An observation on the uniform preconditioners for the mixed Darcy problem*, Numer. Methods PDEs, **36**(6) (2020), 1718–1734.
7. W. Boon, M. Kuchta, K.-A. Mardal, and R. Ruiz-Baier, *Robust preconditioners and stability analysis for perturbed saddle-point problems – application to conservative discretizations of Biot's equations utilizing total pressure*, SIAM J. Sci. Comput., **43** (2021) B961–B983.

# Equal-order finite element method for the Stokes equations with variable viscosity

Abner H. Poza[1] and Ramiro Rebolledo[2]

Universidad Católica de la Santísima Concepción, Concepción, Chile.
apoza@ucsc.cl
Facultad de Ingeniería Agrícola, Universidad de Concepción, Chillán, Chile
ramirorebolledo@udec.cl

**Summary.** In this talk, we discuss the outcomes of [3]. This work builds upon the work outlined in [1], which uses a Taylor–Hood scheme to study the Stokes equations with variable viscosity. Our approach employs a stabilized finite element scheme based on the Galerkin Least Squares method, utilizing equal-order polynomials to approximate both velocity and pressure. The challenge in this study stems from the significant variation in viscosity spanning several orders of magnitude, that appears in some applications as models for the simulation of mantle convection (see, for example, [2]). We address this challenge by establishing optimal *a priori* error estimates for our novel stabilized scheme, which we subsequently validated through numerical tests.

**Keywords**: Non-newtonian flow, incompressible Stokes equations, variable viscosity, stabilized finite element method, dependency on the viscosity.

**Mathematics Subject Classifications (2010)**: 65L60.

## References

1. V. John, K. Kaiser and J. Novo. Finite element methods for the incompressible Stokes equations with variable viscosity ZAMM:*Journal of Applied Mathematics and Mechanics*, 96(2):205-216, 2016.
2. M. Kronbichler, T. Heister and W. Bangerth. High accuracy mantle convection simulation through modern numerical methods *Geophysical Journal International*, 191(1):12-29, 2012.
3. A.H. Poza and R. Rebolledo. Equal-order finite element method for the Stokes equations with variable viscosity *Applied Mathematics Letters*, (submitted).

# MS13: Numerical methods for mineral processing, wastewater treatment, and related applications

# Robust superlinear schemes based on adaptive linearization for solving Richards' equation

Guillermo Albuja[1], Andrés I. Ávila[2], and Miguel Murillo[3]

Facultad de Ciencias, Universidad Central del Ecuador, Quito, 170129, Ecuador
gaalbuja@uce.edu.ec
Departmento de Ingeniería Matemática, Universidad de La Frontera, Temuco, Chile
andres.avila@ufrontera.cl
Facultad de Ciencias, Universidad Central del Ecuador, Quito, 170129, Ecuador
mamurillo@uce.edu.ec

**Summary.** The Richards' equation is a nonlinear degenerate parabolic differential equation with no known analytical solution. Implicit methods are used to obtain nonlinear systems and the linearization methods are necessary. Two of the most valuable linearization schemes are Newton's method, which is it is quadratically, but only locally convergent, and the *L*-scheme, which is linear and global convergent. Also, mixed schemes combine both methods to obtain global quadratically convergent schemes without a clear rule to switch from one to the other.

Using the local error, we develop four finite element adaptive schemes using a convex combination of two types of linearizations schemes: one global and another local convergent. The first case combines the *L*-scheme with Newton's scheme (ALN). For the second case, we first develop an adaptive type-Secant scheme (AtS), which does not compute the derivative, but it is still locally convergent. Next, we use the adaptive convex combination of the *L*-scheme with the type-Secant scheme to obtain a global superlinear convergent scheme (ALS). Finally, the fourth scheme considers an adaptive step size approach of the ALN scheme (ASSLN). We test the four schemes with five examples showing that our schemes are robust, fast, and converge when Newton's scheme does not. Moreover, we consider Gardner exponential nonlinearities and we show that *L*-scheme and *L*2-scheme are too slow as linearization techniques.

**Keywords**: Linearization schemes, Newton method, Degenerate nonlinear equations, Global convergence.

**Mathematics Subject Classifications (2010)**: 65M30, 49M15, 76S05, 35K65.

## References

1. L.A. Richards. Capillary conduction of liquids through porous mediums. *Physics*, 1(5), 318-333, 1931
2. K. Lust and D. Roose. An adaptive Newton–Picard algorithm with subspace iteration for computing periodic solutions. SIAM *Journal on Scientific Computing*, 19(4), 1188-1209, 1998.
3. L. Bergamaschi and M. Putti. Mixed finite elements and Newton-type linearizations for the solution of Richards' equation. *International Journal for Numerical Methods in Engineering*, 45(8), 1025-1046, 1999.
4. D. Kavetski, P. Binning, and S.W. and Sloan. Adaptive time stepping and error control in a mass conservative numerical solution of the mixed form of Richards equation. *Advances in Water Resources*, 24(6), 595-605, 2001.
5. M. Slodicka. A robust and efficient linearization scheme for doubly nonlinear and degenerate parabolic problems arising in flow in porous media. SIAM *Journal on Scientific Computing*, 23(5), 1593-1614, 2002.
6. I.S. Pop, M. Sepúlveda, F.A. Radu, and O.V. Villagrán. Error estimates for the finite volume discretization for the porous medium equation. *Journal of Computational and Applied Mathematics*, 234(7), 2135-2142, 2010.
7. M. Kuráž, P. Mayer, M. Lepš, and D. Trpkošová. An adaptive time discretization of the classical and the dual porosity model of Richards' equation. *Journal of Computational and Applied Mathematics*, 233(12), 3167-3177, 2010.
8. I.S. Pop and B. Schweizer. Regularization schemes for degenerate Richards equations and outflow conditions. *Mathematical Models and Methods in Applied Sciences*, 21(08), 1685-1712, 2011.
9. I.K. Argyros, Y.J. Cho, and S.K. Khattri. On the convergence of Broyden's method in Hilbert spaces. *Applied Mathematics and Computation*, 242, 945-951, 2014.
10. F. List and F.A. Radu. A study on iterative methods for solving Richards' equation. *Computational Geosciences*, 20, 341-353, 2016.

11. V. Baron, Y. Coudière, and P. Sochala. Adaptive multistep time discretization and linearization based on a posteriori error estimates for the Richards equation. *Applied Numerical Mathematics*, 112, 104-125, 2017.
12. J.W. Both, K. Kumar, J.M. Nordbotten, I.S. Pop, and F.A. Radu. Iterative linearisation schemes for doubly degenerate parabolic equations. In *Numerical Mathematics and Advanced Applications* ENUMATH 2017 (pp. 49-63). Springer International Publishing.
13. M. Amrein. A global Newton-type scheme based on a simplified Newton-type approach. *Journal of Applied Mathematics and Computing*, 65(1-2), 321-334, 2021.

# Steady states of a continuous model describing countercurrent decantation

Juan D. Barajas[1], Raimund Bürger[2], Stefan Diehl[3], and Luis Miguel Villada[4]

Universidad del Bío-Bío
juan.barajas2001@alumnos.ubiobio.cl
Universidad de Concepción
rburger@ing-mat.udec.cl
Lund University
stefan.diehl@math.lth.se
Universidad del Bío-Bío
lvillada@ubiobio.cl

**Summary.** In this work, we study the modeling and numerical analysis of the solid-liquid separation process in a countercurrent decantation circuit. The liquid-solid separation is a fundamental part of many processes of hydrometallurgical treatments, in which liquids or settlings have to be recovered with the best possible quality. A system of conservation laws with discontinuous flux in space is proposed to describe the CTs that make up the CCD circuit network, with source term describing the coupling between the different tanks. A particular kind of steady states solutions are studied. Conditions on the control variables are obtained for all units involved in the CCD to be in optimal operation. Some numerical simulations illustrate the behavior of the solutions in particular cases.

**Keywords**: Conservation laws with discontinuous flux, Countercurrent decantation, Steady states, Finite volume method.

**Mathematics Subject Classifications (2010)**: 35L40, 35L65, 65M08, 76T20.

## References

1. R. Bürger, K.H Karlsen, N.H. Risebro, and J.D. Towers. Well-posedness in $BV_t$ and convergence of a difference scheme for continuous sedimentation in ideal clarifier-thickener units. *Numerische Mathematik*, 97:25-65, 2004.
2. S. Diehl. A conservation law with point source and discontinuous flux function modelling continuous sedimentation. *SIAM Journal on Applied Mathematics*, 56:388-419, 1996.
3. S. Diehl. Operating charts for continuous sedimentation I: Control of steady states. *Journal of Engineering Mathematics*, 41:117–144, 2001.

# Froth flotation with drainage: model and steady-state solutions analysis.

Raimund Bürger[1], Stefan Diehl[2], M. Carmen Martí[3], and Yolanda M. Vásquez[4]

CI[2]MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Chile
rburger@ing-mat.udec.cl
Centre for Mathematical Sciences, Lund University, Sweden
stefan.diehl@math.lth.se
Departamento de Matemáticas, Universitat de València, Spain
maria.c.marti@uv.es
Departamento de Ciencias Exactas, Universidad Tecnológica de Panamá, Panamá
yolanda.vasquez@utp.ac.pa

**Summary.** Froth flotation is a common unit operation used in mineral processing to separate valuable mineral particles from worthless gangue particles in finely ground ores. In it, the valuable mineral particles attach to bubbles of air that rise to the top of the column where they are removed, while the gangue particles settle to the bottom of the tank. For the efficiency of the process, it is important that a layer of froth develops near the top of the column. This froth layer works as a filter enhancing the separation process but also reduces the amount of water present in the effluent. In this talk, we will focus on the model for froth flotation introduced in [1], that includes the drainage of liquid occurring at the top of the column, where a froth layer rich in valuable minerals is created. We will detail the construction of steady-state solutions and provide algebraic equations and inequalities that establish the dependence of steady states on the input and control variables.

**Keywords**: froth flotation; sedimentation; drainage; capillarity; three-phase flow; conservation law; second-order degenerate parabolic PDE; steady states.

**Mathematics Subject Classifications (2010)**: 35L65, 35R05, 76T10

## References

1. R. Bürger, S. Diehl, M.C. Martí and Y. Vásquez. A degenerating convection-diffusion system modelling froth flotation with drainage. IMA *J. Appl. Math.*, 87:1151-1190, 2022.

# Front tracking and parameter identification for a conservation law with a space-dependent coefficient modeling granular segregation

Raimund Bürger[1], Yesennia Martínez[2], and Luis Miguel Villada[3]

CI[2]MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Concepción, Chile
rburger@ing-mat.udec.cl
CI[2]MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Concepción, Chile
yesmartinez@udec.cl
CI[2]MA, Universidad de Concepción, and Departamento de Matemática, Universidad del Bío-Bío, Concepción, Chile
lvillada@ubiobio.cl

**Summary.** A well-known experimental setup for the study of segregation by size in a dry granular medium consists of two layers of spheres composed of large and small rigid spheres within an annular region of concentric cylinders covered above and below by plates. As one of the cylinders is rotated and thereby applies shear to the granular mixture, the spheres mix and the large spheres rise while the small ones settle in vertical direction. An established model for this phenomenon of segregation by size [2] can be written as a conservation law whose flux involves a piecewise constant or smooth coefficient that describes dependence of the shear rate on depth. This model can be solved by the hyperfast front tracking method suitably adapted to handle a conservation law with discontinuous flux. It is demonstrated how the problem of identification of the mentioned coefficient from experimental observations can be solved efficiently by the front tracking method. The aim of this paper is to show the efficiency of the Front Trancking method against a numerical scheme, in our case we chose Engquist-Osher, for the identification of parameters in an inverse problem that models the phenomenon of granular flow segregation. Numerical examples are presented for direct and inverse problem.

**Keywords**: Granular media, segregation, conservation law, discontinuous flux, front tracking method, parameter identification

## References

1. R. Bürger. Introducción a Leyes de Conservación. *Centro de Investigación en Ingeniería Matemática, Universidad de Concepción*, 2021.
2. L. May, M. Shearer, and K. Daniels. Scalar conservation laws with nonconstant coefficients with application to particle size segregation in granular flow. *J. Nonlinear Sci*, 20:689-707, 2010.
   2008.
3. H. Risebro. An introduction to the theory of scalar conservation laws with spatially discontinuous flux functions. *Applied Wave Mathematics: Selected Topics in Solids, Fluids, and Mathematical Methods*, 395-464, 2009.

# Froth flotation with drainage: numerical method and simulations.

Raimund Bürger[1], Stefan Diehl[2], M. Carmen Martí[3], and Yolanda M. Vásquez[4]

CI[2]MA and Departamento de Ingeniería Matemática, Universidad de Concepción, Chile
rburger@ing-mat.udec.cl
Centre for Mathematical Sciences, Lund University, Sweden
stefan.diehl@math.lth.se
Departamento de Matemáticas, Universitat de València, Spain
maria.c.marti@uv.es
Departamento de Ciencias Exactas, Universidad Tecnológica de Panamá, Panamá
yolanda.vasquez@utp.ac.pa

**Summary.** Froth flotation is a common unit operation used in mineral processing [2, 5]. It serves to separate valuable mineral particles from worthless gangue particles in finely ground ores. The drainage of liquid due to capillarity is essential for the formation of a stable froth layer [3, 4]. A monotone numerical scheme is derived and employed to simulate the dynamic behaviour of a flotation column [1], under variable operating conditions such as control actions that drive the process to desired states of operation. It is also proven that, under a suitable Courant-Friedrichs-Lewy (CFL) condition, the approximate volume fractions are bounded between zero and one when the initial data are. Dynamic simulations are obtained with the numerical method.

**Keywords**: froth flotation; sedimentation; drainage; capillarity; three-phase flow; conservation law; numerical simulations.

**Mathematics Subject Classifications (2010)**: 35L65, 35R05, 76T10

## References

1. R. Bürger, S. Diehl, M.C. Martí and Y. Vásquez. A degenerating convection-diffusion system modelling froth flotation with drainage. IMA *J. Appl. Math.*, 87:1151-1190, 2022.
2. J.A. Finch and G.S. Dobby, *Column Flotation*, Pergamon Press, London, UK, 1990.
3. S.J. Neethling and J.J. Cilliers, Modelling flotation froths, *Int. J. Mineral Process.* **72** (2003), 267–287.
4. S.J. Neethling and P.R. Brito-Parada, Predicting flotation behaviour — The interaction between froth stability and performance, *Minerals Eng.* **120** (2018), 60–65.
5. P. Quintanilla, S.J. Neethling, and P.R. Brito-Parada. Modelling for froth flotation control: A review. *Minerals Eng.* **162** (2021), paper 106718.

# Coupled finite volume and mixed finite element methods for the viscous model of sedimentation

Julio Careaga[1] and Gabriel N. Gatica[2]

Universidad del Bío-Bío, Chile
jcareaga@ubiobio.cl
Universidad de Concepción, Chile
ggatica@ci2ma.udec.cl

**Summary.** A numerical scheme combining finite volume and mixed finite element methods for the so-called viscous model of sedimentation is presented. A particular feature of the governing equations is given by the fact that the velocity field is non-divergence free. We introduce extra variables such as the pseudostress tensor relating the velocity gradient with the pressure, thus leading to a mixed variational formulation consisting of two systems of equations coupled through their source terms. A result of existence and uniqueness of solutions is shown by means of a fixed-point strategy and the help of the Babuška-Brezzi theory and Banach theorem. Additionally, we employ suitable finite dimensional subspaces to approximate both systems of equations via associated mixed finite element methods. The well-posedness of the resulting coupled scheme is also treated via a fixed-point approach, and hence the discrete version of the existence and uniqueness result is derived analogously to the continuous case. The above is then combined with a finite volume method for the transport equation. Finally, several numerical results illustrating the performance of the proposed model and the full numerical scheme, and confirming the theoretical rates of convergence, are presented.

**Keywords**: solid phase velocity, multidimensional sedimentation, mixed finite elements, fixed-point problem

**Mathematics Subject Classifications (2010)**: 35Q70, 65M08, 65N12, 65N15, 65N30, 70-08, 76T20

## References

1. J. Careaga, and G.N. Gatica. Coupled mixed finite element and finite volume methods for a solid velocity-based model of multidimensional settling. ESAIM: *Mathematical Modelling and Numerical Analysis*, 57(4):2529-2556, 2023.

# A mathematical-ecological model of biofilm growth in slow sand filters

Stefan Diehl[1], Jaime Manríquez[2], Catherine J. Paul[3], and Tage Rosenqvist[4]

Centre for Mathematical Sciences, Lund University, P.O. Box 118, S-221 00 Lund, Sweden
stefan.diehl@math.lth.se
Centre for Mathematical Sciences, Lund University, P.O. Box 118, S-221 00 Lund, Sweden
jaime.manriquez@math.lth.se
Division of Applied Microbiology, Department of Chemistry, Lund University, P.O. Box 124, SE-221 00 Lund, Sweden
catherine.paul@tvrl.lth.se
Division of Applied Microbiology, Department of Chemistry, Lund University, P.O. Box 124, SE-221 00 Lund, Sweden
tage.rosenqvist@tmb.lth.se

**Summary.** Slow Sand Filtration (SSF) is a type of water purification system that consists of a sand bed that acts both as a physical filter and as a settling zone for biological agents to attach and develop a biofilm layer capable of acting as a biological filter. This biofilm layer, usually called *Schmutzdecke*, constitutes the heart of the system and develops in the top 2–5 cm of the sand, growing up to a couple of centimeters above it [4, 3], where it acts as the major pathogen removal mechanism in the filter.

Although SSF has been used for more than two centuries, with early uses reported in the UK in 1804 [2], a comprehensive PDE model for the entire filter is not yet readily available, with most models using either only ODEs or simple diffusion equations. Since it is almost impossible to measure concentrations inside the filter, as it would disrupt the ecosystem formed inside [1], a mathematical model must be developed from physical principles and be flexible enough to account for different ecological models and the change of bacterial population in the filter.

To that end, in this work we have developed a comprehensive model that considers physical mechanisms (e.g. attachment, diffusion, and adsorption) and biological ones (e.g. grazing, photosynthetic growth and death), taking also into account the viscoelastic properties of the biofilm, the movement and growth in the supernatant water of the filter is modeled by a Cahn-Hilliard type PDE. We have implemented a numerical scheme based on a finite differences discretization in space and a semi-implicit method in time, resulting in a splitting scheme between the Cahn-Hilliard type equation in the supernatant water and a system of balance laws throughout the filter. A positivity bound on the time step-size for the balance law system allows us to define an adaptive time step scheme to speed up computations. Simulation results are consistent with the qualitative description of the behaviour of a filter and some scenario simulations under different weather conditions are shown.

**Keywords**: biofilm, drinking water treatment, partial differential equations, slow sand filtration

**Mathematics Subject Classifications (2010)**:

## References

1. F. Hammes, S. Velten, T. Egli, and T. Juhna. 6.41- Biotreatment of drinking water. Comprehensive Biotechnology, pages 517–530. Academic Press, Burlington, secondedition edition, 2011.
2. John K. Maiyo, Sruthi Dasika, and Chad T. Jafvert. Slow sand filters for the 21st century: A review. *Int. J. Environ. Res. Public Health*, 20(2):1019, Jan 2023.
3. Ni' matuzahroh, Nurina Fitriani, Putri Eka Ardiyanti, Eko Prasetyo Kuncoro, Wahid Dian Budiyanto, Dwi Ratri Mitha Isnadina, Febri Eko Wahyudianto, and Radin Maya Saphira Radin Mohamed. Behavior of schmutzdecke with varied filtration rates of slow sand filter to remove total coliforms. *Heliyon, 6(4): e03736*, 2020.
4. Prem Ranjan and Manjeet Prem. Schmutzdecke-A Filtration Layer of Slow Sand Filter. *Int. J. Curr. Microbiol. Appl. Sci.*, 7(07):637-645, 2018.

# Finite volume method in tsunami models and coastal forest interaction

Jorge Moya[1]

Universidad de Concepción
jorgemoya@udec.cl

**Summary.** This research is focused on modeling tsunamis and exploring the potential of coastal vegetation as a means of mitigation. To simulate tsunami propagation and coastal inundation, we employed finite volume methods combined with projection methods for the non-hydrostatic pressure, as described in [1]. The study was validated using field data and experimental observations.

In order to achieve that, we use a multilayer system based on the $\text{LDNH}_0$ model, which approximates the Euler equations under the assumptions of constant velocities and linear pressures [2]. In addition of that we add drag forces, inertia forces, and porosity to model the interaction with the forest, based on [3], and extended them to make them compatible with multilayer systems. This manner, we can more precisely model the vertical properties of the forest, making multilayer systems a valuable tool for future research in this field.

Our partial findings suggest that depending of the vegetation characteristics such as density, height, wood type, and arrangement, coastal vegetation can provide significant mitigation effects for tsunamis and be an effective natural defense against coastal hazards. This research has important implications for coastal planning, management and provides valuable insights into the potential role of ecosystem-based approaches for disaster risk reduction. This is a joint work with Dr. Fernandez-Nieto and Raimund Bürger. Partially supported by ANID/Doctorado Nacional/21211457.

**Keywords**: Tsunami Coastal vegetation Numerical simulation

**Mathematics Subject Classifications (2010)**:

## References

1. MANUEL CASTRO, ENRIQUE FERNANDEZ-NIETO, *A Class of Computationally Fast First Order Finite Volume Solvers: PVM Methods*, SIAM Journal on Scientific Computing, Volume 34, Issue 4, 2012
2. SÁNCHEZ, C.E., FERNÁNDEZ-NIETO, E.D., DE LUNA, T.M. ET AL *Numerical Simulations of a Dispersive Model Approximating Free-Surface Euler Equations* J Sci Comput 89, 55 (2021). https://doi.org/10.1007/s10915-021-01552-6
3. KOSUKE IIMURA, NORIO TANAKA *Numerical simulation estimating effects of tree density distribution in coastal forest on tsunami mitigation* Ocean Engineering, Volume 54, 1 November 2012, Pages 223-232.

# Implicit-explicit schemes for the compressible Cahn-Hilliard-Navier-Stokes equations

Pep Mulet[1]

University of Valencia
mulet@uv.es

**Summary.** In [4] a spinodal decomposition, governed by the Cahn-Hilliard equation [2], is conjectured as the underlying mechanism that explains the layered sedimentations of monodisperse colloidal particles.

Since the Cahn-Hilliard equation cannot explain this phenomenon by itself, the gravitational force is introduced into the model by means of conservation of mass and momentum, which, together with conservation of individual species and ignoring temperature changes, yields a system of equation, the isothermal Navier-Stokes-Cahn-Hilliard equations [3, 1], which are a system of fourth-order partial differential equations that model the evolution of mixtures of binary fluids under gravitational effects.

Although incompressible models for these equations might be more suitable for explaining the cited layering phenomenon, we consider the compressible case for the evolution of, e.g. foams, solidification processes, fluid–gas interface.

The aim of this work is to design implicit-explicit time-stepping schemes to avoid the severe restriction posed by the high order terms for the efficient numerical solution of boundary-initial problems with these equations.

**Keywords**: Cahn-Hilliard-Navier Stokes equations, spinodal decomposition, implicit-explicit schemes

**Mathematics Subject Classifications (2010)**: 65M06 (35K57 35K59 35L65 76M20)

## References

1. Helmut Abels and Eduard Feireisl. On a diffuse interface model for a two-phase flow of compressible viscous fluids. *Indiana Univ. Math. J.*, 57(2):659–698, 2008.
2. JW Cahn and JE Hilliard. Free energy of a nonuniform system .3. nucleation in a 2-component incompressible fluid. *J. Chem. Phys.*, 31(3):688–699, 1959.
3. J. Lowengrub and L. Truskinovsky. Quasi-incompressible Cahn-Hilliard fluids and topological transitions. *Proc. Royal Soc. A*, 454(1978):2617–2654, 1998.
4. Donald B. Siano. Layered sedimentation in suspensions of monodisperse spherical colloidal particles. *J. Colloid and Interface Sci.*, 68(1):111–127, 1979.

# MS14: Numerical methods for particulate and non-newtonian flows

# A Dual-Mixed Approximation for a Huber Regularization of Viscoplastic Flow Problems.

Sergio González-Andrade[1] and Paul E. Méndez[2]

Research Center on Mathematical Modeling (MODEMAT) and Departamento de Matemática - Escuela Politécnica Nacional, Quito, Ecuador.
sergio.gonzalez@epn.edu.ec
Research Center on Mathematical Modeling (MODEMAT) - Escuela Politécnica Nacional, Quito, Ecuador.
paul.mendez01@epn.edu.ec

**Summary.** In the present study, we introduce a dual-mixed formulation tailored to address stationary viscoplastic flows exhibiting yield behavior, exemplified by the Bingham or Herschel-Bulkley flow models. Our approach is rooted in the Huber regularization of the viscosity term, culminating in a two-fold saddle-point nonlinear operator equation governing the resultant weak formulation. We establish the existence and uniqueness of solutions within the continuous framework and advance a discrete computational strategy based in Arnold-Falk-Winther finite elements. This discretization strategy yields a system of nonlinear equations characterized by slant differentiability. To address these nonlinearities, we propose and implement a semismooth Newton algorithm. Furthermore, we present an *a priori* error analysis for the Bingham case. To demonstrate the efficacy and robustness of our methodology, we present a series of numerical experiments, providing insights into the method's performance and behavior.

**Keywords**: Viscoplastic fluids, Dual-mixed methods, Twofold saddle point, Semismooth Newton methods.

**Mathematics Subject Classifications (2010)**: 76A05, 49M29, 47A52, 76M10.

## References

1. S. González-Andrade and P. E. Méndez, *A dual-mixed approximation for a Huber regularization of generalized p-Stokes viscoplastic flow problems*. Comput. Math. Appl. 112 (2022), 76–96.
2. Gatica, Gabriel. *Solvability and Galerkin Approximations of a Class of Nonlinear Operator Equations*. Zeitschrift Für Analysis Und Ihre Anwendungen 21, no. 3 (2002): 761–81.
3. Ervin, Vincent J., Jason S. Howell, and Iuliana Stanculescu. *A Dual-Mixed Approximation Method for a Three-Field Model of a Nonlinear Generalized Stokes Problem*. Computer Methods in Applied Mechanics and Engineering 197, no. 33–40 (June 2008): 2886–2900.

# A comprehensive parametric study of LBM-DEM for immersed granular lows

Geng Chao Yang[1], Lu Jing[2], Chung Yee Kwok[3], and Yuri Dumaresq Sobral[4]

School of Aeronautics and Astronautics, Sun Yat-sen University, Shenzhen, China
yanggch8@sysu.edu.cn
Tsinghua Shenzhen International Graduate School, Tsinghua University, Shenzhen, China
lujing@sz.tsinghua.edu.cn
Department of Civil Engineering, The University of Hong Kong, Hong Kong
fkwok8@hku.hk
Departamento de Matemática, Universidade de Brasília, Brasília, Brazil
ydsobral@unb.br

**Summary.** Simulating the flow of particles fully immersed in a fluid is a difficult computational problema and, despite all the progress that has been achieved in the field, there is still a concern about the accuracy of predictive models for immersed granular flows, especially when complex fluid-particle interactions play a non-negligible role in the dynamics of the flow. In this work, we present a detailed parametric study of a fluid-particle computational model that couples the Lattice Boltzmann Method (LBM) with the Discrete Element Method (DEM) using an immersed moving boundary technique [1, 2, 3]. Benchmark cases with increasing complexity are simulated to understand the numerical accuracy, stability and efficiency of the algorithm. A guideline for a high-quality LBM-DEM model is proposed and applied to a test case of granular collapse in water. The simulation result shows excellent agreement with experiments, which demonstrates the capability of LBM-DEM to describe the dynamics of densely packed and friction dominant immersed granular flows, highlighting its potential to study geophysical mass movements [4].

**Keywords**: Immersed moving boundary, Granular collapse, discrete element method, Verlet, Lattice-Boltzmann

**Mathematics Subject Classifications (2010)**: 76T25, 76M28.

## References

1. S. Chen, G.D. Doolen Lattice Boltzmann method for fluid flows *Ann Rev Fluid Mech*, 30(1), 329-64, 1998.
2. P.A. Cundall, O.D.L. Strack A discrete numerical model for granular assemblies *Geotechnique*, 29(1), 47-65, 1979.
3. D.R. Noble, J.R. Torczynski A Lattice-Boltzmann method for partially saturated computational cells. *Int J Modern Phys C*, 09(08), 1189-201, 1998.
4. G.C. Yang, L. Jing, C.Y. Kwok, , Y.D. Sobral A comprehensive parametric study of LBM-DEM for immersed granular flows *Computers and Geotechnics*, 114, 103100, 2019.

# A mollified version of the Kuwabara-Kono model for 2nd order convergence in DEM

Gabriel Nóbrega Bufolo[1] and Yuri Dumaresq Sobral[2]

Departamento de Matemática/UnB, Brasília, DF
gbufolo7@gmail.com
Departamento de Matemática/UnB, Brasília, DF
ydsobral@unb.br

**Summary.** The Discrete Element Method (DEM) is a technique widely used to simulate multi particle systems, in particular granular materials [1]. For conservative systems, the integration of the equations of motions is often performed via a Verlet-type method of order two [2]. However, when dissipative forces are included, such as in simulations of granular materials, the Verlet method no longer behaves as a second order method. For instance, when using the popular Kuwabara-Kono force scheme [3], the order of the Verlet method decreases to 1.5. In this work, we propose a regularization of the Kuwabara-Kono force model via mollification. We show numerically that the Verlet method combined with this regularized force model can integrate collisions with second order accuracy and that the coefficient of restitution of the system tends to increase as a function of the regularization parameter.

**Keywords**: discrete element method, Verlet Method, Kuwabara-Kono force, mollifier

**Mathematics Subject Classifications (2010)**: 76T25, 65L05, 65L70.

## References

1. P.A. Cundall; O.D.L. Strack A discrete numerical model for granular assemblies *Geotechnique*, 29(1), 47-65, 1979.
2. E. Hairer; C. Lubich; G. Wanner Geometric numerical integration illustrated by the Störmer–Verlet method *Acta Numerica*, 399–450, 2003.
3. G. Kuwabara; K. Kono Restitution Coefficient in a Collision between Two Spheres *Japanese Journal of Applied Physics*, 26, 1230–1233, 1987.

# $\phi$-FEM: an optimally convergent and easily implementable immersed boundary method for particulate flows and Stokes equations

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

MIMESIS team, Inria Nancy - Grand Est, MLMS team, Université de Strasbourg, France.
michel.duprez@inria.fr
IMAG, Univ Montpellier, CNRS, Montpellier, France.
vanessa.lleras@umontpellier.fr
Université de Franche-Comté, Laboratoire de Mathématiques de Besançon, UMR CNRS 6623, 16, route de Gray 25000 Besançon, France.
alexei.lozinski@univ-fcomte.fr

**Summary.** In this talk, we will present an immersed boundary method to simulate the creeping motion of a rigid particle in a fluid described by the Stokes equations discretized thanks to a finite element strategy on unfitted meshes, called $\phi$-FEM, that uses the description of the solid with a level-set function. One of the advantages of our method is the use of standard finite element spaces and classical integration tools, while maintaining the optimal convergence (theoretically in the $H^1$ norm for the velocity and $L^2$ for pressure; numerically also in the $L^2$ norm for the velocity). We will finish with some numerical illustrations.

**Keywords**: Finite element method, numerical analysis, fictitious domain, immersed boundary method, level-set

**Mathematics Subject Classifications (2010)**: 65N30, 65N85, 65N15

## References

1. M. Duprez, A. Lozinski. $\phi$-FEM: a finite element method on domains defined by level-sets *SIAM J. Numer. Anal.*, 58(2):1008-1028, 2020.
2. S. Cotin, M. Duprez, V. Lleras, A. Lozinski and K. Vuillemot. $\phi$-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, Nov 2022.
3. M. Duprez, V. Lleras, A. Lozinski. *$\phi$-FEM: an optimally convergent and easily implementable immersed boundary method for particulate flows and Stokes equations*. *ESAIM: M2AN*, 57:1111-1142, 2023.

# A numerical solution for the saturated wave regime in fluidised beds

Saulo Rodrigo Medrado[1] and Yuri Dumaresq Sobral[2]

Departamento de Matemática, Universidade de Brasília, Brazil
200105639@aluno.unb.br
Departamento de Matemática, Universidade de Brasília, Brazil
ydsobral@unb.br

, Yuri@Sobral, Yuri

**Summary.** Fluidised beds are systems in which a set of particles is suspended by an upward fluid that flows through them. The particles in these flows are modelled as a continuum so that the system can be described by a set of averaged equations composed of continuity and momentum equations for both the fluid and the particles [1]. In a 1D scenario, saturated waves can be observed in experiments, propagating upwards in the flow [2]. In this work, we study these saturated waves by considering the one-dimensional version of the governing equations and recasting them into a nonlinear ODE in the frame moving with the (unknown) velocity of the saturated waves [3]. The boundary value problem defined on the (unknown) wavelength of the saturated wave is solved by an iterative algorithm that finds the concentration profile, the wavelength and the propagation velocity of the waves simultaneously. Different particle pressure models are proposed in order to fit the results to the experimental data available in [2]. We show that a pice-wise particle pressure fucntion that takes into account the the compression and expansion phases of the wave can correctly describe the observations.

**Keywords**: fluidized beds, saturated waves, particle pressure, eigenvalue problem

**Mathematics Subject Classifications (2010)**: 76T20, 76N30, 76A99.

## References

1. Anderson, T. B. and Jackson, R. Fluid Mechanical Description of Fluidized Beds. Equations of Motion. *Industrial & Engineering Chemistry Fundamentals*, 6(4), 527-539, 1967.
2. Duru, P., Nicolas, M., Hinch, E.J., and Guazzelli, É. Constitutive laws in liquid-fluidized beds *Journal of Fluid Mechanics* 452, 371-404, 2002.
3. Sobral, Y. D. and Hinch, E. J. *Finite Amplitude Steady-State One-Dimensional Waves in Fluidized Beds.*, SIAM *J. Appl. Math.*,77(1):247-266, 2017.

# Plateau-Rayleigh instability in superparamagnetic ferrofluids: a simplified 1D theory

Ghylherme Patriota Nunes da Rocha[1], Pavel Zenon Sejas Paz[2], and Yuri Dumaresq Sobral[3]

Departamento de Matemática, Universidade de Brasília, Brazil
ghylherme.patriot@gmail.com
Laboratório de Matemática Aplicada, Universidade Federal de Juiz de Fora, Brazil
psejasp@gmail.com
Departamento de Matemática, Universidade de Brasília, Brazil
ydsobral@unb.br

, Yuri@Sobral, Yuri

**Summary.** In this work, we study the Plateau-Rayleigh instability of a superparamagnetic ferrofluid under the presence of a magneic field. The Plateau-Rayleigh instability [1], which is driven by surface tension, occurs when a thin column of fluid with a predominant axial flow is broken into several drops of fluid. Based on the thin geometry of the flow, we propose a set of 1D governing equations in term of the axial velocity of the flow and of the free surface position. An axial magnetic field is considered and is taken into account in the formulation in the effective pressure in the flow [2]. We perform a linear stability analysis to identify the range of unstable wavenumbers and solve the full nonlinear governing equations with the method of lines [3]. We observe that the simplified theory matches very well the linear theory presented in [4] and that presence of the magnetic field slows down the growth of the instabilities, leading to configurations for which the breakup can be prevented.

**Keywords**:

**Mathematics Subject Classifications (2010)**: 76D45, 76E17, 65M20.

## References

1. Papageorgiou, D. T. On the breakup of viscous liquid threads *Physics of Fluids*, 7(7), 1529-1544, 1995.
2. Paz, P. Z. S. Instabilities in flows of magnetic fluids *PhD Thesis,* Universidade de Brasília, 2021.
3. Furlani, E. P., Hanchak, M. S.. Analysis of the deformation and breakup of the viscous microjets using the method of lines. *International Journal of Numerical Methods in Fluids*, 65, 563-577, 2011.
4. Rosensweig, R. E. *Ferrohydrodynamics* Dover Books, 1985.

# MS15: Recent advances in (hybridizable) discontinuous Galerkin methods and applications

# Discontinuous Galerkin methods for interface problems

Isaac Bermúdez[1], Manuel Solano[2], and Jaime Manríquez[3]

CI$^2$MA and Departamento de Ingeniería Matemática
Universidad de Concepción
Concepción, Chile
ibermudez@udec.cl
CI$^2$MA and Departamento de Ingeniería Matemática
Universidad de Concepción
Concepción, Chile
msolano@ing-mat.udec.cl
Centre for Mathematical Sciences, Lund University, Lund, Sweden
jaime.manriquez@math.lth.se

**Summary.** In many different applications, interfaces divide the domain of interest $\Omega \subset \mathbb{R}^{\mathrm{d}}$, where $\mathrm{d} = 2,3.$, into several subdomains on which the governing equations and/or boundary conditions are different. As the geometrical complexity and required spatial sampling of the subdomains may vary significantly, it is not uncommon to mesh the subdomains separately using different mesh sizes. In this work, we present and analyze a Hybridizable Discontinuous Galerkin (HDG) method for the problem posed by the coupling of the Stokes and Darcy equations, whose domains are discretized by two independent subdomains with different meshes. This causes non-conformity at the intersection of the subdomains or leaves a gap (unmeshed region) between them. To properly couple the two different discretizations, the proposed transmission conditions are based on mass conservation and equilibrium normal forces for matching meshes. For non-matching meshes, we use the transfer technique of the numerical trace/flux and extrapolate the approximate flux in both meshes. Furthermore, we establish the well-posedness of the method and error estimates to show the stability of the HDG method. Finally, we demonstrate the capacities of the method by presenting numerical experiments that validate our theory.

**Keywords**: Non-matching meshes; dissimilar meshes; hybrid method.

## References

1. M. Solano, S. Terrana, N.-C. Nguyen, and J. Peraire. An HDG method for dissimilar meshes. IMA *Journal of Numerical Analysis*. 42(2):1665-1699, 08 2021.
2. J. Manríquez, N.-C. Nguyen, and M. Solano. A dissimilar non-matching hdg discretization for stokes flows. *Computer Methods in Applied Mechanics and Engineering*. 399:115292, 2022.

# Functional inequalities in piecewise Sobolev spaces and applications to (hybrid) discontinuous methods

Michele Botti[1]

Politecnico di Milano
michele.botti@polimi.it

**Summary.** In this talk, we will investigate several functional inequalities that are instrumental to establish the stability and convergence analysis of discontinuous finite element methods supporting polyhedral meshes for a wide class of nonlinear problems. Starting from some preliminary results concerning broken Sobolev spaces, we will develop novel arguments to prove the broken version of Poincaré, Korn, trace inequalities and Sobolev embeddings. The main ingredient is a generalization of the local continuous trace inequality allowing to establish the results without restricting to piecewise polynomials or other discrete functional spaces and without requiring the definition of an interpolator mapping the discontinuous functions to continuous ones. We will apply the functional tools to derive the a priori analysis for discontinuous Galerkin and Hybrid High-Order discretizations of nonlinear creeping flow problems.

**Keywords**: discontinuous Galerkin, polyhedral meshes, functional inequalities, broken Sobolev spaces

**Mathematics Subject Classifications (2010)**: 65J15, 65N30

## References

1. S. Brenner. Korn's inequalities for piecewise $H^1$ vector fields *Math. Comp.*, 2004.
2. A. Buffa, and C. Ortner. Compact embeddings of broken Sobolev spaces *IMA J. Numer. Anal.*, 2009.
3. M. Botti, D. A. Di Pietro, and P. Sochala. A Hybrid High-Order method for nonlinear elasticity *SIAM J. Numer. Anal.*, 2017.
4. M. Botti, D. Castanon Quiroz, D. A. Di Pietro, and A. Harnist. A Hybrid High-Order method for creeping flows of non-Newtonian fluids *ESAIM M2AN*, 2021.
5. M. Botti, D. A. Di Pietro, and M. Salah. A serendipity fully discrete div-div complex on polygonal meshes *Comptes Rendus Mécanique*, 2023.

# Hybrid High-Order methods for incompressible flows of non-Newtonian fluids

Michele Botti[1], Daniel Castañón Quiroz[2], Daniele A. Di Pietro[3], and André Harnist[4]

MOX, Department of Mathematics, Politecnico di Milano, Milano, Italy.
michele.botti@polimi.it
Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas, Universidad Nacional Autónoma de México, México.
daniel.castanon@iimas.unam.mx
IMAG, Univ Montpellier, CNRS, Montpellier, France.
daniele.di-pietro@umontpellier.fr
LMAC, Université de Technologie de Compiègne, Compiègne, France.
andre.harnist@utc.fr

**Summary.** In this presentation we first give a quick introduction to the Hybrid High-Order (HHO) method for the Poisson equation, and mention its connection with the Hybrid Discontinuous Galerkin (HDG) method. We then present a HHO method for the steady motion of non-Newtonian incompressible fluids of small velocities, and then continue with a HHO method for generalized Navier–Stokes equations adapted, not only to non-Newtonian fluids, but also to fluids with non-classical convective behaviour. Both methods have several appealing features such as the support of general meshes and high-order approximation. We present a convergence analysis of both methods under some general assumptions. The final part of the presentation will be dedicated to illustrating the methods with a well-known problem in fluid mechanics, the lid-driven cavity flow.

**Keywords**: hybrid high-order methods; non-Newtonian fluids; Navier–Stokes; general meshes;

**Mathematics Subject Classifications (2010)**: 65N08, 65N30, 65N12, 35Q30, 76D05

# Multisymplectic hybrid finite element methods for Hamiltonian PDEs

Ari Stern[1]

Washington University in St. Louis
stern@wustl.edu

**Summary.** Solutions to Hamiltonian PDEs satisfy a local conservation law, called the *multisymplectic conservation law*, which generalizes the symplectic conservation law for Hamiltonian ODEs. We discuss a class of hybrid finite element methods for Hamiltonian PDEs—including conforming, nonconforming, mixed, and HDG methods—whose numerical solutions satisfy this conservation law locally (i.e., element-by-element) in terms of the numerical trace/flux. This includes methods for canonical Hamiltonian systems in mixed div-grad form [1, 2], as well as a more recent generalization to hybrid methods in finite element exterior calculus [3].

**Keywords**: hybrid finite element methods, hybridizable discontinuous Galerkin (HDG), Hamiltonian, multisymplectic, structure-preserving, finite element exterior calculus (FEEC)

**Mathematics Subject Classifications (2010)**: 65N30, 37K05

## References

1. R. I. McLachlan and A. Stern, *Multisymplecticity of hybridizable discontinuous Galerkin methods*, Found. Comput. Math., 20 (2020), pp. 35–69. doi:10.1007/s10208-019-09415-1.
2. R. I. McLachlan and A. Stern, *Functional equivariance and conservation laws in numerical integration*, Found. Comput. Math., (2022). doi:10.1007/s10208-022-09590-8.
3. A. Stern and E. Zampa, *Multisymplecticity in finite element exterior calculus*. In preparation.

# Hybrid staggered discontinuous Galerkin method on general meshes

Lina Zhao[1] and Eun-Jae Park[2]

Department of Mathematics, City University of Hong Kong, Kowloon Tong, Hong Kong SAR, China.
linazha@cityu.edu.hk
School of Mathematics and Computing (Computational Science and Engineering), Yonsei University, Seoul, Korea.
ejpark@yonsei.ac.kr

**Summary.** In this talk, we present high-order hybrid staggered discontinuous Galerkin method on general meshes to solve general second order elliptic problems. Our formulation is related to standard staggered discontinuous Galerkin method, but more flexible and cost effective: rough grids are allowed and the size of the final system is remarkably reduced thanks to the partial hybridization. Optimal convergence estimates for both the scalar and vector variables are developed. Moreover, superconvergent results with respect to discrete $H^1$ norm and $L^2$ norm for the scalar variable are proved and negative norm error estimates for both the scalar and vector variables are also developed. On the other hand, mesh adaptation is particularly simple since hanging nodes are allowed, which makes the proposed method well suited for adaptive mesh refinement. Therefore, we design a residual type a posteriori error estimator, and the reliability and local efficiency of the error estimator are proved. Numerical experiments confirm the theoretical findings.

**Keywords**: Staggered DG, General polygonal mesh, Locking-free, Fixed stress splitting, Weak symmetry, Biot system, Poroelasticity

**Mathematics Subject Classifications (2010)**:

## References

1. L. Zhao and E.-J. Park A Staggered Discontinuous Galerkin Method of Minimal Dimension on Quadrilateral and Polygonal Meshes, *SIAM J. Sci. Comput.*,40(4), Pages A2543-A2567, 2018.
2. L. Zhao and E.-J. Park A new hybrid staggered discontinuous Galerkin method on general meshes. *J. Sci. Comput.*, 82(1), Paper No. 12, 33 pp. 2020.
3. D. Kim, L. Zhao and E.-J. Park Staggered DG methods for the pseudostress-velocity formulation of the Stokes equations on general meshes. *SIAM J. Sci. Comput.*, 42(4), A2537-A2560, 2020.

# A posteriori error estimates for IPDG discretizations of Helmholtz problems with minimal regularity

Théophile Chaumont-Frelet[1]

Inria, Univ. Lille, CNRS, UMR 8524 – Laboratoire Paul Painlevé
theophile.chaumont@inria.fr

**Summary.** Helmholtz problems model the propagation of time-harmonic waves, and naturally appear in a large array of applications. The design of suitable numerical approximations is therefore paramount, and due to their ability to handle complex propagation media, finite element and discontinuous Galerkin approximations have become very popular to numerically solve Helmholtz problems. In this context, *a posteriori* error estimation appears as an important tool both to accurately control the discretization error and to improve the efficiency by adaptively refining the mesh and/or the polynomial degree. For conforming finite element discretizations, equilibrated and residual-based *a posteriori* estimators have been respectively considered in [2] and [4], with an analysis that holds for very general domains and material coefficients, allowing for minimal regularity of the solution. For discontinuous Galerkin schemes with interior penalization (IPDG) however, the analysis presented in [3] and [5] only holds under a restrictive assumption on the regularity of the solution which excludes important problem configurations. In this talk, I will discuss sharp *a posteriori* error estimates for IPDG discretizations that hold under minimal regularity assumptions. These results have been recently developed in [1], and apply to both equilibrated and residual-based estimators. At the core of the proof lies a duality argument of Aubin–Nitsche type that allows for minimal solution regularity. Beyond its application in *a posteriori* error estimation for Helmholtz problems, this technique should be useful for analyzing other aspects of the IPDG method.

**Keywords**: A posteriori error estimates, Aubin–Nitsche trick, discontinuous Galerkin, Helmholtz problems, interior penalty, minimal regularity.

**Mathematics Subject Classifications (2010)**: 35J05, 65N12, 65N15, 65N30.

## References

1. T. Chaumont-Frelet. Duality analysis of interior penalty discontinuous Galerkin methods under minimal regularity and application to the a priori and a posteriori error analysis of Helmholtz problems. *arXiv 2208.14701*, 2022.
2. T. Chaumont-Frelet, A. Ern and M. Vohralík. On the derivation of guaranteed and $p$-robust a posteriori error estimates for the Helmholtz equation. *Numerische Mathematik*, 148:525-573, 2021.
3. S. Congreve and J. Gedicke and I. Perugia. Robust adaptive $hp$ discontinuous Galerkin finite element methods for the Helmholtz equation. SIAM *Journal on Scientific Computing*, 41(2):A1121-A1147, 2019.
4. W. Dörfler and S.A. Sauter. A posteriori error estimation for highly indefinite Helmholtz problems. *Computer Methods in Applied Mechanics and Engineering*, 13:333-347, 2013.
5. S.A. Sauter and J. Zech. A posteriori error estimation of $hp-dG$ finite element methods for highly indefinite Helmholtz problems. SIAM *Journal on Numerical Analysis*, 53(5):2414-2440, 2015.

# A Divergence-Conforming E-HDG Method for the Linearized Incompressible Resistive MHD equations

Jau-Uei Chen[1], Támás L. Horváth[2], and Tan Bui-Thanh[3]

Department of Aerospace Engineering and Engineering Mechanics, The University of Texas at Austin, Austin, TX 78712, USA
chenju@utexas.edu
Department of Mathematics and Statistics, Oakland University, Rochester, MI 48309, USA
thorvath@oakland.edu
Department of Aerospace Engineering and Engineering Mechanics/Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX 78712, USA
tanbui@oden.utexas.edu

, @Horváth,

**Summary.** Incompressible Magnetohydrodynamics (MHD) models are relevant in low Lundquist number liquid metals, high Lundquist number, large guide field fusion plasmas, and low Mach number compressible flows. Due to its complexity, it is crucial to understand the dynamics of electrically conducting flow in the presence of electromagnetic fields via simulation. In this work, we proposed an Embedded-hybridized discontinuous Galerkin (E-HDG) method for solving linearized incompressible resistive MHD equations.

In particular, the E-HDG method is computationally cheaper than the corresponding HDG method. The benefit is even significant in the three-dimensional scenario. Furthermore, a specific choice of the approximation spaces guarantees that the proposed method is $H(div)$-conforming, meaning that the velocity and magnetic fields are pointwise divergence-free. We implement our approach in the open source library `MFEM` and validate our method using manufactured solutions. The results indicate that convergence rates in the $L^2$ norm for the velocity and magnetic fields are optimal, and divergence error can be reduced to machine zero. Furthermore, the proposed E-HDG discretization is pressure robust.

**Keywords**: discontinuous Galerkin methods, embedded-hybridized, resistive magnetohydrodynamics

**Mathematics Subject Classifications (2010)**: Numerical Analysis (math.NA)

# An energy-dissipative diffusive-interface hybridizable discontinuous Galerkin method for two-phase flows

David C. Del Rey Fernández[1], Sander Rhebergen[2], and Paulo Zúñiga[3]

Department of Applied Mathematics, University of Waterloo, ON, Canada
ddelreyfernandez@uwaterloo.ca
Department of Applied Mathematics, University of Waterloo, ON, Canada
srheberg@uwaterloo.ca
Departamento de Ciencias Matemáticas y Físicas, Universidad Católica de Temuco, Chile
paulo.zuniga@uct.cl

**Summary.** We propose a hybridizable discontinuous Galerkin (HDG) method for a diffusive-interface model of incompressible immiscible two-phase flows with surface tension and non-matching densities. Our method ensures energy dissipation and global mass conservation. Key to this is the divergence-free discretization of the model's entropy functional. This is achieved by employing an HDG method previously used for single-phase Navier-Stokes flows. Numerical examples validate our theoretical results.

**Keywords**: two-phase flow, energy dissipation, hybridizable discontinuous Galerkin

**Mathematics Subject Classifications (2010)**: 65N30, 76T10

## References

1. M.F.P. ten Eikelder and I. Akkerman. *A novel diffuse-interface model and a fully-discrete maximum-principle-preserving energy-stable method for two-phase flow with surface tension and non-matching densities*. *Computer Methods in Applied Mechanics and Engineering*, 379: 113751, 2021.
2. S. Rhebergen and G.N. Wells. *A hybridizable discontinuous Galerkin method for the Navier-Stokes equations with pointwise divergence-free velocity field*. *Journal of Scientific Computing*, 76(3):1484-1501, 2018.
3. G.N. Wells. *Analysis of an interface stabilized finite element method: the advection-diffusion-reaction equation*, SIAM *Journal on Numerical Analysis*, 49(1):87-109, 2011.

# Residual-based a posteriori error estimates for an $hp$-discontinuous Galerkin method of the biharmonic problem

Zhaonan Dong[1], Lorenzo Mascotto[2], and Oliver J. Sutton[3]

SERENA team, INRIA Paris, France
zhaonan.dong@inria.fr
Department of Mathematics and Applications, University of Milano-Bicocca, Italy
lorenzo.mascotto@unimib.it
Department of Mathematics, King's College London, UK
oliver.sutton@kcl.ac.uk

**Summary.** We discuss an *hp*-dG residual error estimator for the biharmonic problem in 2D and 3D. Upper and lower bounds are explicit in the mesh-size and polynomial degree. The lower bound is algebraically suboptimal in terms of the polynomial degree.

[1] is the first reference where an *hp*-dG error estimator is analyzed for fourth order problems. The reason for this is that, in the DG context, one typically needs the existence of a C1-conforming piecewise polynomial space: this does not exist, e.g., on tetrahedral meshes for sufficiently large polynomial degree. We rather use an elliptic reconstruction of the discrete solution to the H2 space and a generalised Helmholtz decomposition of the error.

The theoretical results are confirmed by numerical experiments.

**Keywords**: discontinuous Galerkin methods, adaptivity, hp-Galerkin methods, polynomial inverse estimates, fourth order PDEs, a posteriori error analysis.

**Mathematics Subject Classifications (2010)**:65N12, 65N30, 65N50.

## References

1. Z. Dong, L. Mascotto, O. J. Sutton. Residual-based a posteriori error estimates for hp-discontinuous Galerkin discretisations of the biharmonic problem. SIAM *Journal on Numerical Analysis*,59(3):1273-1298, 2021.

# Structure-preserving Local Discontinuous Galerkin method for nonlinear cross-diffusion system

Sergio Gómez[1]

University of Milano-Bicocca
sergio.gomezmacias@unimib.it

**Summary.** The main difficulty in the design of methods for the numerical approximation of cross-diffusion systems is that the diffusion matrix may be nonsymmetric and not positive semidefinite. In this talk, we present a high-order Local Discontinuous Galerkin method for the discretization of nonlinear cross-diffusion systems. In the spirit of [1], we rewrite the original problem in terms of an entropy variable.

The method is designed so that:

*i)* it naturally preserves the positivity and boundedness of the exact solution, even if a maximum principle is not available;

*ii)* nonlinearities do not appear within differential operators, thus reducing the computational cost of the method;

*iii)* a chain rule involving the auxiliary variables is weakly imposed, which allows us to show a discrete entropy stability estimate.

We present several numerical experiments that validate our theoretical results.

∗ This is a joint work with Ansgar Jüngel and Ilaria Perugia.

**Keywords**: cross-diffusion systems; Local Discontinuous Galerkin method; structure-preserving; entropy variable.

**Mathematics Subject Classifications (2010)**: 65M60; 65M12; 35K55; 35K57.

## References

1. A. Jüngel. The boundedness-by-entropy method for cross-diffusion systems. Nonlinearity, 28:1963–2001, 2015.

# Construction of multigrid solvers for hybridized discontinuous Galerkin discretizations

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

Interdisciplinary Center for Scientific Computing (IWR), Faculty of Engineering Sciences, Heidelberg University, Germany
kanschat@uni-heidelberg.de
Department of Mathematics Sciences, Soochow University, Suzhou, China
pplu@suda.edu.cn
School of Engineering Science, Lappeenranta–Lahti University of Technology, Lappeenranta, Finland
andreas.rupp@lut.fi

**Summary.** Since the approximation spaces of hybridized methods are not nested, the construction of multigrid injection operators is not trivial, see [1]. Starting from analyzing a particular injection operator in [2], we derive general assumptions on HDG methods and injection operators in [3]. With these assumptions, we can prove contraction of multigrid iterations independent of the mesh size. We provide several examples of useful injection operators which fulfil these assumptions. By similar principles, we aslo show the convergence of two-level Schwarz methods in [5]. In addition to standard HDG methods, the structure is applicable to embedded DG methods, where some aspects are even simpler [4].

**Keywords**: HDG, multigrid, GMG, injection operators

**Mathematics Subject Classifications (2010)**: 65F10, 65N30, 65N50

## References

1. B. Cockburn, O. Dubois, J. Gopalakrishnan, and S. Tan. Multigrid for an HDG method. *IMA Journal of Numerical Analysis*, 34(4):1386–1425, 10 2013. DOI: 10.1093/imanum/drt024.
2. P. Lu, A. Rupp, and G. Kanschat. Homogeneous multigrid for HDG. *IMA J. Numer. Anal.*, 2021. DOI: 10.1093/imanum/drab055.
3. P. Lu, A. Rupp, and G. Kanschat. Analysis of injection operators in geometric multigrid solvers for hdg methods. *SIAM J. Numer. Anal.*, 60(4):2293–2317, 2022. DOI: 10.1137/21M1400110.
4. P. Lu, A. Rupp, and G. Kanschat. Homogeneous multigrid for embedded discontinuous Galerkin methods. *BIT Numer. Math.*, 62:1029–1048, 2022. DOI: 10.1007/s10543-021-00902-y.
5. P. Lu, A. Rupp, and G. Kanschat. Two-level Schwarz Methods for Hybridizable Discontinuous Galerkin Methods *J. Sci. Comput.*, 25(9), 2023. DOI: 10.1007/s10915-023-02121-9

# Analysis of an HDG method for Maxwell's equations under minimal regularity

Gang Chen[1], Peter Monk[2], and Yangwen Zhang[3]

Sichuan University, China
cglwdm@uestc.edu.cn
University of Delaware, Newark, USA
monk@udel.edu
University of Louisiana, Lafayette, USA
yangwen.zhang@louisiana.edu

**Summary.** We propose and analyze a hybridizable discontinuous Galerkin (HDG) method combined with the continuous Galerkin (CG) method to approximate Maxwell's equations [1]. We derive optimal convergence estimates for our HGD-CG approximation when the electromagnetic coefficients are piecewise smooth. This requires new techniques of analysis. Second, we use CG elements to approximate the Lagrange multiplier used to enforce the divergence condition and we obtain a discrete system in which we can decouple the discrete the Lagrange multiplier. Because we are using a continuous Lagrange multiplier space, the number of degrees of freedom devoted to this are less than for other HDG methods. We present numerical experiments to confirm our theoretical results.

**Keywords**: Maxwell equations, HDG, Numerical analysis, Frequency domain analysis

**Mathematics Subject Classifications (2010)**: 65Z05, 65L60

## References

1. Gang Chen and Peter Monk and Yangwen Zhang, HDG and CG methods for the Indefinite Time-Harmonic Maxwell's Equations under minimal regularity, arXiv preprint 2002.06139 (2020).

# A robust discontinuous Galerkin scheme on anisotropic meshes

Takahito Kashiwabara[1] and Takuya Tsuchiya[2]

University of Tokyo
tkashiwa@ms.u-tokyo.ac.jp
Osaka University
tsuchiya.takuya.plateau@kyudai.jp

**Summary.** Discontinuous Galerkin (DG) methods are extensions of the usual Galerkin finite element methods. Although there are vast amount of studies on DG methods, most of them have assumed shape-regularity conditions on meshes for both theoretical error analysis and practical computations. In this paper, we present a new symmetric interior penalty DG scheme with a modified penalty term. We show that, without imposing the shape-regularity condition on the meshes, the new DG scheme inherits all of the good properties of standard DG methods, and is thus robust on anisotropic meshes. Numerical experiments confirm the theoretical error estimates obtained.

**Keywords**: discontinuous Galerkin method, symmetric interior penalty, error estimation, anisotropic meshes

**Mathematics Subject Classifications (2010)**: 65N30, 65N50

## References

1. D.N. Arnord. An interior penalty finite element method with discontinuous elements. SIAM *Journal on Numerical Analysis*, 19:742-760, 1982.
2. D.N. Arnold, F. Brezzi, B. Cockburn, L.D. Marini. Unified analysis of discontinuous Galerkin methods for elliptic problems. SIAM *Journal on Numerical Analysis*, 39:1749-1779, 2002.
3. D.A. Di Pietro, A. Ern. Mathematical Aspects of Discontinuous Galerkin Methods. Springer, 2012.
4. A. Ern, J-L Guermond. Theory and Practice of Finite Elements. Springer, 2004.
5. T. Kashiwabara, T. Tsuchiya. A robust discontinuous Galerkin scheme on anisotropic meshes. *Japan Journal of Industrial and Applied Mathematics*, 38:1001-1022, (2021).
6. K. Kobayashi, T. Tsuchiya. Lectures on error analysis of interpolation on simplicial triangulations with the shape regularity assumption, part 1, Lagrange interpolation on triangles. arXiv:1908.03894.
7. K. Kobayashi, T. Tsuchiya. Lectures on error analysis of interpolation on simplicial triangulations with the shape regularity assumption, part 2, Lagrange interpolation on tetrahedrons. arXiv:2103.08101.

# High-order projection-based upwind method for implicit large eddy simulation

Philip L. Lederer[1], Xaver Mooslechner[2], and Joachim Schöberl[3]

University of Twente, Department of Applied Mathematicas
p.l.lederer@utwente.nl
TU Wien, Institute of Analysis and Scientific Computing
xaver.mooslechner@tuwien.ac.at
TU Wien, Institute of Analysis and Scientific Computing
joachim.schöberl@tuwien.ac.at

**Summary.** We assess the ability of high-order (hybrid) discontinuous Galerkin methods to simulate under-resolved turbulent flows. The capabilities of the mass conserving mixed stress-yielding method as structure resolving large eddy simulation (LES) solver are examined. A comparison of a variational multiscale model to no-model or an implicit model approach is presented via numerical results. In addition, we present a novel approach for turbulent modeling in wall-bounded flows which can be interpreted as an extension of the classical variational multiscale idea to implicit LES via discontinuous Galerkin methods. This new technique called high-order projection-based upwind (HOPU) technique provides a more accurate representation of the actual subgrid scales in the near wall region and gives promising results for highly under-resolved flow problems. We consider the turbulent channel flow and periodic hill flow problem as well as a flow over an Eppler airfoil.

**Keywords**: Large eddy simulation, turbulence modeling, hybrid discontinuous Galerkin, mass conserving stress-yielding methods

**Mathematics Subject Classifications (2010)**: 65N30, 76M10.

# Symplectic Hamiltonian hybridizable discontinuous Galerkin methods for linearized shallows-water equations

Cristhian Núñez[1] and Manuel A. Sánchez[2]

Pontificia Universidad Católica de Chile, Facultad de Matemáticas, Santiago, Chile
aanunez6@uc.cl
Pontificia Universidad Católica de Chile, Instituto de Ingeniería Matemática y Computacional IMC, Santiago, Chile
manuel.sanchez@uc.cl

**Summary.** We focus on devising novel numerical methods for solving Linearized Shallow-Water Equations (LSWE) while preserving physical quantities of interest such as energy, vorticity, among others. The Shallow-Water Equations describe the dynamics of a fluid with constant density at low depths, which are entirely determined by the conservative laws for momentum and mass. We employ a suitable rewriting of LSWE in a Hamiltonian form and utilize Hibridizable Discontinuous Galerkin Methods (HDG) for spatial discretization. This approach leverages the Hamiltonian structure of SWE combined with the symplectic time-stepping methods such us SDIRK, which conserve the discrete energy of the system over time. We discuss the main properties of our methodology and present numerical experiments to verify its performance, comparing it with other dissipative approaches found in the bibliography.

**Keywords**: Shallow-Water, HDG, Hamiltonian, symplectic time-stepping.

**Mathematics Subject Classifications (2010)**: 65P10

## References

1. Tan Bui-Thanh. Construction and Analysis of HDG Methods for Linearized Shallow Water Equations. SIAM *Journal on Scientific Computing*, 38:A3696–A3719, 01 2016
2. P.J. Olver. Applications of Lie Groups to Differential Equations. *Graduate Text in Mathematics*, 2000.
3. Rick Salmon. *A General Method for Conserving Quantities related to Potential Vorticity in Numerical Models.* NONLINEARITY Nonlinearity, 18:1–16, 09 2005.
4. Manuel Sánchez, C. Ciuca, Ngoc Nguyen, J. Peraire, and B. Cockburn. *Symplectic Hamiltonian HDG Methods for Wave Propagation Phenomena.* Journal of Computational Physics, 350, 09 2017.
5. Manuel Sánchez, Bernardo Cockburn, Ngoc Nguyen, and Jaime Peraire. *Symplectic Hamiltonian Finite Element Methods for Linear Elastodynamics.* Computer Methods in Applied Mechanics and Engineering, 381:113843, 08 2021.
6. Manuel Sánchez, Shukai Du, Bernardo Cockburn, Ngoc Nguyen, and Jaime Peraire. *Symplectic Hamiltonian Finite Element Methods for Electromagnetics.* Computer Methods in Applied Mechanics and Engineering, 396:114969, 06 2022.

# HDG methods with transmission variables for Helmholtz problems

Simone Pescuma[1], Théophile Chaumont-Frelet[2], Gwenael Gabard[3], and Axel Modave[4]

POEMS, CNRS, Inria, ENSTA Paris, Institut Polytechnique de Paris, 91120 Palaiseau, France
simone.pescuma@ensta-paris.fr
Inria, Université de Lille, CNRS, Laboratoire Paul Painlevé, 59000 Lille, France
theophile.chaumont@inria.fr
LAUM, CNRS, IA-GS, Le Mans Université, 72085 Le Mans, France
gwenael.gabard@univ-lemans.fr
POEMS, CNRS, Inria, ENSTA Paris, Institut Polytechnique de Paris, 91120 Palaiseau, France
axel.modave@ensta-paris.fr

**Summary.** Due to their ability to deliver high-order convergence on unstructured meshes, discontinuous Galerkin finite element methods are well suited for time-harmonic wave propagation problems, where the Helmholtz equation is solved on a variety of complicated physical (*e.g.* with regard to heterogeneous media) and geometrical domains. However, the associated linear system is often very large and poorly conditioned. This renders the use of direct solvers too costly and the convergence of iterative schemes slow.

To overcome these difficulties, a hybridizable discontinuous Galerkin method (CHDG) [1] is proposed. It is based on a standard discontinuous Galerkin scheme with upwind numerical fluxes and high-order polynomial bases. Auxiliary unknowns corresponding to characteristic variables are defined at the interface across the elements, so that the physical fields inside each element are eliminated in order to obtain a reduced system. Eventually, the reduced system can be written in terms of a fixed-point problem that can be solved with stationary iterative schemes, such as CGNR, GMRES and fixed-point.

Numerical results for 2D benchmarks are presented to study the performance of the approach. Compared to the standard HDG approach, the properties of the reduced system are improved with CHDG, which is therefore better suited for iterative solution procedures: the condition number of the reduced system is smaller and both CGNR and GMRES require smaller numbers of iterations.

We are currently investigating extended methods to exploit high-order transmission variables to further reduce the number of iterations (inspired by [2]), as well as to deal with heterogeneous media. Preliminary theoretical and numerical results will be presented.

**Keywords**: Helmholtz equation, Discontinuous finite elements, Hybridization, Iterative solvers.

**Mathematics Subject Classifications (2010)**: 35J05, 65N12, 65N30

## References

1. A. Modave, and T. Chaumont-Frelet. A hybridizable discontinuous Galerkin method with characteristic variables for Helmholtz problems. *Journal of Computational Physics*, 493, 112459, 2023.
2. A. Modave, A. Royer, X. Antoine, and C. Geuzaine. A non-overlapping domain decomposition method with high-order transmission conditions and cross-point treatment for Helmholtz problems. *Computer Methods in Applied Mechanics and Engineering*, 368, 113162, 2020.

# Hybrid discontinuous Galerkin methods for PDEs on hypergraphs and networks of surfaces

Andreas Rupp[1], Markus Gahn[2], and Guido Kanschat[3]

School of Engineering Science, Lappeenranta–Lahti University of Technology, P.O. Box 20, 53851 Lappeenranta, Finland
andreas@rupp.ink
Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University, Mathematikon, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany
markus.gahn@fau.de
Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University, Mathematikon, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany
kanschat@uni-heidelberg.de

**Summary.** We introduce a general, analytical framework to express and to approximate partial differential equations (PDEs) numerically on graphs and networks of surfaces – generalized by the term hypergraphs. To this end, we consider PDEs on hypergraphs as singular limits of PDEs in networks of thin domains (such as fault planes, pipes, etc.), and we observe that (mixed) hybrid formulations offer useful tools to formulate such PDEs. Thus, our numerical framework is based on hybrid finite element methods (in particular, the class of hybrid discontinuous Galerkin methods).

**Keywords**: hybrid finite elements, hypergraphs, continuity equations

**Mathematics Subject Classifications (2010)**: Numerical Analysis (math.NA)

# An adaptive residual minimization method based on HDG formulations in primal form

Liliana Camargo[1], Sergio Rojas[2], and Patrick Vega[3]

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile
liliana.camargo@pucv.cl
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile
sergio.rojas.h@pucv.cl
Departamento de Matemática y Ciencia de la Computación, Universidad de Santiago de Chile, Chile
patrick.vega@usach.cl

**Summary.** The aim of this talk is to present a residual minimization method based on hybridizable discontinuous Galerkin (HDG) schemes in primal form (see [1, 3]). The method is stated in terms of a minimization problem, where the discrete solution is obtained as the minimizer, in an adequate conforming discrete space, of the residual in a discrete dual space. This methodology leads to a discrete saddle point problem that delivers a residual representative in addition to the discrete solution. The residual measured in an energy norm can automatically drive adaptive mesh refinements. We verify that, under a saturation assumption, this kind of error estimator has the properties of reliability and efficiency. The main advantage of the proposed method is that the HDG nature of the formulation allows for static condensation, with a notorious reduction of the global degrees of freedom required for its resolution (see [2]). We demonstrate the method's performance using numerical experiments in the setting of diffusion problems.

**Keywords**: hybridizable discontinuous Galerkin methods, residual minimization, saddle point problem, saturation assumption, implicit estimator, diffusion problems.

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N30, 65N50

## References

1. M. Ainsworth, G. Fu, *Fully computable a posteriori error bounds for hybridizable discontinuous Galerkin finite element approximations*, Journal of Scientific Computing, Springer **77**, pp. 443-466 (2018)
2. V.M. Calo, A. Ern, I. Muga, S. Rojas, *An adaptive stabilized conforming finite element method via residual minimization on dual discontinuous Galerkin norms*, Computer Methods in Applied Mechanics and Engineering, Elsevier **363**, p. 112891 (2020)
3. G. Chen, J. Cui, *On the error estimates of a hybridizable discontinuous Galerkin method for second-order elliptic problem with discontinuous coefficients*, IMA Journal of Numerical Analysis, JSTOR **40**, pp. 1577–1600 (2020)

# Minimum-residual a posteriori error estimates for a hybridizable discontinuous Galerkin discretization of the Helmholtz equation

Liliana Camargo[1], Sergio Rojas[2], and Patrick Vega[3]

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile.
liliana.camargo@pucv.cl
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, Chile.
sergio.rojas.h@pucv.cl
Departamento de Matemática y Ciencia de la Computación, Universidad de Santiago de Chile, Chile.
patrick.vega@usach.cl

**Summary.** We propose reliable and efficient a posteriori error estimators for a hybridizable discontinuous Galerkin (HDG) discretization of the Helmholtz equation with mixed boundary conditions based on residual minimization. Such residual minimizations are performed on local postprocessing schemes of the approximation of the scalar solution provided by the HDG scheme. As a result, we obtain new postprocessed approximations for the scalar solution and residual representatives in the Riesz sense, which are further employed to derive a posteriori estimators. We illustrate our theoretical findings and the behavior of the a posteriori error estimators through two ad-hoc numerical experiments.

**Keywords**: residual minimization, postprocessing, a posteriori error analysis, adaptive mesh refinement.

**Mathematics Subject Classifications (2010)**: 65N12, 65N15, 65N22, 65N30, 65N50.

**Funding**: LC was supported by the Chilean grant DI Postdoctorado 2022 (PUCV). SR was supported by the Chilean National Agency for Research and Development (ANID) through FONDECYT project 3210009. PV was funded by the Chilean grant ANID FONDECYT 3220858.

## References

1. L. Camargo, S. Rojas, and P. Vega. Minimum-residual a posteriori error estimates for a hybridizable discontinuous Galerkin discretization of the Helmholtz equation *arXiv preprint*, arXiv:2304.00418, 2023.
2. I. Muga, S. Rojas, and P. Vega. An adaptive superconvergent mixed finite element method based on local residual minimization *SIAM Journal on Numerical Analysis*, 61(5):2084-2105, 2023.

## MS16: Recent advances in BEM for complex domains

# Implementation of local multiple traces formulation for electromagnetic scattering by complex objects

Timo Betcke[1], Paul Escapil-Inchauspé[2], Carlos Jerez-Hanckes[3], and Matthew Scroggs[4]

University College London, Department of Mathematics, London, UK
t.betcke@ucl.ac.uk
Data Observatory Foundation, Santiago, Chile
paul.escapil@dataobservatory.net
Universidad Adolfo Ibáñez, Santiago, Chile
carlos.jerez@uai.cl
University College London, Department of Mathematics, London, UK
matthew.scroggs.14@ucl.ac.uk

**Summary.** We consider the three-dimensional time-harmonic scattering transmission problem for complex scatterers. To approximate the fields, we introduce a local multiple-trace formulation [1, 2, 3], allowing the handling of junction points between sub-domains and resulting in efficient and parallel schemes. However, its practical implementation can be challenging, particularly in the context of 3D electromagnetic scattering. Therefore, we propose a new framework based on a skeleton (union of interfaces) approach and on swapping normal vectors' orientations. This enables the description of Calderón and transmission operators in their natural function spaces, thus resulting in a straightforward implementation of the local multiple-trace formulation. Consequently, we conduct multiple numerical experiments on increasingly complex objects, thereby demonstrating the method's scalability and applicability. Finally, we provide suggestions for future research avenues.

**Keywords**: Maxwell scattering, multiple-traces formulation, Boundary element methods.

**Mathematics Subject Classifications (2010)**: 65N38, 45A05, 35Q61.

## References

1. R. Hiptmair, and C. Jerez-Hanckes. Multiple traces boundary integral formulation for Helmholtz transmission problems. *Advances in Computational Mathematics*, 39:91, Springer, 2012.
2. X. Claeys, R. Hiptmair, and C. Jerez-Hanckes. *Multitrace boundary integral equations, in: Direct and inverse problems in wave propagation and application*, volume 14. Radon Set. Comput. Appl. Math., De Gruyter, Berlin, 2013.
3. A. Ayala, X. Claeys, P. Escapil-Inchauspé, and C. Jerez-Hanckes. Local multiple traces formulation for electromagnetics: Stability and preconditioning for smooth geometries. *Journal of Computational and Applied Mathematics*, 413:114356, 2022.
4. J.-C. Nedelec. *Acoustic and electromagnetic equations: integral representations for harmonic problems*, volume 144. Springer Science & Business Media, 2001.
5. A. Buffa, R. Hiptmair. *Galerkin boundary element methods for electromagnetic scattering, in: Topics in computational wave propagation*. Springer, 2003.
6. A. Kleanthous, T. Betcke, D. P. Hewett, P. Escapil-Inchauspé, C. Jerez-Hanckes, A. J. Baran. Accelerated Calderón preconditioning for Maxwell transmission problems. *Journal of Computational Physics*, 458:111099, 2022.

# Spectral Galerkin method for solving elastic wave scattering problems with multiple open arcs

Carlos Jerez-Hanckes[1], José Pinto[2], and Tao Yin[3]

Facultad de Ingeniería y Ciencias, Universidad Adolfo Ibáñez
carlos.jerez@uai.cl
Facultad de Ingeniería y Ciencias, Universidad Adolfo Ibáñez
jose.pinto@uai.cl
Institute of Computational Mathematics and Scientific Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences
yintao@lsec.cc.ac.cn

**Summary.** We study the elastic time-harmonic wave scattering problems on unbounded domains with boundaries composed of finite collections of disjoint finite open arcs (or cracks) in two dimensions [1]. Specifically, we present a fast spectral Galerkin method for solving the associated weakly- and hypersingular boundary integral equations (BIEs) arising from Dirichlet and Neumann boundary conditions, respectively. Discretization bases of the resulting BIEs employ weighted Chebyshev polynomials that capture the solutions' edge behavior [2]. We show that these bases guarantee exponential convergence in the polynomial degree when assuming analyticity of sources and arcs geometries. Numerical examples demonstrate the accuracy and robustness of the proposed method with respect to number of arcs and wavenumber.

**Keywords**: Boundary Integral Equations, Elastic Waves, Wave Scattering, Open arcs, Spectral Methods, Cracks

**Mathematics Subject Classifications (2010)**: 35J25, 65R20, 65N38, 74B05.

## References

1. C. Jerez-Hanckes, J. Pinto, T. Yin. Spectral Galerkin Method for Solving Elastic Wave Scattering Problems with Multiple Open Arcs. http://arxiv.org/abs/2205.04842
2. C. Jerez-Hanckes, J. Pinto. High-order Galerkin method for Helmholtz and Laplace problems on multiple open arcs. *ESAIM: Mathematical Modelling and Numerical Analysis*, 54(6):1975–2009, 2020.
3. O. Bruno, T. Yin. Regularized integral equation methods for elastic scattering problems in three dimensions. *Journal of Computational Physics*, 410:109350, 2020.
4. O. Bruno, L. Xu, T. Yin. Weighted integral solvers for elastic scattering by open arcs in two dimensions. *International Journal of Numerical Methods in Engineering*, 122:2733–2750, 2021.
5. R. Hiptmair, C. Jerez-Hanckes, C. Urzua-Torres. Mesh-independent operator preconditioning for boundary elements on open curves. SIAM Journal on Numerical Analysis, 52:2295–2314, 2014.

# Coupled Volume and Boundary Integral Equations for Electromagnetic Scattering

Ignacio Labarca[1] and Ralf Hiptmair[2]

Seminar for Applied Mathematics, ETH Zurich
ignacio.labarca@sam.math.ethz.ch
Seminar for Applied Mathematics, ETH Zurich
ralf.hiptmair@sam.math.ethz.ch

**Summary.** We study frequency domain electromagnetic scattering at a bounded, penetrable, and inhomogeneous obstacle. By defining constant reference coefficients, a new representation formula for interior and exterior vector fields is proposed, based on the general form of the Stratton-Chu integral representation. The final integral equation system consists of surface integral operators arising from a Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) formulation and compact volume integral operators with weakly singular kernels. The problem is solved with a Galerkin approach with usual Curl-conforming and Div-conforming finite elements on the surface and in the volume. Compression techniques and special quadrature rules for singular integrands are required for an efficient and accurate solution. Numerical experiments provide evidence that our new formulation enjoys promising properties.

**Keywords**: volume integral equations, boundary integral operators, boundary elements, finite elements, electromagnetic waves.

**Mathematics Subject Classifications (2010)**: 31B10, 65N80, 78M10, 78M15.

# Quasi-Periodic Boundary Integral Model of Nerve Electrical Stimulation

José Pinto[1] and Isabel Martinez[2]

Universidad Adolfo Ibañez
jose.pinto@uai.cl
Pontificia Universidad Catolica de Chile
iamartinez@uc.cl

**Summary.** We present a model for the electrical activity of a nerve under external stimulation. The nerve is composed of many axons, each consisting of alternating myelinated and unmyelinated regions, as well as ions channels that giving rise to nonlinear bioelectrical phenomena.

Due to the complexity of the underlying geometry, a direct discretization of the model is unfeasible. Therefore, it is necessary to introduce some simplifications.

Our approach builds upon [1],[2] where the nerve is reduced to a set of two-dimensional axons, and boundary integral formulations are used to obtain significant results. However, the two-dimensional truncation greatly reduces the applicability of the model.

In our study, we depart from dimensional reduction. Instead, we approximate the entire problem by a family of quasi-periodic problems and demonstrate an effective discretization technique using the boundary integral method.

**Keywords**: Quasi-Periodic Problem, Boundary Integral Formulation.

**Mathematics Subject Classifications (2010)**: 65M38, 65M12,65R20

## References

1. F. Henriquez, C. Jerez-Hanckes, and F. Altermatt. Boundary integral formulation and semi-implicitscheme coupling for modeling cells under electrical stimulation. Numer. Math. 136, 101–145 (2017).
2. F. Henriquez, and C. Jerez-Hanckes. Multiple traces formulation and semi-implicit scheme for modelling biological cells under electrical stimulation. M2AN 52 659–703 (2018) .

# Quantifying Atomic Position Uncertainty in Molecular Electrostatics with Poisson-Boltzmann and Boundary Elements

Paul Escapil-Inchauspé[1], Miguel Godoy Díaz[2], Carlos Jerez-Hanckes[3], and Christopher D. Cooper[4]

Data Observatory, Universidad Adolfo Ibañez
paul.escapil@dataobservatory.net
Departmento de Ingeniería Mecánica, Universidad Técnica Federico Santa María
miguel.godoy.13@sansano.usm.cl
Facultad de Ingeniería y Ciencias, Universidad Adolfo Ibañez
carlos.jerez@uai.cl
Departmento de Ingeniería Mecánica, Universidad Técnica Federico Santa María
christopher.cooper@usm.cl

**Summary.** Electrostatic interactions are fundamental to molecular processes, structure, and function. Accurately modeling these interactions is essential for understanding molecular behavior. The Poisson-Boltzmann equation is a widely used tool to this end, applied to model scenarios where a dissolved solute is represented as a low dielectric region in an infinite solvent domain, containing Dirac deltas to represent partial charges. Traditional Poisson-Boltzmann calculations often assume structural rigidity, overlooking thermal fluctuations that significantly impact atomic positions. These fluctuations result in structural variations, introducing inherent uncertainty into solvation energy predictions.

We present a methodology that integrates the solution of the Poisson-Boltzmann equation with the boundary element method, with quasi-Monte Carlo sampling techniques to accommodate the dynamic nature of solute molecules in solution. This way, we quantify the uncertainty arising from these thermal fluctuations, providing a more realistic representation of solvation energies. We validate our approach using a large dataset of realistic molecules, leveraging from molecular dynamics simulations for benchmarking. Furthermore, we extend our method to estimate uncertainty in solvation energies for larger structures, like proteins.

Importantly, our research contributes to an open-source and FAIR (Findable, Accessible, Interoperable, Reusable) software infrastructure, promoting transparency, collaboration, and accessibility. This work enhances the accuracy of solvation energy calculations and underscores the importance of incorporating uncertainty quantification in molecular modeling.

**Keywords**: Poisson-Boltzmann, Uncertainty Quantification, Molecular Electrostatics, Boundary Element Method.

**Mathematics Subject Classifications (2010)**: 92E10, 92C40, 45A05

## References

1. S.D. Search, C.D. Cooper, and E. van't Wout. Towards optimal boundary integral formulations of the Poisson–Boltzmann equation for molecular electrostatics *Journal of Computational Chemistry*, 43 (10): 674-691, 2022.
2. P. Escapil-Inchauspé and C. Jerez Hanckes. Shape Uncertainty Quantification for Electromagnetic Wave Scattering via First-Order Sparse Boundary Element Approximation *arXiv preprint arXiv:2308.01457*, 2023.
3. X. Yang, H. Lei, P. Gao, D.G. Thomas, D.L. Mobley, and N.A. Baker, Atomic radius and charge parameter uncertainty in biomolecular solvation energy calculations. *Journal of Chemical Theory and Computation*, 14(2), 759-767, 2018.

# MS17: Session of Communications

# Tensor Networks Space-time Spectral Elements Method for Solving Heat Equation

Dibyendu Adak[1]

Theoretical Division, Los Alamos National Laboratory
dadak@lanl.gov

**Summary.** In this work, we have coupled Spectral Methods with tensor train format for the efficient low- rank approximation of the multi-dimensional elliptic equation. For the discretization of the model problem, we have employed collocation spectral methods, which are justified for applying the tensor train format. We propose two different discretization for the global space-time formulation, resulting in a large block linear system, encapsulating all time steps, and solve it at once in the TT/QTT-formats. The linear complexity of storage and the solution time is observed in both spatial and time grid sizes. Further, we develop the theory without assuming the separable condition of the force function, which leads to function train decomposition of the force function. In addition, we have studied the cross-tensor train decomposition for the general solution while avoiding the rank-1 assumption of the solution. The method is applied to the Richards equation arising from the unsaturated water flow in the soil.

**Keywords**: Multi-dimensional PDEs, Tensor-Train Format, Quantized Tensor-Train Format, Richards Equations.

**Mathematics Subject Classifications (2010)**: 35K20, 65F50, 15A69, 65D15, 33F05, 65F10

## References

1. I. V. Oseledets. Tensor-train decomposition. SIAM *Journal Scientific Computing*, 33:2295–2317, 2011.
2. I. V. Oseledets and E. E. Tyrtyshnikov. Breaking the curse of dimensionality, or how to use SVD in many dimensions. SIAM *Journal Scientific Computing*, 31:3744–3759, 2009.
3. I. V. Oseledets and E. E. Tyrtyshnikov. TT-cross approximation for multidimensional arrays. Linear Algebra Application, 432: 70–88, 2010.

# Error estimation for the FEM solution with a few bad elements

Kenta Kobayashi[1]

Hitotsubashi University, Japan
kenta.k@r.hit-u.ac.jp

**Summary.** Let $\Omega$ be a convex polygonal domain. For $f \in L^2(\Omega)$, we consider $P^1$ finite element solution of the following Poisson equation:

$$\begin{cases} -\Delta u = f & \text{in} \quad \Omega \\ u = 0 & \text{on} \quad \partial\Omega \end{cases}.$$

In conventional error analysis for the finite element method, typical error estimation for the finite element solution $u_h$ is obtained by the following form [1]:

$$|u_h - u|_{H^1(\Omega)} \leq \max_{\tau_j} C(\tau_j)|u|_{H^2(\Omega)}$$

where $H^1$ semi-norm and $H^2$ semi-norm are defined as follows

$$|v|^2_{H^1(\Omega)} = |v_x|^2_{L^2(\Omega)} + |v_y|^2_{L^2(\Omega)}, \qquad |v|^2_{H^2(\Omega)} = |v_{xx}|^2_{L^2(\Omega)} + 2|v_{xy}|^2_{L^2(\Omega)} + |v_{yy}|^2_{L^2(\Omega)},$$

$\tau_j$ are triangular elements which composing a mesh division, and $C(T)$ is a constant which only depends on triangle $T$.

Concerning this error estimation, even one bad element results in poor error estimation because we take maximum of $C(\tau_j)$. However, numerical results suggest that a few bad elements do not lead to an increase in error. We have provided theoretical proof for this fact with the concrete error estimation. In other words, under certain conditions, we proved that the presence of a few bad elements does not worsen the error of the finite element method.

**Keywords**: finite element method, error estimation, triangular elements

**Mathematics Subject Classifications (2010)**: 65N30

## References

1. S. C. Brenner , L. R. Scott. *The Mathematical Theory of Finite Element Methods*, Springer, New York, 2008.

# A finite differences scheme for a Camassa-Holm type equation.

Héctor Torres Apablaza[1] and Rodrigo Véjar Asem[2]

Departamento de Matemáticas, Universidad de La Serena
htorres@userena.cl
Departamento de Matemáticas, Universidad de La Serena
rodrigo.vejar@userena.cl

**Summary.** A finite differences scheme for a Camassa-Holm type equation will be presented. In particular, we will find approximate solutions for the Cauchy problem

$$\begin{cases} u_t - 2u_{xxt} + u_{xxxxt} = -3uu_x + 4uu_{xxx} - uu_{xxxxx} + 5u_xu_{xx} \\ \qquad\qquad\qquad\qquad -2u_xu_{xxxx} - 6u_{xx}u_{xxx} + 2u_{xxx}u_{xxxx} + u_{xx}u_{xxxxx}, \\ u(x,0) = u_0(x). \end{cases} \tag{1}$$

The equation was first proposed by Qiao and Reyes in [2], and it is a variation of the original Camassa-Holm equation first proposed in [3], which is a dispersive shallow water equation that possess special soliton solutions known as *peakons*.

In this talk, the numerical scheme will be presented, along with a preview of some of its properties and numerical examples of its performance.

**Keywords**: Finite difference scheme, Camassa-Holm equation, hyperbolic-elliptic system.

**Mathematics Subject Classifications (2010)**: 35G25, 35L05, 65M06, 65M12

## References

1. M. DELFOUR, M. FORTIN, G. PAYRE, *Finite-Difference Solutions of a Non-linear Schrödinger Equation.* Journal of Computational Physics 44 (1981), 277-288.
2. Z. QIAO, E. G. REYES, *Fifth-order equations of Camassa-Holm type and pseudo-peakons*, Applied Numerical Mathematics, https://doi.org/10.106/j.apnum.2022.12.015
3. CAMASSA, ROBERTO AND HOLM, DARRYL D.. *An integrable shallow water equation with peaked solitons*. Physical Review Letters, 71 (1993), 1661 - 1664.

# MS18: Structure preserving methods for nonlinear conservation equations

# Active flux for triangular meshes for non linear hyperbolic problems

Rémi Abgrall[1], Jianfang Lin[2], and Yongle Liu[3]

Institute of Mathematics, University of Zürich, Switzerland
remi.abgrall@math.uzh.ch
Institute of Mathematics, University of Zürich, Switzerland

Institute of Mathematics, University of Zürich, Switzerland

**Summary.** In this article, we show how to construct a numerical method for solving hyperbolic problems, whether linear or nonlinear, using a continuous representation of the variables and their mean value in each triangular element. This type of approach has already been introduced by Roe, and others, in the multidimensional framework under the name of Active flux, see [1, 2, 3, 4, 5]. Here, the presentation is more general and follows [6, 7]Various examples (linear advection, KPP, Euler equations) show the good behavior of the method in both linear and nonlinear cases, including non-convex problems. The expected order of precision is obtained in the linear case. This work represents a step towards the development of methods in the spirit of virtual finite elements for linear or nonlinear hyperbolic problems, including the case where the solution is not regular.

**Keywords**:

**Mathematics Subject Classifications (2010)**:

## References

1. T.A. Eyman and P.L. Roe. Active flux. 49th AIAA Aerospace Science Meeting, 2011.
2. T.A. Eyman and P.L. Roe. Active flux for systems. 20 th AIAA Computationa Fluid Dynamics Conference, 2011.
3. T.A. Eyman. *Active flux*. PhD thesis, University of Michigan, 2013.
4. C. Helzel, D. Kerkmann, and L. Scandurra. A new ADER method inspired by the active flux method. *Journal of Scientific Computing*, 80(3):35–61, 2019.
5. W. Barsukow. The active flux scheme for nonlinear problems. *J. Sci. Comput.*, 86(1):Paper No. 3, 34, 2021.
6. R. Abgrall. A combination of residual distribution and the active flux formulations or a new class of schemes that can combine several writings of the same hyperbolic problem: application to the 1d Euler equations. *Commun. Appl. Math. Comput.*, 5(1):370–402, 2023.
7. Remi Abgrall and Wasilij Barsukow. Extensions of active flux to arbitrary order of accuracy. *ESAIM, Math. Model. Numer. Anal.*, 57(2):991–1027, 2023.

# An asymptotic preserving method for the linear transport equation on general meshes

Pierre Anguill[1], Patricia Cargo[2], Cedric Énaux[3], Philippe. Hoch[4], Emmanuel Labourasse[5], and Gerald Samba[6]

CEA, DAM, DIF, F-91297 Arpajon, France.
pierre.anguill@cea.fr
CEA, DAM, DIF, F-91297 Arpajon, France.
patricia.cargo@cea.fr
CEA, DAM, DIF, F-91297 Arpajon, France.
cedric.enaux@cea.fr
CEA, DAM, DIF, F-91297 Arpajon, France.
philippe.hoch@cea.fr
CEA, DAM, DIF, F-91297 Arpajon, France.
emmanuel.labourasse@cea.fr
CEA, DAM, DIF, F-91297 Arpajon, France.
gerald.samba@cea.fr

**Summary.** This talk presents a finite-volume scheme [1] for a linear transport equation derived from a linearization of the radiative transfer equations. This scheme has been implemented on 2D unstructured meshes, and satisfies the following properties:

**P1** to be consistent on general meshes,
**P2** to enforce the conservation of radiative energy,
**P3** to be able to handle all the radiation regimes from free-streaming to diffusion (Asymptotic Preserving),
**P4** to have the radiative energy degrees of freedom located at the centers of the elements to ensure the compatibility with the hydrodynamic scheme.
**P5** to allow us to use the limit diffusion scheme of our choice.

As our scheme is implicit, we used a system of sub-iterations to avoid to solve a global linear system (of size equal to the cells number $\times$ directions number), while remaining stable. In addition, this sub-iterations system is acting as a fixed point loop, in order to get rid of the non-linearity of the diffusion scheme. Thanks to the properties of our diffusion scheme, we enforce the energy to remain positive in this regime, for which radiation and matter temperature are strongly coupled. We have conducted numerical 1D tests on structured and unstructured 2D meshes, which assess that the expected properties are respected. Finally, we carried out the Lattice problem test to compare our results with existing methods, in particular the Discontinuous Finite Element (DFE) discretization.

**Keywords**: Finite Volume, radiative transfer, asymptotic analysis, computational transport, monotone anisotropic diffusion, unstructured meshes.

**Mathematics Subject Classifications (2010)**: 65M08, 65M22.

## References

1. Anguill, P., Cargo, P., Énaux, C., Hoch, P., Labourasse, E., and Samba, G. (2022). An asymptotic preserving method for the linear transport equation on general meshes. *Journal of Computational Physics*, 450:110859.

# Boundary stabilization of the Korteweg-de Vries-Burgers equation with an infinite memory-type control and applications: a qualitative and numerical analysis

Boumediene Chentouf[1], Aissa Guesmia[2], Mauricio Sepúlveda[3], and Rodrigo Véjar Asem[4]

Kuwait University, Faculty of Science, Department of Mathematics Safat 13060, Kuwait
boumediene.chentouf@ku.edu.kw
Institut Elie Cartan de Lorraine, UMR 7502, Université de Lorraine, France
aissa.guesmia@univ-lorraine.fr
CI$^2$MA and DIM, Universidad de Concepción, Concepción-Chile
maursepu@udec.cl
Departamento de Matemáticas, Universidad de La Serena, La Serena, Chile
rodrigo.vejar@userena.cl

**Summary.** This work is intended to present a qualitative and numerical analysis of well-posedness and boundary stabilization problems of the well-known Korteweg-de Vries-Burgers equation. Assuming that the boundary control is of memory type, the history approach is adopted in order to deal with the memory term. Under sufficient conditions on the physical parameters of the system and the memory kernel of the control, the system is shown to be well-posed by combining the semigroups approach of linear operators and the fixed point theory. Then, energy decay estimates are provided by applying the multiplier method. An application to the Kuramoto-Sivashinsky equation will be also given. Moreover, we present a numerical analysis based on a finite differences method and provide numerical examples illustrating our theoretical results.

**Keywords**: Korteweg-de Vries-Burgers equation, Kuramoto-Sivashinsky equation, boundary infinite memory, well-posedness, stability, numerical analysis, semigroups approach, fixed point theory, energy method, finite differences method.

**Mathematics Subject Classifications (2010)**: 35B40, 35G31, 35Q35, 65M06.

## References

1. B. Chentouf and A. Guesmia, Well-posedness and stability results for the Korteweg-de Vries-Burgers and Kuramoto-Sivashinsky equations with infinite memory: a history approach, *Nonlinear Analysis,* 65 (2022), 30 pages.
2. Boumediene Chentouf, Aissa Guesmia, Mauricio Sepúlveda, Rodrigo Véjar-Asem: *Boundary stabilization of the Korteweg-de Vries-Burgers equation with an infinite memory-type control and applications: a qualitative and numerical analysis* Pre-print DIM 2023-10 y Pre-print CI$^2$MA 2023-21.
3. Raul Nina Mollisaca, Mauricio Sepúlveda Cortés, Rodrigo Véjar Asem, Octavio Vera Villagrán *Gain of regularity for a coupled system of generalized nonlinear Schrödinger equations* eprint arXiv:2301.07816, 2023.

*MS was supported by Fondecyt-ANID project 1220869, ANID (Chile) through project Centro de Modelamiento Matemático (BASAL projects ACE210010 and FB210005), ECOS-Sud project C20E03 (France - Chile), INRIA Associated team ANACONDA, and Jean d'Alembert fellowship program, Université de Paris-Saclay.

# A geometrically and thermodynamically compatible finite volume scheme for continuum mechanics on unstructured Voronoi meshes

Walter Boscheri[1]

Department of Mathematics and Computer Science, University of Ferrara, Ferrara, Italy
walter.boscheri@unife.it

**Summary.** We consider a first order hyperbolic formulation of the equations of continuum mechanics [1], that includes fluid mechanics as well as solid mechanics. This system falls into the larger class of overdetermined hyperbolic and thermodynamically compatible (HTC) systems of partial differential equations. They satisfy an entropy inequality (second principle of thermodynamics) and conserve total energy (first principle of thermodynamics). Furthermore, the governing equations involve a geometric constraint that links the determinant of deformation gradient to the density of the material under study. This is also known as the Geometric Conservation Law (GCL), which can be regarded as an extra conservation law admitted by the governing equations. The aim of this talk is to present a novel geometrically and thermodynamically compatible cell-centered finite volume scheme on unstructured Voronoi meshes. First, the governing equations are written in fluctuation form. Next, the non-compatible numerical fluxes of the deformation gradient are corrected using a scalar correction factor that is defined at the faces of the grid. This allows to achieve full compatibility with the GCL, hence ensuring positivity of density. Eventually, another scalar factor takes into account thermodynamic compatibility by a correction which only acts on the momentum and the total energy equation, in order not to destroy the geometric compatibility previously obtained. This exhibits a direct link with thermodynamic compatibility in Lagrangian coordinates [2]. Entropy preservation can then be attained on general unstructured meshes. The novel schemes are provably compatible at the semi-discrete level and their accuracy and robustness are validated against a set of benchmarks for fluid and solid mechanics.

**Keywords**: thermodynamically compatible finite volume schemes, Geometric Conservation Law, cell entropy inequality, positivity preserving, unstructured mesh

**Mathematics Subject Classifications (2010)**: please, name your files after the lastname of the first author, that is `lastname.tex`, and send both the .tex and .pdf files.

## References

1. I. Peshkov and E. Romenski. A hyperbolic model for viscous Newtonian flows. 28 (2016) 85–104 *Contin. Mech. Thermodyn.*, 28: 85-104, 2016.
2. W. Boscheri, M. Dumbser, P.-H. Maire. A NEW THERMODYNAMICALLY COMPATIBLE FINITE VOLUME SCHEME FOR LAGRANGIAN GAS DYNAMICS. SIAM *Journal of Scientific Computing*, submitted, 2023.

# Implicit discretization of Lagrangian gas dynamics

Setéphane Del Pino[1], Bruno Després[2], and Alexiane Plessier[3]

CEA, DAM, DIF, F-91297 Arpajon, France and Université Paris-Saclay, LIHPC, France
stephane.delpino@cea.fr
LJLL (UMR 7598) – Laboratoire Jacques-Louis Lions, France
bruno.despres@sorbonne-universite.fr
Université Paris-Saclay, CEA, STMF, 91191, Gif-sur-Yvette, France
alexiane.plessier@cea.fr

**Summary.** We have recently proposed an implicit discretization of the Lagrangian gas dynamics in 1D in [1]. Whichever the time step $\Delta t > 0$ is, we proved that the scheme is well defined, conservative and stable. More precisely, the scheme ensures that the solution obtained at time $t^{n+1}$ belongs to the invariant domain of Euler's equation and that it satisfies the desired entropy inequality.

In short, the method proposed and analyzed in [1] is a predictor-corrector scheme. Following [2], the implicit predictor step approximates isentropic Euler equations, and the corrector explicit step restores the conservation of total energy using the implicit fluxes computed in the predictor.

In this presentation, we show how this method extends to higher-dimension and explain the new difficulties in this case. We insist on the discrepancy of the volumes calculation computed by the scheme and using the new node positions. We explain how to modify the scheme to retrieve the same stability properties as in the 1D case. The behavior of the scheme is illustrated using representative numerical tests.

**Keywords**: Lagrangian, Finite volume, gas dynamics, implicit method, nonlinear stability.

**Mathematics Subject Classifications (2010)**: 65M08, 65M22.

## References

1. A. Plessier and S. Del Pino and B. Després, Implicit discretization of Lagrangian gas dynamics. *ESAIM: M2AN*, 57(2):717-743, 2023.
2. C. Chalons, F. Coquel and C. Marmignon, Time-implicit approximation of the multipressure gas dynamics equations in several space dimensions. *SIAM Journal on Numerical Analysis* 48:1678-1706, 2010.

# An exactly curl-free scheme for a hyperbolic model of compressible two-fluid flows

Laura del Río Martín[1] and Firas Dhaouadi[2]

Department of Information Engineering and Computer Science, University of Trento, via Sommarive 9, Povo, 38123, Trento, Italy
laura.delrio@unitn.it
Laboratory of Applied Mathematics, DICAM, University of Trento, Via Mesiano 77, 38123, Trento, Italy
firas.dhaouadi@unitn.it

**Summary.** We present a structure-preserving scheme for the compressible two-velocity two-pressure two-fluid model of Romenski *et. al* [1, 2] in the barotropic case. The governing equations are derived in the scope of symmetric hyperbolic thermodynamically compatible models and consist in a set of first-order hyperbolic conservation laws. In the absence of algebraic sources terms, the model is submitted to a curl-free constraint affecting the relative velocity, which nevertheless allows to recover strong hyperbolicity in multiple space dimensions. Thus, in order to preserve this structure at the numerical level, the model is solved numerically using a second-order exactly curl-free finite volume scheme. The method is based on a staggered grid discretization where the curl-bound vector is stored in the cell vertexes while all the remaining variables are stored in the cell centers. This allows to define specific discrete compatible gradient and curl operators that ensure the discrete curl errors are zero at the machine level precision. Lastly, we present a set of numerical results further emphasizing this property.

**Keywords**: Multiphase flows, Hyperbolic models, curl-free schemes, structure-preserving,

**Mathematics Subject Classifications (2010)**: 65M08; 35L40; 76M12; 76T10

## References

1. E Romenski, A Resnyansky, and E Toro. Conservative hyperbolic formulation for compressible two-phase flow with different phase pressures and temperatures. *Quarterly of applied mathematics*, 65(2):259–279, 2007.
2. Evgeniy Romenski, Dimitris Drikakis, and Eleuterio Toro. Conservative models and numerical methods for compressible two-phase flow. *Journal of Scientific Computing*, 42:68–95, 2010.

# Particle dynamics with shocks on Voronoï meshes

Bruno Després[1]

LJLL/ Sorbonne Université, Paris
bruno.despres@sorbonne.universite.fr

**Summary.** As discussed in [1] for astrophysical applications, there always has been interesting questions at the intersection of standard discretization of PDEs in view of applications and the use of meshes with various given structures. See also the seminal work [4]. In this direction, we present a new first order numerical method [2] on lagrangian and moving Voronoï meshes for the numerical simulation of compressible flows with shocks and internal interfaces between different gas. The scheme can be seen either as a particle method (the mass of particles is constant and there is no connectivity between particles) or as specific finite volume solver.

The method is based on the closed form formula of the partial derivative of the volume of Voronoï cells with respect to the generators. The mathematical proof of the formula with partition functions comes from applied statistical physics [3], and it seems original with respect to the mathematical literature. A corollary is that the volume of Voronoï cells is generically of class $C^1$ with respect to the generators. The final scheme is conservative in local mass, total momentum and total energy, and it is endowed with an entropy inequality which insures the correctness of shocks calculations. Numerical illustrations in dimension $d = 2$ will be shown for basic problems on coarse meshes. The implementation developed to obtain the numerical illustrations uses a freely available library for the generation of the Voronoï cells at all time steps.

Other open problems will be discussed, in particular wether the closed form formula can be used for the discretization of other PDEs.

**Keywords**:

**Mathematics Subject Classifications (2010)**:

## References

1. V. Springel, E pur si muove: Galilean-invariant cosmological hydrodynamical simulations on a moving mesh, Mon. Not. R. Astron. Soc., 2009.
2. B. Després, Lagrangian Voronoï meshes and particle dynamics with shocks, 2023, https://hal.sorbonne-universite.fr/hal-04166811v2
3. M. Serrano and P. Espanol, Thermodynamically consistent mesoscopic fluid particle model, Physical Review E, Vol 64, 046115, 2000.
4. M. Shashkov and A. Solovjov, Numerical simulation of two-dimensional flows by the free-Lagrangian method, TUM Mathematishes institut report 1991.

# A structure-preserving scheme for a hyperbolic approximation of the Navier-Stokes-Korteweg equations

Firas Dhaouadi[1] and Michael Dumbser[2]

Laboratory of Applied Mathematics, DICAM, University of Trento, Via Mesiano 77, 38123 Trento, Italy
firas.dhaouadi@unitn.it
Laboratory of Applied Mathematics, DICAM, University of Trento, Via Mesiano 77, 38123 Trento, Italy
michael.dumbser@unitn.it

**Summary.** We present an explicit second-order accurate structure-preserving finite volume scheme for the hyperbolic approximation of the Navier-Stokes-Korteweg equations. The model combines the unified Godunov-Peshkov-Romenski model of continuum mechanics with a recently proposed hyperbolic reformulation of the Euler-Korteweg system. The considered PDE system includes an evolution equation for a gradient field that is by construction endowed with a curl-free constraint. The numerical scheme presented here relies on the use of vertex-based staggered grids and is proven to preserve the curl constraint *exactly* at the discrete level, up to machine precision. We show evidence of this property via a set of numerical tests, including non-condensing bubbles as well as non-stationary Ostwald ripening test cases with several bubbles. We present quantitative and qualitative comparisons of the numerical solution, both, when the new structure-preserving discretization is applied and when it is not. In particular we show that some numerical solutions blow up in finite time when the curl-free constraint is not respected.

**Keywords**: Navier-Stokes-Korteweg system, hyperbolic systems, compressible multi-phase flows, structure-preserving curl-free schemes, staggered finite volume method, augmented Lagrangian approach,

**Mathematics Subject Classifications (2010)**: 65M08; 35L40; 76M12; 76T10

## References

1. Dhaouadi F, Dumbser M. 2023 A structure-preserving finite volume scheme for a hyperbolic reformulation of the Navier–Stokes–Korteweg equations. *Mathematics* **11**, 876.
2. Dhaouadi F, Dumbser M. 2022 A first order hyperbolic reformulation of the Navier-Stokes-Korteweg system based on the GPR model and an augmented Lagrangian approach. *Journal of Computational Physics* **470**, 111544.

# Continuously bounds-preserving limiting methods for high-order discontinuous Galerkin schemes

Tarik Dzanic[1]

Lawrence Livermore National Laboratory, Livermore, CA 94550, United States of America
dzanic1@llnl.gov

**Summary.** The efficient and accurate computation of complex transport phenomena remains a driving force in the development of high-fidelity numerical discretization techniques. Within this broad field of research, the use of finite element methods such as discontinuous Galerkin (DG) schemes has grown in prevalence due to their high-order accuracy, geometric flexibility, and computational efficiency. However, their accuracy and robustness can become severely degraded when the physical systems in question must abide by strict constraints, which is frequently the case in multi-physics applications. Standard DG implementations do not generally guarantee that these constraints are satisfied by the discrete solution, which may result in inaccurate and physically inconsistent predictions or, more typically, the failure of the scheme altogether.

A typical remedy for this problem is to enforce these constraints via some form of *a posteriori* limiting on the discrete solution, combining the solution of the high-order scheme with a more robust, low-order scheme [1]. One critical drawback of these limiting approaches is that they are typically performed *discretely*, whereas the DG solution is represented piecewise continuously, such that the schemes are only provably bounds-preserving at the discrete spatial locations where the limiting was performed. For many applications, this is not sufficient – it is common in FEM to have to evaluate the solution at some other points which, in some cases, may not even be known *a priori* (e.g., in the remap stage of an arbitrary Lagrangian-Eulerian solver [2]).

In this talk, I will present a limiting technique for convex constraints in DG schemes which ensures that the solution is *continuously bounds-preserving* (i.e., across the entire solution polynomial) for any arbitrary choice of basis and approximation order. The proposed approach relies on utilizing the ability of DG schemes to preserve convex invariants on the element-wise mean [3] along with modified formulations of the constraint functionals which reduce the limiting operation to a single spatial minimization problem for each element in the mesh. As a result, the approach can be efficiently and straightforwardly implemented in general DG codebases and can be applied to a wide variety of governing equations and user-specified constraint functionals. The results of the proposed approach will be shown for high-order, unstructured DG schemes applied to nonlinear scalar transport problems and the compressible Euler equations.

**Keywords**: discontinuous Galerkin schemes, bounds preserving, limiting, structure preserving, hyperbolic conservation laws

**Mathematics Subject Classifications (2010)**: 65M60, 65M12, 35L65

## References

1. J. P. Boris and D. L. Book. Flux-corrected transport. *Journal of Computational Physics*, 135(2):172-186, 1997.
2. R. Anderson, V. Dobrev, Tz. Kolev, D. Kuzmin, M. Quezada de Luna, R. Rieben, and V. Tomov. High-order local maximum principle preserving (MPP) discontinuous Galerkin finite element method for the transport equation. *Journal of Computational Physics*, 334:102-124, 2008.
3. X. Zhang and C.W. Shu. High-order local maximum principle preserving (MPP) discontinuous Galerkin finite element method for the transport equation. *Journal of Computational Physics*, 229(9):3091-3120, 2010.

# Spectral correctness of the discontinuous Galerkin approximation of the first-order form of Maxwell's equations with discontinuous coefficients

Jean-Luc Guermond[1] and Alexandre Ern[2]

Department of Mathematics, Texas A&M University, College Station, TX 77843, USA
guermond@tamu.edu
CERMICS, Ecole des Ponts, 77455 Marne-la-Vallee Cedex 2, France and INRIA Paris, 75589 Paris, France
alexandre.ern@enpc.fr

**Summary.** The paper analyzes the discontinuous Galerkin approximation of Maxwell's equations written in first-order form and with non-homogeneous magnetic permeability and electric permittivity. Although the Sobolev smoothness index of the solution may be smaller than $\frac{1}{2}$, it is shown that the approximation is spectrally correct. The convergence proof is based on a duality argument. One essential idea is that the smoothness index of the dual solution is always larger than $\frac{1}{2}$ irrespective of the regularity of the material properties. Discrete involutions also play a key role in the analysis.

**Keywords**: Curl-curl problem, duality argument, involution, spectral approximation, finite elements, Maxwell's equations

**Mathematics Subject Classifications (2010)**: 65M60, 65M12, 65N30, 35L02, 35L05, 35Q61

# Proximal Galerkin: A structure-preserving finite element method for pointwise bound constraints

Brendan Keith[1] and Thomas M. Surowiec[2]

Brown University
brendan_keith@brown.edu
Simula Research Laboratory
thomasms@simula.no

**Summary.** The proximal Galerkin finite element method is a high-order, nonlinear numerical method that preserves the geometric and algebraic structure of bound constraints in infinite-dimensional function spaces. In this talk, we will introduce the proximal Galerkin method and apply it to solve free-boundary problems, enforce discrete maximum principles, and develop scalable, mesh-independent algorithms for optimal design. The proximal Galerkin framework is a natural consequence of the latent variable proximal point (LVPP) method: an unconditionally stable alternative to the interior point method. LVPP is an infinite-dimensional optimization algorithm that may be viewed as having an adaptive barrier function that is updated with a new informative prior at each (outer loop) optimization iteration. One of the main benefits of this algorithm is witnessed when analyzing the classical obstacle problem. Therein, we find that the original variational inequality can be replaced by a sequence of semilinear partial differential equations (PDEs) that are readily discretized and solved with, e.g., high-order finite elements. Throughout the talk, we will arrive at several unexpected contributions that may be of independent interest. These include (1) a semilinear PDE we refer to as the entropic Poisson equation; (2) an algebraic/geometric connection between high-order positivity-preserving discretizations and an infinite-dimensional Lie group; and (3) a gradient-based, bound-preserving algorithm for two-field density-based topology optimization. The complete latent variable proximal Galerkin methodology combines ideas from nonlinear programming, functional analysis, tropical algebra, and differential geometry and can potentially lead to new synergies among these areas as well as within variational and numerical analysis. This talk is based on [1].

**Keywords**: pointwise bound constraints, bound-preserving discretization, entropy regularization, proximal point

**Mathematics Subject Classifications (2010)**: 49M37, 65K15, 65N30

## References

1. B. Keith, T.M. Surowiec. Proximal Galerkin: A structure-preserving finite element method for pointwise bound constraints arXiv preprint arXiv:2307.12444 2023.

# Reduction of material diffusion in multi-material ALE remap: conservative and bounded matrix-free method

Tzanio V. Kolev[1], Robert N. Rieben[2], Vladimir Z. Tomov[3], and Arturo Vargas[4]

Lawrence Livermore National Laboratory
kolev1@llnl.gov
Lawrence Livermore National Laboratory
rieben1@llnl.gov
Lawrence Livermore National Laboratory
tomov2@llnl.gov
Lawrence Livermore National Laboratory
vargas45@llnl.gov

**Summary.** We propose a new method for remap of material volume fractions, densities, and specific internal energies in the context of multi-material compressible ALE hydrodynamics [1]. The remap is based on advection in pseudotime. As the volume fraction approach may diffuse materials over many mesh elements, we introduce a sharpening modification on PDE level. We explain the effects of the modification and how it produces results that are still conservative for volume, mass, internal energy, and bounded with respect to the volume fraction, density, and specific internal energy. The latter involves FCT-type methods. The second major contribution, in addition to sharpening, is that all remap methods avoid assembly of global matrices. This avoids data motion and enables higher computational efficiency [2, 3].

**Keywords**: advection remap, volume fractions, material diffusion, bounds preservation, matrix-free

**Mathematics Subject Classifications (2010)**: 65M60, 76N15, 76L05

Performed under the auspices of the U.S. Department of Energy under Contract DE-AC52-07NA27344 (LLNL-ABS-847808).

## References

1. R. Anderson and V. Dobrev and T. Kolev and R. Rieben and V. Tomov. High-Order Multi-Material ALE Hydrodynamics. *SIAM J. Sci. Comp.*, 40(1):B32-B58, 2018.
2. A. Vargas and T. Stitt and K. Weiss and V. Tomov and J.-S. Camier and T. Kolev and R. Rieben. Matrix-free approaches for GPU acceleration of a high-order finite element hydrodynamics application using MFEM, Umpire, and RAJA. *Int. J. High Perform. Comput. Appl.*, 36(4):492-509, 2022.
3. P. Bello-Maldonado and T. Kolev and R. Rieben and V. Tomov. A Matrix-Free Hyperviscosity Formulation for High-Order ALE Hydrodynamics. *Comput. Fluids*, 205:104577, 2020.

# Structure-preserving finite-element schemes for coupled Euler-Poisson and Euler-Maxwell systems

Matthias Maier[1], Jordan Hoffart[2], and Ignacio Tomas[3]

Department of Mathematics, Texas A&M University, College Station 77843 TX, USA
maier@tamu.edu
Department of Mathematics, Texas A&M University, College Station 77843 TX, USA
jordanhoffart@tamu.edu
Department of Mathematics & Statistics, Texas Tech University, 2500 Broadway Lubbock 79409 TX, USA
igtomas@ttu.edu

**Summary.** We discuss structure-preserving numerical discretizations for the Euler-Poisson and Euler-Maxwell systems. The schemes are fully discrete and structure preserving in the sense that they maintains a discrete energy law, as well as hyperbolic invariant domain properties, such as positivity of the density and a minimum principle of the specific entropy.

We discuss the underlying algebraic discretization technique based on collocation and convex limiting that maintain hyperbolic invariants and a discrete energy law, and discuss recovery strategies to maintain the discrete Gauss law.
**Keywords**:

**Mathematics Subject Classifications (2010)**:

# A high-order explicit Runge-Kutta approximation technique for the Shallow Water Equations

Eric J. Tovar[1]

Los Alamos National Laboratory
ericjtovar@lanl.gov

**Summary.** We introduce a higher-order in time approximation of the Shallow Water Equations that is invariant-domain preserving and well-balanced. The employed time-stepping technique is a novel explicit Runge-Kutta (ERK) approach which is an extension of the class of ERK-IDP methods introduced in [1] for systems of non-linear conservation equations. Moreover, we show that any explicit Runge-Kutta method applied to the Shallow Water Equations, supplemented with a higher-order in space discretization, can be made mass conservative, invariant-domain preserving and well-balanced with respect to rest states. The resulting method is then numerically illustrated through verification and validation

**Keywords**: shallow water equations, well-balanced, higher-order accuracy, convex limiting, explicit Runge-Kutta, time discretization

**Mathematics Subject Classifications (2010)**: 65M60, 65M12, 35L50, 35L65, 76M10

## References

1. Alexandre Ern and Jean-Luc Guermond Invariant-Domain-Preserving High-Order Time Stepping: I. Explicit Runge–Kutta Schemes. SIAM *Journal on Scientific Computing*, 44(5):A3366-A3392, 2022.

# A simple and efficient convex optimization based bound-preserving high order accurate limiter for Cahn–Hilliard–Navier–Stokes system

Chen Liu[1], Beatrice Riviere[2], Jie Shen[3], and Xiangxiong Zhang[4]

Department of Mathematics, Purdue University, West Lafayette, IN, USA
liu3373@purdue.edu
Department of Computational Applied Mathematics and Operations Research, Rice University, Houston, Texas, USA
riviere@rice.edu
Department of Mathematics, Purdue University, West Lafayette, IN, USA
shen7@purdue.edu
Department of Mathematics, Purdue University, West Lafayette, IN, USA
zhan1966@purdue.edu

**Summary.** For time-dependent PDEs, the numerical schemes can be rendered bound-preserving without losing conservation and accuracy, by a post processing procedure of solving a constrained minimization in each time step. Such a constrained optimization can be formulated as a nonsmooth convex minimization, which can be efficiently solved by first order optimization methods, if using the optimal algorithm parameters. By analyzing the asymptotic linear convergence rate of the generalized Douglas–Rachford splitting method, optimal algorithm parameters can be approximately expressed as a simple function of the number of out-of-bounds cells. We demonstrate the efficiency of this simple choice of algorithm parameters by applying such a limiter to cell averages of a discontinuous Galerkin scheme solving phase field equations for 3D demanding problems. Numerical tests on a sophisticated 3D Cahn–Hilliard–Navier–Stokes system indicate that the limiter is high order accurate, very efficient, and well-suited for large-scale simulations. For each time step, it takes at most 20 iterations for the Douglas–Rachford splitting to enforce bounds and conservation up to the round-off error, for which the computational cost is at most $80N$ with $N$ being the total number of cells.

**Keywords**: Douglas–Rachford splitting, nearly optimal parameters, bound-preserving limiter, discontinuous Galerkin method, Cahn–Hilliard–Navier–Stokes, high order accuracy

**Mathematics Subject Classifications (2010)**: 65K10, 65M60, 65M12, 90C25

## References

1. C. Liu, B. Riviere, J. Shen and X. Zhang, A simple and efficient convex optimization based bound-preserving high order accurate limiter for Cahn–Hilliard–Navier–Stokes system. arXiv:2307.09726

# MS19: Theoretical and numerical advances for mixed-dimensional 3d-1d coupling

# Multiscale modeling of partial discharges and electrical treeing

Beatrice Crippa[1], Anna Scotti[2], and Andrea Villa[3]

MOX, Department of Mathematics, Politecnico di Milano, Italy
beatrice.crippa@polimi.it
MOX, Department of Mathematics, Politecnico di Milano, Italy
anna.scotti@polimi.it
Ricerca Sul Sistema Energetico (RSE), Italy
villa.andrea@rse-web.it

**Summary.** Electric power is a key component of the energetic system, and one of the main causes of ageing and deterioration of solid insulating components in the electric cables consists in Partial Discharges (PD). They are caused by the effect of high electrical fields acting on dielectric domains for a long time, leading to the formation of gas-filled fractures, in which charged particles are free to move and generate an internal electric field that contributes to the increase of the external one. This process gives rise to the Electrical Treeing, a self-propagating internal defect due to the interaction of PDs and the polymeric surface, that can be fully described by a coupled system of Partial Differential Equations (PDEs) [1]. The key aspects of this problem take into account the movement of charges in the gas-filled fracture and the evolution of the electric field and potential in both materials. The main drawback in this framework is the computational time needed for the numerical simulation of the problem, due to both the strong coupling among PDEs and the geometric complexity of the gas domain. Indeed, the crack produced by the Electrical Treeing consists of a ramification with very small diameter, compared to its length and the size of the dielectric domain, implying the need for a very fine mesh around and inside the defect for the 3D discretization. We can model this phenomenon as a coupled hybrid-dimensional 3D-1D problem, where the movement of charges in the gas is described by a system of one-dimensional diffusion-transport and pure transport equations, coupled with Maxwell's equation for electrostatics in both domains. This approach leads to a simpler geometry with much less degrees of freedom. Reducing the gas domain to a line is equivalent to considering a one-dimensional charge distribution, which produces a non-negligibile radial component of the electric fields. The correct treatment of this component when passing to the limit, together with the branched structure of the 1D domain, which allows the presence of bifurcations, were the main challenges in our work. We have derived the reduced-dimensional formulation of the presented problems and developed numerical schemes for their solution, based on Finite Volumes in 1D and mixed Finite Elements in 3D, in order to improve the performance of the numerical simulation of this physical phenomenon.

**Keywords**: mixed-dimensions, 3d-1d coupling, multiscale, electrical treeing **Mathematics Subject Classifications (2010)**: 65M08,65M60

## References

1. A. Villa, L. Barbieri, M. Gondola, A. R. Leon-Garzon and R. Malgesini A PDE-based partial discharge simulator *Journal of Computational Physics*, 345: 687-705, 2017.

# A mixed-dimensional model for simulating direct current with a high-resistivity liner

Alessio Fumagalli[1], Lorenzo Panzeri[2], Luca Formaggia[3], Anna Scotti[4], and Diego Arosio[5]

Politecnico di Milano, Italy
alessio.fumagalli@polimi.it
Politecnico di Milano, Italy
lorenzo.panzeri@polimi.it
Politecnico di Milano, Italy
luca.formaggia@polimi.it
Politecnico di Milano, Italy
anna.scotti@polimi.it
Università degli Studi di Modena e Reggio Emilia, Italy
diego.arosio@unimore.it

**Summary.** In this study, we introduce a mathematical model that combines different dimensions to analyze the electric potential and current density in direct current simulations, particularly when incorporating a thin liner within the modeled area. This liner is employed in landfill management to prevent leachate leakage from the waste body into the underground, and it is constructed from a highly impermeable, high-resistivity plastic material. Given that the electrodes and the liner possess significantly smaller diameters and thickness compared to their other dimensions, conducting numerical simulations for these elements in an equi-dimensional context could be prohibitively costly. Therefore, our approach involves approximating them as objects with reduced dimensions and subsequently deriving the corresponding equations. We validate the resulting mixed-dimensional model by comparing it to progressively complex laboratory experiments, demonstrating the reliability of our proposed mathematical framework. Our experiments also indicate that configurations involving current and voltage electrodes on opposite sides of the liner, enclosing the landfill, may be effective for detecting damage to the membrane.

**Keywords**: mixed-dimensional modeling, direct current simulations, sensitivity, laboratory comparison

## References

1. Alessandro Aguzzoli, Alessio Fumagalli, Anna Scotti, Luigi Zanzi, and Diego Arosio. Inversion of synthetic and measured 3d geoelectrical data to study the geomembrane below a landfill. In *4th Asia Pacific Meeting on Near Surface Geoscience & Engineering*, volume 2021, pages 1–5. European Association of Geoscientists & Engineers, 2021.
2. Alessio Fumagalli, Lorenzo Panzeri, Luca Formaggia, Anna Scotti, and Diego Arosio. A mixed-dimensional model for direct current simulations in presence of a thin high-resistivity liner. Submitted to International Journal for Numerical Methods in Engineering. Available at arXiv:2303.12469 [math.NA], 2023.
3. Lorenzo Panzeri, Alessio Fumagalli, Alessandro Aguzzoli, Luigi Zanzi, Laura Longoni, Monica Papini, and Diego Arosio. Lab and modelling dc resistivity tests to analyse the response of a high resistivity liner. In *5th Asia Pacific Meeting on Near Surface Geoscience & Engineering*, volume 2023, pages 1–5. European Association of Geoscientists & Engineers, 2023.

# An optimization based 3D-1D coupling for tissue perfusion and chemical transport in growing capillary networks

Stefano Berrone[1], Chiara Giverso[2], Denise Grappein[3], Luigi Preziosi[4], and Stefano Scialò[5]

Department of Mathematical Sciences G. L. Lagrange, Politecnico di Torino (Italy)
stefano.berrone@polito.it
Department of Mathematical Sciences G. L. Lagrange, Politecnico di Torino (Italy)
chiara.giverso@polito.it
Department of Mathematical Sciences G. L. Lagrange, Politecnico di Torino (Italy)
denise.grappein@polito.it
Department of Mathematical Sciences G. L. Lagrange, Politecnico di Torino (Italy)
luigi.preziosi@polito.it
Department of Mathematical Sciences G. L. Lagrange, Politecnico di Torino (Italy)
stefano.scialo@polito.it

**Summary.** The application of an optimization based 3D-1D coupling strategy is proposed for the simulation of tissue perfusion and chemical transport in evolving micro-vascular structures [1]. In particular the process of angiogenesis is taken into account, consisting in the formation of new capillaries from existing ones.

Angiogenesis simulations can become very complex and computationally expensive, especially if the blood flow inside the nascent vessels and the exchanges with the surrounding tissue are accounted for as the network grows. It is a common practice in the modeling of the interactions between a capillary network and the surrounding tissue to adopt a 3D-1D coupling strategy, in which, under proper assumptions on the regularity of the solution, the computational cost of the simulation is reduced by approximating the capillaries by their centerlines. The novelty of the proposed approach lies in the strategy adopted to solve the resulting 3D-1D set of equations [2]: two auxiliary variables are introduced, approximating the value of the unknowns on the capillary wall, and a properly designed cost functional is minimized constrained by the 3D-1D system of PDEs. This PDE-constrained optimization approach appears to be highly robust and flexible in handling geometrical complexities and hence it fits particularly well angiogenesis simulations. First of all, no conformity between the 3D and the 1D meshes is required, so that remeshing is never needed as the network grows. Furthermore, a proper choice of the interface variables yields a well conditioned discrete problem, regardless of the mutual sizes of the 3D and 1D partitions. Finally, interface variables are directly available, without the need of post processing. We propose the use of the optimization based 3D-1D coupling for the modeling of fluid pressure and oxygen concentration in the tissue and inside the growing capillaries. The model also accounts for the dispersion of a chemotactic growth factor (VEGF) which is responsible for the vessel growth and which is modeled by a 3D equation with a singular sink term.

**Keywords**: 3D-1D coupling, domain-decomposition, non conforming mesh, optimization methods for PDE problems, mathematical model of angiogenesis, fluid and chemical transport in evolving networks

**Mathematics Subject Classifications (2010)**: 65N30, 65N50, 68U20, 35Q92, 92B05, 92C17

## References

1. S. Berrone, C. Giverso, D. Grappein, L. Preziosi, S. Scialò *An optimization based 3D-1D coupling strategy for tissue perfusion and chemical transport during tumor-induced angiogenesis*, (2023) https://arxiv.org/abs/2212.00692
2. S. Berrone, D. Grappein, S. Scialò, *A PDE-constrained optimization method for 3D-1D coupled problems with discontinuous solutions*, Numerical Algorithms (2023), 10.1007/s11075-023-01579-w

# Coupled Flow and Transport in the Liver Organ

Bilyana Tzolova[1]

Rice University, United States
bilyana@rice.edu

**Summary.** In contrast to many other types of cancer, the incidence of hepatocellular carcinoma (HCC) is on the rise. Unfortunately, surgical intervention is not a viable option for most HCC patients, leaving them reliant on chemotherapy treatments, specifically transarterial chemoembolization (TACE), for relief. Since these treatments can potentially obstruct blood flow to healthy liver tissue, there exists a finite number of procedures patients can undergo. Therefore, our study hopes to understand how these treatments unravel in the liver and how they affect the tumor growth. Building upon existing research in the field of computational fluid flow, we aim to model the flow and transport of chemotherapy drugs and embolic agents in the liver. Using CT images of liver cancer patients, we extract a 1D centerline of the hepatic vascular structures that deliver blood to the tumors and then construct a 3D mesh of the liver from the liver segmentation. We use the singularity subtraction technique to model the flow of blood in the liver, specially studying the flow of blood in the parts of the liver that have been affected by the embolic agent. We then extend the singularity subtraction technique to the time-dependent advection-diffusion equation to model the concentration of chemotherapy drugs in the liver and tumors. We obtain optimal convergence rates. The resulting coupled flow and transport model gives us an insight to the evolving dynamics of TACE within the liver. We use this model to evaluate the impact of TACE treatments on HCC tumors, with the hope that it will expose opportunities to improve the efficacy of these treatments in the future.

**Keywords**: singularity subtraction technique, coupled flow and transport

## References

1. I. Gjerde, K. Kumar, J. M. Nordbotten, and B. Wohlmuth. Splitting method for elliptic equations with line sources. *ESAIM: Mathematical Modelling and Numerical Analysis*, 53(5):1715–1739, 2019.

# Author Index

# Index