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# The 21st Workshop on Numerical Methods for Problems with Layer Phenomena

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## Book of Abstracts **DRAFT**

*Workshop Organisers:*

- Niall Madden (Chair)
- Nanda Poddar
- Jekaterina Mosalska
- Sean Tobin

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## ABSTRACTS

# AN EVOLVE-FILTER-RELAX REGULARIZED REDUCED ORDER MODEL FOR BUOYANCY-DRIVEN FLOWS

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The a priori error analysis of reduced order models (ROMs) for buoyancy-driven flows is relatively scarce. In this study, we take a step in this direction and conduct numerical analysis of the evolve-filter-relax ROM (EFR-ROM), which uses spatial filtering to stabilize ROMs for convection-dominated flows. This study extends the EFR-ROM model of [1] for the Navier-Stokes equations to the Boussinesq equations with the spectral element discretization framework. Specifically, we prove stability, and an a priori error bound for the EFR-ROM. Our numerical investigation shows that the theoretical convergence rates are recovered numerically. In addition, we show that EFR-ROM yields more accurate solutions and quantity of interest than the Galerkin-ROM (G-ROM) in two test problems.

*This is joint work with Ping-Hsuan Tsai (VA, USA).*

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# ON A POSTERIORI ESTIMATION IN THE ENERGY NORM FOR CONVECTION-DIFFUSION PROBLEMS

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We consider a singularly perturbed convection-diffusion problem

$$Lu = -\varepsilon \Delta u + b \cdot \nabla u + cu = f$$

in a domain  $\Omega \subset \mathbb{R}^2$  with Dirichlet and Neumann boundary conditions. A result by Verfürth showed that the classical residual and jump estimators

$$\begin{aligned}\eta(T) &= \sqrt{\eta_{Vol}(T)^2 + \eta_{jump}(T)^2}, \\ \eta_{Vol}(T) &= \alpha_T \|f - Lu_h\|_{L_2(T)}, \\ \eta_{jump}(T) &= \sqrt{\beta_T \varepsilon} \|u_h\|_{L_2(\partial T)}\end{aligned}$$

can be used as a posteriori error estimator. However, the associated norm contains a dual norm which is not computable.

We present a different norm that bounds this estimator, is efficient and computable. A mesh adaptation algorithm using this estimator can be applied to problems with boundary and interior layers to solve them and produce reliable results.

*This is joint work with Natalia Kopteva (Limerick).*

# NOVEL MESHES FOR THE SOLUTION OF A PROBLEM WITH INTERIOR PARABOLIC LAYERS

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In [1] a numerical algorithm was proposed to solve singularly perturbed convection diffusion problems on curvilinear domains. Constraints were imposed on the data so that only regular exponential boundary layers appear in the solution. A domain decomposition method was used, comprising a rectangular grid outside the boundary layer and a Shishkin mesh, aligned to the curvature of the outflow boundary, near the boundary layer. We now wish to examine how this algorithm can be modified to treat a problem with interior layers. Numerical results will be presented to test the convergence of the modified algorithm.

*This is joint work with Eugene O’Riordan (DCU).*

## References

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# POINTWISE-IN-TIME ERROR BOUNDS FOR A FRACTIONAL-DERIVATIVE PARABOLIC PROBLEM ON QUASI-GRADED MESHES.

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An initial-boundary value, subdiffusion problem involving a Caputo time derivative of fractional order  $\alpha \in (0, 1)$  is considered. The solutions of which typically exhibit a singular behaviour at initial time. We propose an extension to the approach, by Kopteva and Meng [1], used to analyse the error of L1-type discretizations on both graded and uniform temporal meshes. We broaden the assumption on the regularity of the solution to incorporate more general solution behaviour, such that  $|\delta_t^l u(\cdot, t)| \lesssim 1 + t^{\sigma-l}$  for some  $\sigma \in (0, 1) \cup (1, 2)$  and any  $l = 0, 1, 2$ . Under this more general assumption on the solution, we give sharp pointwise-in-time error bounds on quasi-graded temporal meshes with arbitrary degree of grading (including uniform meshes, also considered by Li, Qin, and Zhang [2]). Extensions to the semilinear case will also be considered.

*This is joint work with Professor Natalia Kopteva (University of Limerick).*

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# THE BOUND PRESERVING METHOD APPLIED TO THE 2D INDUCTION HEATING PROBLEM

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Induction heating is a process widely used in the metallurgical manufacturing industry to heat conductive materials. Using an alternating current with a very high frequency, a magnetic field generates a current in the material, which produces heat due to the Joule heating process. This current is concentrated in a very thin layer near the boundary of the material, and as such there is a boundary layer in the magnetic field. This creates a highly irregular source term ( $f \in L^1(\Omega)$ ) in the heat equation, and in the time-dependent case, generates a boundary layer in temperature near  $t = 0$ .

In this talk, I will describe the application of the Nodally Bound Preserving Method [1] to the induction heating equations. This method is designed to satisfy given bounds on the solution and guarantees stability for meshes for which standard methods do not guarantee bound preservation. The main technical result shows that when imposing non-physical bounds on the discrete solution, the method converges to the best approximation in the infinite-dimensional constrained convex set. As a result, for the induction heating problem, where the bounds are not explicit, this leads to a method that converges without imposing a restriction on the mesh.

*This is joint work with Gabriel R. Barrenechea.*

*Supported by a University of Strathclyde SEA scholarship with EPSRC and additional support by Bifrangi UK Ltd.*

## References

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# A TUTORIAL ON SOLVING SINGULARLY PERTURBED PROBLEMS IN FIREDRAKE

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Firedrake is a Python-based system for solving partial differential equations, by finite element methods. It is built on the FEniCS *Unified Form Language*, and the PETSc toolkit.

In this hands-on tutorial you'll be introduced to using Firedrake for solving some singularly perturbed ordinary and partial differential equations. We've cover constructing layer-adapted meshes, discretization by high-order methods, and estimation of errors.

No previous experience of Firedrake is required. It would be useful, but not essential, to have a reading knowledge of Python. You will require you own laptop, and should sign up to Google colab: <https://colab.google/>

*This is a joint presentation with Sean Tobin (Galway)*



# A STABILIZED SCHEME FOR AN OPTIMAL CONTROL PROBLEM GOVERNED BY CONVECTION–DIFFUSION–REACTION EQUATION

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It is well-known that convection-diffusion equations may exhibit layers, which can render standard finite element methods inadequate for accurately approximating the exact solution. These layers can cause issues such as spurious oscillations, violating physical properties of the solution. To address this, nonlinear discretizations have been developed that preserve the maximum principle of the solution and accurately capture the position of these layers.

In this talk, we will consider an optimal control problem on a bounded domain  $\Omega \subset \mathbb{R}^2$ , governed by a time-dependent convection–diffusion–reaction equation with pointwise control constraints. Following the optimize–then–discretize approach, the resulting optimality conditions yield a coupled system of two time-dependent convection–diffusion–reaction equations.

To stabilize the fully–discrete scheme derived from the optimality conditions, we employ the algebraic flux correction method. Additionally, we discuss the well-posedness of the resulting fully–discrete scheme and present a priori and residual-type a posteriori error estimates.

## References

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# INTERPLAY OF DYNAMIC BOUNDARY ABSORPTION AND LAYER-LIKE PHENOMENA IN REACTIVE SOLUTE TRANSPORT: A DUAL NUMERICAL APPROACH

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The role of time and space-dependent boundary absorption in hydrodynamic solute dispersion [1, 2, 3] remains underexplored despite its significance in environmental, biological, and industrial systems. This study investigates how dynamic boundary absorption influences solute transport under oscillatory flow conditions, where rapid spatial and temporal changes can generate steep concentration gradients near reactive boundaries.

Through numerical simulation, a dual modeling framework is developed: a deterministic advection-diffusion solver (using a finite difference method) and a stochastic Brownian dynamics simulation, capturing both macroscopic and particle-scale transport behavior. Numerical results show that as boundary reactivity increases, solute concentration near the reactive wall decreases sharply, eventually reaching a steady profile for high absorption values. These effects are strongly time-dependent: longer dispersion times allow significantly more particles to be absorbed in the same boundary condition, revealing a cumulative interaction between flow unsteadiness and boundary reactions.

By analyzing the evolution of concentration profiles and dispersion statistics under varying Péclet and Schmidt numbers, oscillation frequencies, and boundary absorption strengths, this study highlights how dynamic boundary interactions induce layer-like features in solute distribution. The comparative strengths of the deterministic and stochastic models offer a comprehensive understanding of reactive solute transport in unsteady systems, with implications for filtration, microfluidics, and environmental flow applications.

*This is joint work with Niall Madden (University of Galway).*

*Supported by the Irish Research Council (now Research Ireland), Grant GOIPD/2024/226.*

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- [3] Saha G., Poddar N., Mondal K.K., Wang P.: Evolution of concentration distribution and removal of a solute in magnetohydrodynamics channel flow: effects of buoyancy-driven force and induced magnetic field. *Proc. R. Soc. Lond. A* **480**, 20240091 (2024)

# ADAPTIVE REGULARISATION FOR PDE-CONSTRAINED OPTIMAL CONTROL

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PDE-constrained optimal control problems require regularisation to ensure well-posedness. This typically involves a small regularisation parameter and the resulting optimal control problem is equivalent to solving a singularly perturbed PDE. We propose an adaptive strategy for regularising PDE-constrained optimal control problems. This method leverages rigorous a posteriori error estimates to adaptively vary the regularisation parameter across the computational domain. This allows the regularisation to be varied elementwise, dynamically balancing induced regularisation and discretisation errors, offering a robust and efficient method for solving these problems. We demonstrate the efficacy of our analysis with several numerical experiments.

## References

- [1] Jenny Power and Tristan Pryer. *Adaptive Regularisation for PDE-Constrained Optimal Control*. arXiv preprint arXiv:2503.11386 (2025).

# NODALLY BOUND-PRESERVING DISCONTINUOUS GALERKIN METHODS FOR CHARGE TRANSPORT

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Preserving the positivity of charge density variables is often critical to ensuring the well-posedness of models describing the transport of charged particles. A prototypical example is the coupled nonlinear *Poisson–Nernst–Planck* (PNP) equations, or *drift-diffusion* equations, which provide a continuum description for the two-way interaction between charged particle densities and an associated electric field. Motivated by the PNP system, and its extension to fluidic media through the *Navier–Stokes–PNP* model, in this talk I will present recent work [2] adopting the nodally bound-preserving method first introduced in [1] to the context of discontinuous Galerkin methods for charge transport.

*This is joint work with Tristan Pryer (University of Bath) and Gabriel R. Barrenechea (University of Strathclyde).*

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# ON THE DECOMPOSITION OF THE SOLUTION TO REACTION-DIFFUSION TWO-POINT BOUNDARY VALUE PROBLEMS WITH DATA OF FINITE REGULARITY

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We consider reaction-diffusion two-point boundary value problems with data of finite regularity, i.e.  $H^2$ . It is well known that the solution may be decomposed into a smooth part, two boundary layers at the endpoints, and a remainder. We provide a proof of the regularity of each term in the decomposition that *does not use the maximum principle*, but rather utilizes *exponentially weighted* spaces. Even though the end result is known, our method of proof may be extended to problems for which the maximum principle does not hold, e.g. fourth order problems, Reissner-Mindlin plate model, etc. Using our result, we show how the  $h$  version of the Finite Element Method (with piece-wise linears) on the exponentially graded (eXp) mesh from [2], converges uniformly at the optimal rate. The results presented in this talk appear in [1].

*This is joint work with Ch. Schwab (ETH, Zürich).*

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- [2] Xenophontos, C.: Optimal mesh design for the finite element approximation of reaction-diffusion problems, Int. J. Numer. Meth. Eng., Vol. 53, No 4, pp. 929–943 (2002).

# GRADIENT-ROBUST FINITE ELEMENT - FINITE VOLUME SCHEME FOR THE COMPRESSIBLE STOKES EQUATIONS

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We consider a steady compressible Stokes problem on a domain  $\Omega \subset \mathbb{R}^d$ , where  $d \in \{2, 3\}$ , in primitive variables velocity, pressure and non-constant density  $(\mathbf{u}, p, \varrho)$ . A *barotropic flow* is assumed, where the pressure depends solely on the density under an exponential *equation of state*  $p = c_M \varrho^\gamma$  for  $\gamma \geq 1$ .

A finite element scheme for the momentum balance, coupled to a finite volume discretization for the continuity equation  $\nabla \cdot (\varrho \mathbf{u}) = 0$ , was proposed in [1] for a linear equation of state ( $\gamma = 1$ ). In this talk, we present an extension of the scheme to the nonlinear equation of state ( $\gamma > 1$ ). The scheme satisfies several desired structural properties, namely stability, convergence, the preservation of non-negativity and mass constraints for the density, and gradient-robustness. The latter property is related to the locking phenomenon observed in incompressible flow at high Reynolds number regimes, which carries over to the compressible setting. To achieve gradient-robustness, we employed the reconstruction operator proposed in [2]. The structural properties of the scheme were tested using various numerical benchmark problems.

*This is joint work with Volker John and Christian Merdon (Berlin).*

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