International Conference in Boundary and Interior Layers

BAIL 2022

Conference Programme

Universidad de Buenos Aires, Buenos Aires

28th of November - 2nd of December, 2022

Note : All talks will take place in room 1401, building $0 + \infty$, Ground Floor. Lunches will take place in the buffet of building 1.

Monday 28^{th} of November

10.00-11.00 Registration

11.10-11.30 Opening

Session 1 (chair: R. Durán)

11.30-12.30 Jens Markus Melenk - Plenary talk. *hp-FEM for spectral fractional diffusion.*

12.30-14.30 Lunch

14.30-15.00 Torsten Linß. *Resolving singularities in parabolic initial-boundary value problems.*

15.00-15.30 Tristan Pryer. *Structure preserving finite element schemes for a non-Newtonian flow.*

15.30-16.00 Coffee Break.

16.00-16.30 Lucia Gastaldi. *A Lagrange multiplier formulation for the finite element discretization of FSI.*

16.30-17.00 Daniel Quero. *Error estimates for the pointwise tracking optimal control problem of the Stokes equation.*

Tuesday 29^{th} of November

Session 2 (chair: I. Ojea)

10.00-10.30 Rodolfo Araya. *A stabilized finite element method for the Stokes–Temperature coupled problem.*

10.30-11.00 Roisin Hill. *Generating graded layer-adapted meshes using mesh partial differential equations.*

11.00-11.30 Coffee-break.

11.30-12.30 Gabriel Barrenechea - Plenary talk. *Positivity-preserving discretisations in general meshes.*

12.30-14.30 Lunch

Session 3 (chair: G. Acosta)

14.30-15.00 Volker John. *Finite element methods respecting the discrete maximum principle for convection-diffusion equations I.*

15.00-15.30 Petr Knobloch. *Finite element methods respecting the discrete maximum principle for convection-diffusion equations II.*

15.30-16.00 Coffee Break.

16.00-16.30 Julia Novo. *Reduced order models for incompressible flows.*

16.30-17.00 Joshua Vedral. *Dissipation-based WENO stabilization of high-order continuous Galerkin approximations to scalar conservation laws.*

Wednesday 30th of November

Session 4 (chair: A. Lombardi)

10.00-10.30 Thomas Führer. *MINRES methods for the singularly perturbed Darcy equations.*

10.30-11.00 Cecilia Penessi. *Robust error estimates in a balanced norm for the approximation of reaction-diffusion equations on graded meshes.*

11.00-11.30 Coffee-break.

11.30-12.30 Norbert Heuer - Plenary talk. *The DPG method and its application to problems with layers.*

12.30-14.30 Lunch

Thursday 1st of December

Session 5 (chair: A. Lombardi)

10.00-10.30 Ignacio Ojea. *Anisotropic regularity of solutions of elliptic problems with Dirac measures as data.*

10.30-11.00 Alexandre Ern. *A new perspective on time-stepping schemes: Beyond strong stability.*

11.00-11.30 Coffee-break.

11.30-12.30 Natalia Kopteva - Plenary talk. *A posteriori error estimates for singularly perturbed equations.*

12.30-14.30 Lunch

Session 6 (chair: G. Acosta)

14.30-15.00 Ben Ashby. *Adaptive regularisation applied to Richards' equation.*

15.00-15.30 Patricio Farrell. *Challenges for non-Boltzmann drift-diffusion charge transport simulations in semiconductors.*

15.30-16.00 Coffee Break.

16.00-17.00 International BAIL Assembly. Meeting room, Building I, mezzanine.

20.30- Conference Dinner. Besares Restaurant. 11 de Septiembre 3301 - Núñez, Buenos Aires.

Friday 2nd of December

Session 7 (chair: M. G. Armentano)
Minisymposium on Numerical approximation of nonlocal and fractional problems.

10.00-10.30 Juan Pablo Borthagaray. *Constructive approximation on graded meshes for the fractional Laplacian.*

10.30-11.00 Francisco Bersetche. *Coupling local and nonlocal equations with Neumann boundary conditions.*

11.00-11.30 Coffee-break.

11.30-12.00 Jens Markus Melenk *Weighted analytic regularity for the integral fractional Laplacian in polygons and application to hp-FEM.*

12.00-12.30 Gabriel Acosta *An iterative method for local/nonlocal coupled systems.*

12.30-14.30 Lunch

Abstracts

hp-FEM for spectral fractional diffusion

Jens Markus Melenk, *Technische Universität Wien*
Lehel Banjai, *Heriot Watt University*
Alexander Rieder, *Technische Universität Wien*
Christoph Schwab, *ETH Zürich*

The numerical treatment of fractional differential operators is challenging due to their non-local nature. Additional numerical challenges arise in particular in the case of bounded domains from strong singularities of the solution at the boundary. In this talk we present recent results for high order finite element discretizations (*hp*-FEMs) of the spectral fractional Laplacian in bounded domains, in particular on polygonal domains. In this situation the solution has strong boundary singularities as well as corner singularities. We present mesh design principles that are based on geometric refinement towards the corners and anisotropic geometric refinement towards the boundary. We show that *hp*-FEM on such meshes can deliver exponential convergence. We discuss in more detail two high order discretization schemes. The first one is based on the Caffarelli-Silvestre extension, which realizes the non-local fractional Laplacian as a Dirichlet-to-Neumann map of a (degenerate) elliptic boundary value problem (BVP). This BVP is amenable to a discretization by high order finite element method (*hp*-FEM). The second discretization is based on the so-called "Balakrishnan" formula, an integral representation of the inverse of the spectral fractional Laplacian. The discretization of the integral leads to a collection of BVPs, which can be discretization by *hp*-FEM. For both discretization schemes, exponential convergence of *hp*-FEM is established. Extensions to time-dependent problems will also be given.

Resolving singularities in parabolic initial-boundary value problems

Torsten Linß, *FernUniversität in Hagen*
Brice Girol, *FernUniversität in Hagen*

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

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

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 (potentially small,) positive parameters μ and ε and $\phi_0(0) \neq 0$.

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

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

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.

Structure preserving finite element schemes for a non-Newtonian flow

Tristan Pryer, *University of Bath*

We propose a finite element discretisation of a three-dimensional non-Newtonian flow whose dynamics are described by an Upper Convected Maxwell model. The scheme preserves structure in the sense that the velocity is divergence free and the overall discretisation is energy consistent with the underlying problem. We investigate the problem's complexity and devise relevant timestepping strategies for efficient solution realisation. We showcase the method with several numerical experiments, confirm the theory and demonstrate the efficiency of the scheme.

A Lagrange multiplier formulation for the finite element discretization of FSI

Lucia Gastaldi, *Università di Brescia*

We provide a general variational framework for the finite element discretization of fluid-structure interaction problems. In this talk we consider the case of an elastic body immersed in an incompressible fluid, it can be either a thick or a thin body. Our formulation originates from the so called Finite Element Immersed Boundary Method (FE-IBM) and can be interpreted as a fictitious domain approach. It is based on the introduction of a Lagrange multiplier so that the problem fits in the framework of saddle point systems. We present a recent result on the existence and uniqueness of the solution in a linearized case. Moreover, we discuss the finite element discretization, which requires proper choices for the finite elements spaces and an accurate analysis in order to obtain the solvability of the problem at each time step. With the aid of the simpler interface problem presenting the same features as the saddle point problem resulting from the time discretization of the FSI system, we analyze new choices for the finite element spaces and obtain error estimates.

The results presented here have been obtained in collaboration with Daniele Boffi, Fabio Credali, and Najwa Alshehri.

Error estimates for the pointwise tracking optimal control problem of the Stokes equations

Daniel Quero, *Universidad Técnica Federico Santa María*
Alejandro Allendes, *Universidad Técnica Federico Santa María*
Francisco Fuica, *Universidad Técnica Federico Santa María*
Enrique Otárola, *Universidad Técnica Federico Santa María*

In this work we consider the pointwise tracking optimal control problem of the Stokes equations. This problem entails the minimization of a linear-quadratic cost functional that involves point evaluations of the velocity field that solves the Stokes equations. Control constraints are also considered. The purpose of this work is to derive a priori and a posteriori error estimates for a finite element discretization of the aforementioned optimal control problem. We utilize the lowest-order Taylor Hood scheme for the discretization of the state and the adjoint equations. To approximate the control variable, we consider piecewise quadratic and piecewise constant functions.

A stabilized finite element method for the Stokes-Temperature coupled problem

Rodolfo Araya, *Universidad de Concepción*
Cristian Cárcamo, *Universidad de Concepción*
Abner H. Poza, *Universidad Católica de la Santísima Concepción*

In this work, 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 [1]. 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 [2].

References

[1] Alvarez, M., Gatica, G.N., Ruiz–Baier, R., 2015. An augmented mixed-primal finite element method for a coupled flow-transport problem. ESAIM: M2AN 49, 1399–1427. doi:10.1051/m2an/2015015.

[2] van Keken, P.E., Currie, C., King, S.D., Behn, M.D., Cagnioncle, A., He, J., Katz, R.F., Lin, S.C., Parmentier, E.M., Spiegelman, M., Wang, K., 2008. A community benchmark for subduction zone modeling. Phys. Earth Planet. Inter. 171, 187–197. doi:10.1016/j.pepi.2008.04.015.

Generating graded layer-adapted meshes using mesh partial differential equations

Róisín Hill, *University of Limerick*
Niall Madden, *University of Galway*

We consider the numerical solution, by finite elements methods, of singularly-perturbed differential equations (SPDEs) whose solutions exhibit boundary layers. Our interest lies in developing parameter-robust methods, where the quality of the solution is independent of the value of the perturbation parameter. One way of achieving this is to use layer resolving methods based on meshes that concentrate their mesh points in regions of large variations in the solution. We investigate the use of Mesh PDEs (MPDEs), based on Moving Mesh PDEs first presented in [2], to generate layer resolving meshes that yield parameter robust solutions to SPDEs. Specifically, we present MPDEs based on the derivative to the numerical solution to the related SPDE. Their solutions yields meshes that are similar to Bakhvalov meshes [1]. The algorithms and code build on those presented in [4]. Since the MPDEs are non-linear problems, we use a fixed-point iterative method to solve them numerically. We present an approach involving alternating between h- and r-refinement which is highly efficient, especially for larger meshes. We demonstrate the flexibility of the approach with numerical examples implemented in FEniCS [3]. Acknowledgements: My research is supported by the Irish Research Council, GOIPG/2017/463 and GOIPD/2022/284.

References

[1] N. S. Bakhvalov. *On the optimization of the methods for solving boundary value problems in the presence of a boundary layer.* Ž. Vyčisl. Mat i Mat. Fiz., 9:841-859, 1969.

[2] W. Huang, Y. Ren, and R.D. Russell. Moving mesh partial differential equations (MMPDES) based on the equidistribution principle. SIAM J. on Numer. Anal.,31(3):709-730, 1994.

[3] M.S. Alnæs, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M.E. Rognes, and G. N. Wells. The FEniCS project version 1.5. Archive of Numerical Software, 3(100), 2015.

[4] R. Hill and N. Madden. Generating layer-adapted meshes using mesh partial differential equations, Numer. Maths. Theory MethodsAppl., 14(3):559-588, 2021.

Positivity-preserving discretisations in general meshes

Gabriel R. Barrenechea, *University of Strathclyde*

The quest for physical consistency in the discretisation of PDEs started as soon as the numerical methods started being proposed. By physical consistency we mean a discretisation that *by design* satisfies a property also satisfied by the continuous PDE. This property might be positivity of the discrete solution, or preservation of some bounds (e.g., concentrations should belong to the interval $[0, 1]$), or can also be energy preservation, or exactly divergence-free velocities for incompressible fluids.

Regarding positivity preservation, this topic has been around since the pioneering work by Ph. Ciarlet in the late 1960s and early 1970s. In the context of finite element methods, it was shown in those early works (and not significantly improved since), that in order for a finite element method to preserve positivity the mesh needs to satisfy certain geometrical restrictions, e.g., in two space dimensions with simplicial elements the triangulation needs to be of Delaunay type (in higher dimensions or quadrilateral meshes the restrictions are more involved). Throughout the years several conclusions have been reached in this topic, but in the context of finite element methods the discretisations tend to be of first order in space. So, many important problems still remain open. In particular, one open problem is how to build a discretisation that will lead to a positive solution regarless of the geometry of the mesh and the order of the finite element method.

In this talk I will review recent results addressing the last question posed in the last paragraph. More precisely, I will present a method that enforces bound-preservation (at the degrees of freedom) of the discrete solution. 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, then the outcome is a finite element function that satisfies the bounds at the degrees of freedom. Another important observation to make is that this approach is related to variational inequalities, and this fact will be exploited in the error analysis. 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).

Finite element methods respecting the discrete maximum principle for convection-diffusion equations I

Volker John, *Weierstrass Institute for Applied Analysis and Stochastics and Freie Universität Berlin*

Gabriel R. Barrenechea, *University of Strathclyde*

Petr Knobloch, *Charles University*

Convection-diffusion-reaction equations model the conservation of scalar quantities. From the analytic point of view, solution of these equations satisfy under certain conditions maximum principles, which represent physical bounds of the solution. That the same bounds are respected by numerical approximations of the solution is often of utmost importance in practice. The mathematical formulation of this property, which contributes to the physical consistency of a method, is called Discrete Maximum Principle (DMP). In many applications, convection dominates diffusion by several orders of magnitude. It is well known that standard discretizations typically do not satisfy the DMP in this convection-dominated regime. In fact, in this case, it turns out to be a challenging problem to construct discretizations that, on the one hand, respect the DMP and, on the other hand, compute accurate solutions.

This talk starts to presents a survey on finite element methods, with a main focus on the convection-dominated regime, that satisfy a local or a global DMP. The concepts of the underlying numerical analysis are explained. All available linear discretizations with P_1 finite elements satisfying DMPs are described. Linear discretizations for other finite elements are discussed briefly.

Part II of this talk will be presented by Petr Knobloch.

Finite element methods respecting the discrete maximum principle for convection-diffusion equations II

Petr Knobloch, *Charles University*
Gabriel R. Barrenechea, *University of Strathclyde*
Volker John, *Weierstrass Institute for Applied Analysis and Stochastics, Berlin*

This talk is a second part of a joint presentation with Volker John (see the abstract of Part I for an introduction into the topic). The talk will be devoted to the numerical solution of both steady-state and time-dependent convection-diffusion-reaction equations and, in contrast to Part I, it will present examples of nonlinear finite element methods methods satisfying the discrete maximum principle (DMP). In fact, it turns out that, for steady-state problems, all successful finite element approaches satisfying the DMP are nonlinear, which will be also illustrated by numerical results.

This talk is based on a joint review paper with Gabriel R. Barrenechea and Volker John (see https://arxiv.org/abs/2204.07480).

Reduced order models for incompressible flows

Julia Novo, *Universidad Autónoma de Madrid*

We consider proper orthogonal decomposition (POD) methods to approximate the incompressible Navier-Stokes equations. Our aim is to get error bounds with constants independent of inverse powers of the viscosity parameter. This type of error bounds are called robust. In the case of small viscosity coefficients and coarse grids, only robust estimates provide useful information about the behavior of a numerical method on coarse grids. To this end, we compute the snapshots with a full order stabilized method (FOM). We also add stabilization to the POD method.

In practical simulations one can apply some given software to compute the snapshots. It could then be the case that a different discretization for the nonlinear term is used in the FOM and the POD methods. We analyze the influence of using different discretizations for the nonlinear term.

Finally, we also analyze the influence of including snapshots that approach the velocity time derivative. We study the differences between projecting onto L^2 and H^1 and prove pointwise in time error bounds in both cases.

Dissipation-based WENO stabilization of high-order continuous Galerkin approximations to scalar conservation laws

Joshua Vedral, *Institute of Applied Mathematics (LS III), TU Dortmund*
Dmitri Kuzmin, *Institute of Applied Mathematics (LS III), TU Dortmund*

In this work, we introduce a new nonlinear stabilization approach for high-order continuous finite element discretizations of scalar conservation laws. The proposed methodology is based on the weighted essentially non-oscillatory (WENO) framework. Unlike Runge-Kutta discontinuous Galerkin (RKDG) schemes that overwrite the finite element solution with a WENO reconstruction, our scheme uses a reconstruction-based smoothness sensor to blend the numerical viscosity coefficients of high- and low-order dissipative stabilization terms. The so-defined WENO approximation introduces low-order nonlinear diffusion in the vicinity of shocks and retains high-order accuracy of a continuous Galerkin scheme with linear stabilization in regions where the solution is sufficiently smooth. The reconstructions that we use include Lagrange and Hermite interpolation polynomials. The amount of numerical viscosity depends on the differences between partial derivatives of candidate polynomials. All derivatives are taken into account by our smoothness sensor. The preliminary results for standard linear and nonlinear test problems in one and two dimensions are promising. In our numerical experiments, we observe crisp resolution of shocks and optimal convergence behavior even for high polynomial degrees.

MINRES methods for the singularly perturbed Darcy equations

Thomas Führer, *Pontificia Universidad Católica de Chile*
Juha Videmann, *Instituto Superior Técnico, Universidade de Lisboa*

In this talk I present recent results on minimum residual methods (MINRES) for solving a scaled Brinkman model of fluid flow through porous media. We consider a first-order reformulation using a pseudostress variable that allows to eliminate the pressure variable from the system. Based on this formulation we define a least-squares finite element method (FOSLS) and a discontinuous Petrov–Galerkin method with optimal test functions (DPG). Our proposed numerical schemes are inf–sup stable for any choice of discrete spaces. Furthermore, the minimum residual functionals are norm equivalent to a generic norm induced by the model problem and the equivalence constants are independent of the singular perturbation parameter. Therefore, the approximation properties only depend on the choice of discrete spaces. We analyze the use of some common finite element spaces. Numerical results for benchmark problems will be presented.

Robust error estimates in a balanced norm for the approximation of reaction-diffusion equations on graded meshes

Cecilia Penessi, *Universidad Nacional de Rosario - CONICET*
María Gabriela Armentano, *Universidad de Buenos Aires - IMAS CONICET*
Ariel L. Lombardi, *Universidad Nacional de Rosario - CONICET*

For the reaction-diffusion problem

$$\begin{aligned} -\varepsilon^2\Delta u + b(x)u &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

where $b(x) \geq b_0 > 0$ on Ω and ε is a small positive parameter, we consider the weighted variational formulation introduced in [N. Madden, M. Stynes, Calcolo, vol. 58, 2021]: find $u \in H_0^1(\Omega)$ such that

$$B_\beta(u,v) = \varepsilon^2(\nabla u, \nabla(\beta v)) + (b(x)u, \beta v) = (f(x), \beta v) \quad \forall v \in H_0^1(\Omega)$$

where the weight β is defined by

$$\beta(x) = 1 + \frac{1}{\varepsilon} exp\Big(-\gamma\frac{d(x)}{\varepsilon}\Big)$$

with $d(x)$ the distance from x to the boundary of Ω and $0 < \gamma \leq b_0$. The bilinear form B_β is coercive and continuous in the weighted norm

$$|||v|||_\beta = \left(\varepsilon^2 \|\nabla v\|_\beta^2 + \|v\|_\beta^2\right)^{\frac{1}{2}}$$

where $\|v\|_\beta = (\beta v, v)^{\frac{1}{2}}$. It turn out that this norm is balanced for the problem under consideration. In the case of Ω being a rectangle, we consider the approximation by continuous piecewise bilinear functions based on this variational formulation on graded meshes, which depend on a graduation parameter which controls how refined becomes the mesh near the boundary layers. We prove that, by using appropriate graded meshes, we obtain numerical solutions with error estimates almost robust in ε and quasi-optimal in the number of degrees of freedom for the balanced norm $|||\cdot|||_\beta$.

The DPG method and its application to problems with layers

Norbert Heuer, *Pontificia Universidad Católica de Chile*

The discontinuous Petrov–Galerkin method with optimal test functions (DPG method) was proposed in 2009 by Demkowicz and Gopalakrishnan, initially to solve transport equations. During the last decade it has evolved into a framework to develop robust Galerkin approximations for challenging problems from engineering sciences and physics. In this talk we discuss its application for the solution of advection-reaction-diffusion problems and mechanical thin structure models, with emphasis on problems of low regularity that exhibit layer phenomena.

The presentation is based on results from various collaborations, including Leszek Demkowicz (U Texas, Austin), Thomas Führer (UC, Chile), Michael Karkulik (USM, Chile), and Antti Niemi (U Oulu, Finland). Suppport by ANID-Chile through Fondecyt project 1190009 is gratefully acknowledged.

Anisotropic regularity of solutions of elliptic problems with Dirac measures as data.

Ignacio Ojea, *Universidad de Buenos Aires - IMAS CONICET*

We consider the problem:

$$\begin{cases} -\Delta u &= q\delta_\Lambda & \text{in } \Omega \\ u &= 0 & \text{in } \partial\Omega, \end{cases} \tag{1}$$

where $\Omega \subset \mathbb{R}^3$ is a bounded domain that can be a polyhedron, Λ is a simple, open, smooth curve strictly contained in Ω, δ_Λ is the Dirac measure supported on Λ and q is a density function.

We prove regularity results for the solution u. In a first step, we obtain regularity in Kondratiev spaces, with weights given by powers of the distance to Λ. For this, we use a classical approach: we consider a regularized version of the data, depending on a regularization parameter ρ, and obtain a regularized solution u_ρ. Then, we analyze the weighted norms of u_ρ and its derivatives in order to deduce the weights that allows us to take limit with ρ tending to zero. In a second step, we show that if Λ is a straight line the derivatives of u in a direction parallel to Λ are *smoother* than the derivatives in a direction orthogonal to Λ. This leads to a regularity result in *anisotropic* spaces, with two weights: one given by a power of the distance to Λ and the other given by a power of the distance to the extreme points of Λ.

Our estimates can be easily extended to more general contexts. For example: the isotropic regularity holds for closed curves. More interestingly, the anisotropic regularity can be extended to polygonals, where the distance to the extreme points of Λ should be replaced by the distance to the extreme point of each segment, i.e: the vertices of the polygonal.

A new perspective on time-stepping schemes: Beyond strong stability

Alexandre Ern, *CERMICS, Ecole des Ponts and INRIA*
Jean-Luc Guermond, *Texas A&M University*

We introduce a technique that makes every explicit Runge–Kutta time stepping method invariant-domain preserving when applied to high-order discretizations of the Cauchy problem associated with nonlinear conservation equations. The main advantage over the popular strong stability preserving (SSP) paradigm is more flexibility in the choice of the ERK scheme, thus allowing for a less stringent restriction on the time step and circumventing order barriers. The technique is agnostic to the space discretization. In a second step, we extend the technique to implicit-explicit (IMEX) time-stepping schemes for the Cauchy problem where the evolution operator comprises a hyperbolic part and a parabolic part with diffusion and stiff relaxation terms. Numerical experiments are presented to illustrate the theory.

A posteriori error estimates for singularly perturbed equations

Natalia Kopteva, *University of Limerick*

Solutions of singularly perturbed partial differential equations typically exhibit sharp boundary and interior layers, as well as corner singularities. To obtain reliable numerical approximations of such solutions in an efficient way, one may want to use meshes that are adapted to solution singularities using a posteriori error estimates.

In this talk, we shall discuss residual-type a posteriori error estimates singularly perturbed reaction-diffusion equations and singularly perturbed convection-diffusion equations. The error constants in the considered estimates are independent of the diameters of mesh elements and of the small perturbation parameter. Some earlier results will be briefly reviewed, with the main focus on the recent preprints [1, 2].

References

[1] N. Kopteva, R. Rankin, Pointwise a posteriori error estimates for discontinuous Galerkin methods for singularly perturbed reaction-diffusion equations, May 2022.

[2] A. Demlow, S. Franz and N. Kopteva, Maximum norm a posteriori error estimates for convection-diffusion problems, July 2022.

Adaptive regularisation applied to Richards' equation

Ben Ashby, *Heriot-Watt University*
Tristan Pryer, *University of Bath*

Richards' equation models infiltration and subsurface flow of water in soils, and it is well known that numerical methods for solving it are prone to convergence failure in the nonlinear iteration. In this talk, we consider situations in which this failure is due to sharp fronts that appear in the solution under heavy infiltration due to the nature of the parametrisation of the soil permeability. A regularisation, controlled by a length parameter ε, of the nonlinear relations that describe permeability is introduced with the aim of stabilising the nonlinear iteration without adversely affecting the rate of convergence of the numerical method. A posteriori error estimates are derived for a finite element method applied to linear elliptic and parabolic test problems with regualrised data to determine the effect of regularisation on the overall discretisation error. Since these estimates are computable, they can provide insight into the cause of numerical issues, and for this reason are often used as the basis for adaptive mesh refinement. The results motivate the regularisation of Richards' equation, and simulations are presented to show the performance of the scheme, both in convergence rate and iteration stability.

Challenges for non-Boltzmann drift-diffusion charge transport simulations in semiconductors

Patricio Farrell, *Weierstrass Institute for Applied Analysis and Stochastics (WIAS)*

The thermodynamically consistent Scharfetter-Gummel flux approximation has been proven to be a very effective tool in finite volume drift-diffusion simulations of semiconductor devices. Recently, its basic limitations to Boltzmann statistics have been overcome. In this talk, new thermodynamically consistent schemes are presented which can be employed when it is no longer sufficient to assume Boltzmann statistics, for example when the device operates at low temperatures or organic semiconductor materials are used. In the latter case, the Blakemore or Gauss-Fermi functions most accurately reflect the physical statistics. Furthermore, we discuss the impact of three additional challenges which may slow down the convergence of the numerical solution: boundary layers at Ohmic contacts, discontinuities in the doping profile and corner singularities. Differences between the proposed finite volume method and a finite-element based will be examined.

Constructive approximation on graded meshes for the fractional Laplacian

Juan Pablo Borthagaray, *Universidad de la República*
Ricardo H. Nochetto, *University of Maryland*

In this talk, we consider the homogeneous Dirichlet problem for the integral fractional Laplacian. We discuss optimal Sobolev regularity estimates in Lipschitz domains satisfying an exterior ball condition. We present the construction of graded bisection meshes by a greedy algorithm and derive quasi-optimal convergence rates for approximations to the solution of such a problem by continuous piecewise linear functions. The nonlinear Sobolev scale dictates the relation between regularity and approximability.

Coupling local and nonlocal equations with Neumann boundary conditions.

Francisco Bersetche, *Universidad Técnica Federico Santamaría*
Gabriel Acosta, *Universidad de Buenos Aires - IMAS CONICET*
Julio Rossi, *Universidad de Buenos Aires - IMAS CONICET*

We introduce two different ways of coupling local and nonlocal equations with Neumann boundary conditions in such a way that the resulting model is naturally associated with an energy functional. For these two models we prove that there is a minimizer of the resulting energy that is unique modulo adding a constant.

Weighted analytic regularity for the integral fractional Laplacian in polygons and application to hp-FEM

Jens Markus Melenk, *Technische Universität Wien*
Markus Faustmann, *Technische Universität Wien*
Carlo Marcati, *Università di Pavia*
Christoph Schwab, *ETH Zürich*

We study the Dirichlet problem for the integral fractional Laplacian in a polygon Ω with analytic right-hand side. We show the solution to be in a weighted analyticity class that captures both the analyticity of the solution in Ω and the singular behavior near the boundary. Near the boundary the solution has an anisotropic behavior: near edges but away from the corners, the solution is smooth in tangential direction and higher order derivatives in normal direction are singular at edges. At the corners, also higher order tangential derivatives are singular. This behavior is captured in terms of weights that are products of powers of the distances from edges and corners.

The proof of the regularity assertions is based on the Caffarelli-Silvestre extension, which realizes the non-local fractional Laplacian as a Dirichlet-to-Neumann map of a (degenerate) elliptic boundary value problem.

We employ our analytic regularity to show exponential convergence of high order finite element methods (hp-FEM) on meshes that are geometrically refined towards both edges and corners. The geometric refinement towards edges results in anisotropic meshes away from corners. The use of such anisotropic elements is crucial for the exponential convergence result.

An iterative method for local/nonlocal coupled systems

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We explore an iterative method for solving systems arising from couplings between local and nonlocal models of the kind given in [1]. The proposed technique resembles the so-called Schwarz method and can be successfully treated within the framework developed by P.L. Lions.

References

[1] Acosta G.; Bersetche F.; Rossi J., Local and nonlocal energy-based couplings models, to appear in SIAM J. Math. Anal. https://arxiv.org/pdf/2107.05083.pdf