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INTERNATIONAL CONFERENCE ON
BOUNDARY AND INTERIOR LAYERS,
COMPUTATIONAL AND ASYMPTOTIC
METHODS



BOOK OF ABSTRACTS

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Introduction

Dear Participant,

On behalf of the University of A Coruña and the Scientific and Organizing Committees, it is with immense pleasure that we extend a warm welcome to you for the International Conference on Boundary and Interior Layers: Computational and Asymptotic Methods - BAIL 2024. This conference continues the long tradition of the BAIL meetings, which started 44 years ago in Dublin. We are particularly honored that A Coruña has been chosen as the city to host the second one of this prestigious series to be held in Spain, following Zaragoza in 2010. We eagerly anticipate the gathering of delegates from across the globe.

We are privileged to present a distinguished lineup of invited speakers who will delve into various topics related to the numerical solution of problems presenting layers. With such diversity, we trust there will be something of interest to every attendee. While the conference is primarily funded through the registration fees, we are grateful for the additional financial support extended by our sponsors: the University of A Coruña, the Galician Centre for Mathematical Research and Technology (CITMaga), the Centre for Information and Communications Technology Research (CITIC), and the Spanish Society of Applied Mathematics (SEMA).

Beyond the scientific sessions, we encourage you to take advantage of the opportunities to reconnect with colleagues and forge new connections during the communal meals and social program. We extend our heartfelt appreciation to the A Coruña City Council for generously receiving us at the City Hall on Monday evening. The City Hall is well worth a visit, featuring a vast range of ornate decorations complete with a large exhibition of the last two centuries' wall clocks.

On Wednesday afternoon, we invite you to join us for an excursion, exploring the historic charm of A Coruña's old town and visiting the Mega Museum, intricately linked to the renowned Estrella Galicia brewery. The Wednesday evening conference dinner will be hosted at one of A Coruña's finest restaurants, offering a breathtaking view of Riazor's beach as you indulge in a delightful culinary experience.

Thank you for coming, and we hope you enjoy the meeting!

The BAIL 2024 Organizing Committee

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INVITED SPEAKERS

Recent advances in reduced order models based on proper orthogonal decomposition for incompressible flows

Bosco García Archilla

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Abstract. In this talk we review the latest results concerning reduced order models (ROM) based on proper orthogonal decomposition (POD) to approximate the solutions of the incompressible Navier-Stokes equations. These include, among other topics, error bounds independent of the Reynolds number, pointwise in time error estimates, the inclusion of time derivatives in the set of snapshots, higher-order estimates in time, and POD approximation to the pressure.

Algebraic stabilizations of convection-diffusion-reaction equations

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Abstract. Convection-diffusion-reaction equations appear in many mathematical models of physical, technical or biological processes and are also often used as model problems for developing numerical techniques for more complicated applications in which the interplay among convection, diffusion and reaction is important. Often, the diffusion is very small in comparison with the convection or reaction, which causes that the solutions comprise layers. It is well known that standard numerical methods then provide approximate solutions polluted by spurious oscillations unless the underlying mesh resolves the layers. Therefore, special numerical techniques have to be applied which are usually called stabilized methods. In what follows, we will consider only finite element approaches.

During the last five decades, many various stabilized methods have been developed. Their stabilizing effect can be characterized by the artificial diffusion they add to the underlying Galerkin discretization. To diminish the spurious oscillations to a sufficient extent, the artificial diffusion has to be sufficiently large. However, to avoid an excessive smearing of the layers, the artificial diffusion is not allowed to be too large. Consequently, the design of a proper stabilization is very difficult and it turns out that, due to the multiscale character of the problem, accurate approximate solutions can be obtained only if the amount of the artificial diffusion locally depends on the character of the exact solution. Consequently, numerical methods for convection-diffusion-reaction equations should be nonlinear. Many of these approaches are indeed quite successful in suppressing spurious oscillations without smearing the layers too much. However, in general, some spurious oscillations are often still present, which may be not acceptable in many applications. For example, concentrations should be in the interval $[0, 1]$ to avoid a blow-up if they are used as data of other equations. To guarantee that approximate solutions satisfy such global bounds, discretizations satisfying the discrete maximum principle (DMP) have to be used.

A recent survey revealed that there are only a few discretizations that at the same time satisfy the DMP and compute reasonably accurate solutions. An example are algebraically stabilized schemes. In contrast to many other stabilized methods which modify the variational formulation of the problem, the starting point of algebraic stabilizations is the system of linear algebraic equations corresponding to the Galerkin discretization. Then, a nonlinear algebraic term is added to the linear system in order to enforce a DMP without an excessive smearing of the layers. These methods have been intensively developed in recent years and we will formulate an abstract framework that enables the analysis of algebraically stabilized discretizations for steady-state problems in a unified way. We will present general results on local and global DMPs, existence of solutions, and error estimation. Then, various examples of algebraic stabilizations fitting into the abstract framework will be given and applied to discretizations of steady-state convection-diffusion-reaction equations. The properties of these particular algebraic stabilizations will be discussed both theoretically and by means of numerical examples.

Rigorous justification of the effective boundary condition on a porous wall

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Abstract. Porous boundaries appear naturally in many applications. Concrete, wood, stone, soil and most biological tissues (including human skin) are porous materials. If their porosity is large enough to be taken into account in the model, then we need an appropriate effective boundary condition. The goal of our work is to derive rigorously the new effective boundary condition for the fluid flow in domain with porous boundary. Starting from the Newtonian fluid flow through a domain with an array of small holes on the boundary, using the homogenization and the boundary layers, we find an effective law in the form of generalized Darcy law. The effective law states that the velocity on the boundary is proportional to the difference between the interior and the exterior stresses on the boundary. That law describes, not only the leaking/perspiration through the boundary (the normal velocity) but also the slipping of the fluid in direction tangential to the boundary. The proportionality is given by a symmetric positive tensor, corresponding to the permeability of the boundary and depending on the form and the distribution of the pores. If the pores geometry is isotropic, then the condition splits in Beavers–Joseph type condition for the tangential flow and the standard Darcy condition for the normal flow.

Keywords: Porous boundary; viscous fluid; homogenization; Darcy-type boundary condition; boundary layers.

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Tropical cyclone fundamentals: The rotating-convection paradigm and a new book

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Abstract. Understanding how tropical cyclones form, intensify, mature and decay requires first and foremost a conceptual model. Without such a model, forecasters and researchers must rely entirely on numerical model predictions from, in essence, a black box. In this talk, I review briefly the conceptual models available, focusing on a new framework that my colleagues and I have developed progressively over the last two decades. This framework, which we refer to as the "Rotating-convection paradigm", emphasizes the intrinsic three-dimensional nature of tropical cyclone evolution, principally as a result of the stochastic and localized nature of deep convection. However, the framework includes a simplified azimuthally-averaged perspective to connect it with previous paradigms, all of which have been based on strictly axisymmetric models. Unlike previous paradigms, the new one recognizes the importance of nonlinear boundary layer dynamics and the mostly overlooked fact that all of the air converging in the boundary layer may not be able to be ventilated to the upper troposphere by deep convection, especially as the storm matures and in the subsequent stages of its life cycle. Decoupling of the boundary-layer inflow from the deep-convective mass flux leads to a richness of storm behavior not described by previous conceptual frameworks.

Advances in Filtering for Boundary Layers

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Abstract. Utilizing filtering to extract extra information from data allows for interaction between disparate scales while minimising error and decreasing noise in data. While the ability to move data from fine resolutions to coarser resolutions is straight forward, moving data from a coarse resolution to a finer resolution while reducing errors is more challenging. This relies on utilizing ideas from multi-resolution analysis combined with symmetric convolutional filters [1, 2]. This approach has the further advantage of requiring fewer computations to gain insight into calculations such as for Bohm speed [3]. Advances in non-symmetric filtering, especially for boundary layers, have become increasingly necessary in order to understand the detailed physics in applications such as hypersonics. In this talk, we review the necessary properties for effective filters and the difficulties in constructing useful non-symmetric filters, especially for boundary layers. As basis for discussion, we utilize the Smoothness-Increasing Accuracy-Conserving (SIAC) filtering framework, which inherently takes advantage of the underlying physics and allows for the full resolution of the approximation and its derivatives in both the physical domain and Fourier signal space. We discuss recent advances in non-symmetric filtering and reliance of the approach on the underlying numerical method that generated the data.

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MINISYMPOSIUM

Numerical Approaches to Singularly Perturbed Problems with the Aid of Machine Learning

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MS abstract. This mini-symposium proposes to explore the cutting-edge integration of numerical methods and machine learning (ML) in addressing singularly perturbed problems, a significant area in the field of boundary and interior layers. Singular perturbation problems are prevalent in various scientific and engineering fields, characterized by the presence of small parameters that lead to solutions with boundary layers or rapidly changing features. Traditional numerical approaches often struggle with these problems due to issues like numerical instability and the need for extremely fine meshes in certain regions. Our symposium will address innovative techniques where machine learning algorithms assist in overcoming these challenges. We will present studies where ML algorithms have been used to predict solution behavior in critical regions, and open a new avenue of numerical approaches.

MS keywords: singular perturbation, machine learning, boundary layer, semi-analytic method.

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Analysis and computation of plane-parallel flows at a small viscosity

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**Speaker author*

Abstract. Singular perturbations occur when a small coefficient affects the highest order derivatives in a system of partial differential equations. From the physical point of view, singular perturbations lead to the formation of narrow regions close to the boundary of a domain, known as boundary layers, where numerous crucial physical processes occur. This presentation explores the analysis of viscous boundary layers in plane-parallel flows and their utilization in developing efficient Physics Informed Neural Networks (PINNs).

Keywords: Boundary layers; Navier-Stokes equations; Vanishing viscosity limit

Operator Learning for Parametric PDEs Without Data Reliance

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Abstract. Partial differential equations (PDEs) underlie our understanding and prediction of natural phenomena across numerous fields, including physics, engineering, and finance. However, solving parametric PDEs is a complex task that necessitates efficient numerical methods. In this paper, we propose a novel approach for solving parametric PDEs using a Finite Element Operator Network (FEONet). Our proposed method leverages the power of deep learning in conjunction with traditional numerical methods, specifically the finite element method, to solve parametric PDEs in the absence of any paired input-output training data. We performed various experiments on several benchmark problems and confirmed that our approach has demonstrated excellent performance across various settings and environments, proving its versatility in terms of accuracy, generalization, and computational flexibility. Our FEONet framework shows potential for application in various fields where PDEs play a crucial role in modeling complex domains with diverse boundary conditions and singular behavior. Furthermore, we provide theoretical convergence analysis to support our approach, utilizing finite element approximation in numerical analysis.

Keywords: Operator network; boundary layer; spectral element method; finite element method; deep learning.

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Semi-analytic PINN methods for boundary layer problems in a rectangular domain

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Abstract. Singularly perturbed boundary value problems pose a significant challenge for their numerical approximations because of the presence of sharp boundary layers. These sharp boundary layers are responsible for the stiffness of solutions, which leads to large computational errors, if not properly handled. It is well-known that the classical numerical methods as well as the Physics-Informed Neural Networks (PINNs) require some special treatments near the boundary, e.g., using extensive mesh refinements or finer collocation points, in order to obtain an accurate approximate solution especially inside of the stiff boundary layer. In this article, we modify the PINNs and construct our new semi-analytic SL-PINNs suitable for singularly perturbed boundary value problems. Performing the boundary layer analysis, we first find the corrector functions describing the singular behavior of the stiff solutions inside boundary layers. Then we obtain the SL-PINN approximations of the singularly perturbed problems by embedding the explicit correctors in the structure of PINNs or by training the correctors together with the PINN approximations. Our numerical experiments confirm that our new SL-PINN methods produce stable and accurate approximations for stiff solutions.

Keywords: PINN; Semi-analytic methods; SL-PINN; singular perturbations; boundary layers

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Neural Networks for Singularly Perturbed Problems

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*Speaker author

Abstract. We consider Neural Networks (NNs) for the approximation of the solution to singularly perturbed reaction-diffusion boundary value problems (BVPs), in one-dimension. The solution to such problems features, in general, boundary layers at the two end-points of the domain, and under the assumption of analytic input data, regularity estimates for the solution components are readily available from the literature [1]. First we present the general framework of NNs, including the different choices of the so-called activation functions, and then we show that there exists a NN that approximates the solution to such problems at an exponential rate of convergence, as the number of neurons is increased and the error is measured in the natural energy norm, as well as a balanced norm. The implementation of such an NN is also discussed, and we conclude with some numerical experiments, illustrating the theory.

Keywords: Singularly Perturbed Problem; Boundary Layers; Neural Networks; Exponential Convergence.

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CONTRIBUTED ABSTRACTS

A nodally bound-preserving finite element method for time-dependent reaction-convection-diffusion equations

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Abstract. In this research we introduce a stabilized finite element method for time dependent convection-diffusion-reaction equations. The basic idea of stabilized finite element methods is that after temporal discretization of the time dependent convection-diffusion-reaction equations, the equation has the form of a steady-state convection-diffusion-reaction equation at each time step. It is well-known that the finite element (FE) Galerkin approximation for the space discretization of the steady state convection-diffusion problem in the convection-diffusion regime generates highly oscillatory results, and additional numerical stabilization must be introduced. The most common stabilization methods are adding nonconsistent terms, e.g., homogeneous artificial diffusion or a penalty term called stabilization term to the spatial discretization problem (Galerkin method). But even using stabilization does not guarantee the preserving of the *Discrete Maximum principles (DMP)* and/or *monotonicity properties*, i.e. even by using the stabilization term, it is possible that the approximation solution at each time step does not respect the bounds of the exact solution.

Following the same line as in [1, 2], we use the following property: There is a correspondence between the imposition of bounds on the numerical solution and searching for the numerical solution on a convex subset of the finite element space of the steady state convection-diffusion-reaction equation at each time step consisting of the discrete functions satisfying those bounds at their nodal values. So, to propose a finite element method which respects the boundary conditions, we first project the finite element solution of the steady state problem onto the subset of admissible finite element functions (that is, those that respect the bounds of the continuous problem). To eliminate the non-trivial kernel generated by this process, a stabilization term is incorporated into the discretized equations at each time step to remove this kernel (that is, the negative part of the solution). To improve the general stability of the method we also add a linear stabilizing term (in this work, CIP stabilization). Additionally, we have presented the stability and also the error analysis of the finite element method.

Keywords: Finite element method; Reaction-convection-diffusion equation; Stabilising term; Space discretization; Time discretization.

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Adaptive mixed FEM combined with the method of characteristics for stationary convection–diffusion–reaction problems

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Abstract. We examine a stationary convection–diffusion–reaction model within a bounded domain of two or three dimensions. We propose an approximation method for this model, transforming it into a non-stationary problem, and introduce a numerical approach that integrates the method of characteristics with an augmented mixed finite element technique. We demonstrate the existence of a unique solution for this scheme. Additionally, we develop a residual-based a posteriori error estimator and establish its reliability and local efficiency. Furthermore, we conduct numerical experiments to showcase the rates of convergence of the adaptive algorithm.

Keywords: Convection-diffusion-reaction; dominant convection; mixed finite element; method of characteristics; residual a posteriori estimates.

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Stokes problem with slip boundary conditions

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Abstract. We discuss how slip conditions for the Stokes equation can be handled using the Nitsche method [2] for a stabilized finite element discretization. Emphasis is made on the interplay between stabilization and Nitsche terms. Well-posedness of the discrete problem and optimal convergence rates are established and illustrated with various numerical experiments. [1]

Keywords: Nitsche method; Stokes equation; Stabilized methods.

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Asymptotic Analysis of Wear Phenomena in Elastic Elliptic Membrane Shells

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Abstract. We consider a family of linearly elastic elliptic membrane shells, all sharing the same middle surface, with thickness 2ε , clamped along their entire lateral face. Moreover, tractions may act on the upper face of a shell and it may become in frictional contact along its lower face with a moving deformable foundation. Friction is modeled taking into account the effect of material wear on contact surfaces [1]. By using asymptotic analysis, we show that when the small parameter ε tends to zero, the solution of the three-dimensional variational contact problem converges to a limit that is independent of the transverse variable and which can be identified with the solution of a two-dimensional variational problem describing deformations and wear on the common middle surface.

Keywords: Shells; Contact; Elasticity; Wear; Asymptotic Analysis

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A positivity-preserving discretisation of an Oldroyd-B viscoelastic fluid

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Abstract.

In this talk we present a numerical method for the Stokes flow of an Oldroyd-B fluid. Oldroyd-B is a non-Newtonian fluid for which the stress includes an addition to the usual Newtonian stress tensor, the *conformation tensor* σ , which evolves according to a constitutive law formulated in terms of the upper convected time derivative:

$$\frac{\partial}{\partial t} \sigma + (\mathbf{u} \cdot \nabla) \sigma - (\nabla \mathbf{u}) \sigma - \sigma (\nabla \mathbf{u})^T = -\frac{1}{Wi} (\sigma - \mathbf{I}), \quad (1)$$

where \mathbf{u} is the fluid velocity and \mathbf{I} is the identity tensor. The dimensionless Weissenberg number Wi quantifies the effects of nonlinearities that arise due to non-Newtonian stresses. This is a hyperbolic partial differential equation, and its numerical solution remains a challenge, especially for large Wi . From the derivation of (1) from kinetics, one sees that the conformation tensor must remain positive definite for all flows, and violation of this condition often leads to numerical blowup.

We present a discretisation that preserves positive definiteness of the conformation tensor to increase stability of computations. The method consists of a finite element method for the fluid flow coupled to a finite difference method for a Lie derivative formulation of the constitutive law. In this framework, the advection and deformation terms of the upper convected derivative are discretised along fluid particle trajectories in a simple, cheap and cohesive manner, ensuring that the discrete conformation tensor is positive definite. We demonstrate the performance of this method with detailed numerical experiments in a lid-driven cavity setup. Numerical results are benchmarked against published data, and the method is shown to perform well in this challenging case.

Keywords: Non-Newtonian fluid dynamics; Upper convected time derivative; Finite element methods; Finite difference methods.

Implicit-explicit schemes for incompressible flow problems with variable viscosity

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Abstract. This talk is devoted to the study of different Implicit-Explicit (IMEX) schemes for incompressible flow problems with variable viscosity. Unlike most previous work on IMEX schemes, which focuses on the convective part, we here focus on treating parts of the diffusive term explicitly to reduce the coupling between the velocity components. We present different, both monolithic and fractional-step, IMEX alternatives for the variable-viscosity Navier–Stokes system, analysing their theoretical and algorithmic properties. Stability results are proven for all the methods presented, with all these results being unconditional, except for one of the discretisations using a fractional-step scheme, where a CFL condition (in terms of the problem data) is required for showing stability. Our analysis is supported by a series of numerical experiments. The results presented in this talk are based on the manuscript [1].

Keywords: Implicit-explicit scheme; stability analysis; generalised Newtonian flows.

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On the stability of a fictitious domain approach for fluid structure interaction problems

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Abstract. In this talk I will review the main stability property of a fictitious domain approach for the modeling of fluid-structure interaction problems [2]. We will focus on several aspects, including implementation details [1], and stability results. In particular, I will discuss the stability in presence of small intersection cells.

Keywords: Fluid structure interactions; Fictitious domain; Distributed Lagrange multiplier; Stability.

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A vorticity wave packet breaking within a rapidly rotating vortex

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Abstract. This study considers a critical-layer like interaction between a free vorticity wave packet and a linearly stable, columnar, and axisymmetric rapidly rotating vortex on the f -plane, in the quasi-steady regime, a long time after the initial, unsteady and strong interaction. Though the motion in intense atmospheric vortices such as tropical cyclones can be considered highly axisymmetric above the surface boundary layer, observation often shows asymmetric features. Through a radiating wave-induced axisymmetric adjustment, these asymmetries are believed to play a significant role in the intensification of these vortices [1]. Latent heat release, for example, creates asymmetric potential vorticity (PV) anomalies that outward propagate in the form of PV waves; their breaking was recently related to the inner spiral rainbands. Observation and numerical simulations indeed show that inner spiral bands mainly exhibit vorticity wave characteristics described by continuous vortical modes [2]. In this study, the interaction-induced vertically sheared three-dimensional mean flow is of higher amplitude than the wave packet and makes the helical critical layer asymmetric and spiraling. The pattern asymmetry is here enhanced by modeling a critical layer whose streamwise symmetry axis does not coincide with the critical radius, which is a space-time slowly evolving spiraling surface. This model permits one to consider retrograde vorticity wave packets whose angular phase speed is less than the angular wind rotation and whose radial group velocity is directed outward. Through matched asymptotic expansions, we find an analytical solution of the leading-order motion equations inside the critical layer. Owing to this new asymmetry, the interaction is strengthened with respect to previous studies [4]. The outer-flow equation singularity becomes higher on the resonant surface; the equivalent Richardson number at the critical radius is larger, of order the square root of the neutral-mode amplitude. The inviscid eigenmode is no longer continuous across the critical layer. The Prandtl-Batchelor theorem generalization to the quasi-steady three-dimensional critical-layer flow inside the separatrices is not true any more. The leading-order axial vorticity is indeed no longer a function of only the slow modulation variables, it now rapidly varies with the wave phase, its magnitude is increased and its azimuthal symmetry is broken. The wave and mean flow motions become less helical but more spiraling and distorted in the neighborhood of the critical layer [3].

Keywords: Nonlinear critical layer; Spiral vorticity band; Tropical cyclone; Vorticity wave packet; Wave-vortex interaction.

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Supercloseness of the local discontinuous Galerkin method for a singularly perturbed convection-diffusion problem

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Abstract. The Local Discontinuous Galerkin (LDG) method is a very popular finite element method for high order partial differential equations. Its basic idea is to rewrite the PDE as an equivalent first-order system to which one then applies the original DG method. In the LDG method one must specify a numerical flux on the boundary of each mesh element; if this is done appropriately, then the auxiliary variables that approximate the derivatives of the solution can be eliminated locally, which explains the name LDG. The LDG method is superior to many other numerical methods because of its strong stability, high-order accuracy, flexibility for hp -adaptivity, and high parallelizability. It is well suited to problems whose solutions have boundary layers. Furthermore, it can produce high-order accuracy for both the solution itself and its gradient

In this talk, we give some supercloseness results of the LDG method using tensor-product piecewise polynomials of degree at most $k > 0$ for two singularly perturbed convection-diffusion problems posed on the unit square in \mathbb{R}^2 , whose solutions have exponential boundary layers and have both exponential and characteristic layers. On Shishkin-type meshes this method is known to be no greater than $O(N^{-(k+1/2)})$ accurate in the energy norm induced by the bilinear form of the weak formulation, where N mesh intervals are used in each coordinate direction. (Note: all bounds in this abstract are uniform in the singular perturbation parameter and neglect logarithmic factors that will appear in our detailed analysis.) A delicate argument is used in this paper to establish $O(N^{-(k+1)})$ energy-norm superconvergence on all three types of mesh for the difference between the LDG solution and a local Gauss-Radau projection of the true solution into the finite element space. This supercloseness property implies a new bound for the error between the LDG solution on each type of mesh and the true solution of the problem; this bound is optimal (up to logarithmic factors). Numerical experiments confirm our theoretical results.

Keywords: Local discontinuous Galerkin method; Singularly perturbed; Supercloseness; Gauss-Radau projectors; Shishkin mesh.

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A uniformly convergent method for solving one-dimensional parabolic singularly perturbed systems with turning points

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Abstract. In this work, we design and analyze a uniformly convergent method for solving a type of parabolic singularly perturbed systems, given by

$$\begin{cases} \mathbf{L}_\varepsilon \mathbf{u} \equiv \frac{\partial \mathbf{u}}{\partial t}(x, t) + \mathcal{L}_{x, \varepsilon}(t) \mathbf{u}(x, t) = \mathbf{f}(x, t), & (x, t) \in (-1, 1) \times (0, T], \\ \mathbf{u}(-1, t) = \mathbf{g}_0(t), \mathbf{u}(1, t) = \mathbf{g}_1(t), & t \in [0, T], \mathbf{u}(x, 0) = \boldsymbol{\varphi}(x), & x \in (-1, 1), \end{cases} \quad (1)$$

where $\mathbf{u} = (u_1, u_2)^T$ and the spatial differential operator $\mathcal{L}_{x, \varepsilon}(t)$ is defined as

$$\mathcal{L}_{x, \varepsilon}(t) \mathbf{u} \equiv -\mathcal{D}_\varepsilon \frac{\partial^2 \mathbf{u}}{\partial x^2} + x^q \mathcal{B}(x) \frac{\partial \mathbf{u}}{\partial x} + \mathcal{A}(x, t) \mathbf{u}, \quad (2)$$

or as

$$\mathcal{L}_{x, \varepsilon}(t) \mathbf{u} \equiv -\mathcal{D}_\varepsilon \frac{\partial^2 \mathbf{u}}{\partial x^2} - x^q \mathcal{B}(x) \frac{\partial \mathbf{u}}{\partial x} + \mathcal{A}(x, t) \mathbf{u}, \quad (3)$$

where $\mathcal{D}_\varepsilon = \text{diag}(\varepsilon_1, \varepsilon_2)$ is the diffusion matrix, $\mathcal{B}(x) = \text{diag}(b_{11}(x), b_{22}(x))$, with $b_{kk} \geq \beta > 0$, $k = 1, 2$, is the convection matrix, the reaction matrix $\mathcal{A}(x, t) = (a_{kp}(x, t))$, $k, p = 1, 2$ is an M -matrix and q is a positive odd integer. We assume that $0 < \varepsilon_1 \leq \varepsilon_2 \leq 1$ and also that they can have different order of magnitude.

In the case (2), it is said that (1) has a turning point of repulsive type at $x = 0$. Conversely, in the case (3), it is said that the turning point $x = 0$ is of attractive type. In the first case, for arbitrary values of the diffusion parameters, in general, the exact solution has overlapping boundary layers at $x = -1$ and $x = 1$ of widths $O(\varepsilon_1)$ and $O(\varepsilon_2)$. In the second case, if the source term is a continuous function, there are neither interior nor boundary layers; however, overlapping internal layers appear at $x = 0$, of widths $O(\sqrt{\varepsilon_1})$ and $O(\sqrt{\varepsilon_2})$, if we include a discontinuity jump at $x = 0$ in the source term.

To approximate the exact solution of (1), we use a time integrator of type fractional steps combined with a decomposition in components for the differential operator; on the other hand, the spatial discretization uses the upwind scheme, which is defined on appropriate piecewise uniform meshes of Shishkin type, depending on the case which we are considering. The resulting fully discrete scheme is uniformly convergent with respect to both diffusion parameters, reaching first order in time and almost first order in space. We show the numerical results obtained for several test problems which corroborate in practice the efficiency and the reliability of the numerical algorithm.

Keywords: Singular Perturbed Systems, Turning Points, Shishkin Meshes, Uniform Convergence.

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Minimally implicit Runge-Kutta (MIRK) methods and applications

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Abstract. We present the Minimally-Implicit Runge-Kutta (MIRK) methods for the numerical resolution of hyperbolic equations with stiff source terms. Diffusion and convection-diffusion equations are very well known examples of this kind of equations. Previous approaches rely on using the so-called Implicit-Explicit (IMEX) Runge-Kutta schemes [1]. Instead, we apply the MIRK methods to the resistive relativistic magnetohydrodynamic (RRMHD) [2] and the M1 neutrino transport [3] equations. We will also present the preliminary results of applying the MIRK methods in the shallow water equations. The MIRK methods are able to deal with stiff terms producing stable numerical evolutions and their computational cost is similar to the standard explicit methods.

Keywords: Hyperbolic equations with stiff terms; implicit schemes; resistive relativistic magnetohydrodynamic equations; neutrino transport equations; shallow water equations.

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Numerical study of an inverse problem for a reaction-diffusion system arising in epidemiology

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Abstract. In this talk, we study the inverse problem of coefficients identification in reaction and diffusion terms of a reaction-diffusion system arising from the mathematical modeling of disease transmission. The direct problem is given by an initial boundary value problem for a reaction diffusion system where the unknowns are the population densities for susceptible and infected individuals living in a bounded domain and the boundary condition models the migration or emigration during the time of epidemics process, or equivalently we consider the boundary condition modeling the population flux across the boundary for both the susceptible and infected individuals. The coefficients of the reaction term are the rates of disease transmission and disease recovery. The inverse problem consists in the determination of disease rate, recovery transmission rate and the diffusion from observed measurement of the direct problem solution at the end time. We begin our analysis by reformulating the inverse problem as an optimization problem for an appropriate cost functional. Then we develop an analytical analysis and a numerical analysis. In the case of analytical analysis we obtain the following results: the existence of solutions of the inverse problem, which deduced by proving the existence of a minimizer for the cost functional; a first order necessary optimality condition; the stability of the inverse problem unknowns with respect to the observations; and the uniqueness up an additive constant of identification problem. Meanwhile, in the case of numerical analysis we introduce a finite volume scheme to approximate the direct problem and prove that is positive preserving, unconditionally stable and convergent; we define the numerical cost function; introduce a discrete adjoint scheme; and define a numerical gradient. Additionally, we present several numerical experiments focused on the convergence and the stability of the numerical scheme for parameter identification.

Keywords: Inverse problem; Numerical identification; SIS epidemic reaction–diffusion model.

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Singularly perturbed elliptic problems of convection-diffusion type with non-smooth data

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Abstract. A singularly perturbed elliptic problem with non-smooth data is examined. A decomposition of the continuous solution is constructed and parameter-explicit pointwise bounds on the first order partial derivatives of these components are established. An appropriate Shishkin mesh is identified for the problem and this is combined with upwinding to form a numerical method. Parameter-uniform error bounds are deduced and numerical results are presented to illustrate the performance of the numerical method.

Keywords: Convection diffusion; Elliptic problem; Interior layer; Shishkin mesh.

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A higher order numerical method for problems with characteristic boundary layers

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Abstract. A Petrov-Galerkin finite element method is constructed for a singularly perturbed elliptic problem in two space dimensions. The solution comprises a regular boundary layer and two characteristic boundary layers [1]. Exponential splines are used as test functions in one coordinate direction and are combined with bilinear trial functions defined on a Shishkin mesh. The method is shown to be a stable parameter-uniform numerical method with higher order of convergence, measured in L_∞ and energy norms, compared to simple upwinding on the same mesh.

Keywords: Convection-diffusion; Shishkin mesh; Petrov-Galerkin, Higher order.

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A posteriori error estimate for a reduced-order model totally based on Legendre collocation

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Abstract. This study presents an a posteriori error estimation of a reduced-order model for the study of bifurcations in a Rayleigh-Bard problem. The reduced method follows the reduced basis paradigm, which consists of using several low-dimensional bases to create a reduced-order problem. The high fidelity discretization underlying the reduced order method is a spectral Legendre Collocation method. This problem is formulated as a least-squares problem based on a high-fidelity discretization, avoiding the variational formulation. The resulting reduced solutions are certified by an a posteriori error estimator, which follows the standard pattern of dividing the norm of the residual by a stability factor [3]. Overall, the proposed methodology computes accurately, quickly and reliably, the bifurcation diagram [4].

Keywords: Reduced-order methods; a posteriori error estimation; Proper Orthogonal Decomposition; Legendre Collocation; Bifurcation problems; Rayleigh Bénard instability.

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Equation with boundary feedback damping

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Abstract. In this paper we consider PDE problems in which certain terms of the equations are concentrated, when a parameter tends to zero. Usually near the domain boundary.

This implies that the problem in question is subject to singular perturbations that drastically change the nature of the problem, by passing the limit on this parameter. The objective is then to identify the form of the limit problem and to describe the process of convergence of solutions, when this parameter tends to zero. Here we consider a nonlinear PDE problem that is a generalization from previous works such as [1, 2].

Keywords: Transmission problem; Singular limit; Concentrating terms.

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A multisplitting method for solving 2D parabolic convection-diffusion systems

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Abstract. In this work, we design and analyze a new numerical algorithm for solving efficiently two dimensional parabolic singularly perturbed coupled convection-diffusion systems given by

$$\begin{cases} \mathcal{L}_\varepsilon(t)\mathbf{u} \equiv \frac{\partial \mathbf{u}}{\partial t}(\mathbf{x},t) + \mathcal{L}_{\mathbf{x},\varepsilon}(t)\mathbf{u}(\mathbf{x},t) = \mathbf{f}(\mathbf{x},t), (\mathbf{x},t) \in \mathcal{Q} \equiv \Omega \times (0,T], \\ \mathbf{u}(\mathbf{x},t) = \mathbf{g}(\mathbf{x},t), (\mathbf{x},t) \in \partial\Omega \times [0,T], \\ \mathbf{u}(\mathbf{x},0) = \varphi(\mathbf{x}), \mathbf{x} \in \Omega, \end{cases} \quad (1)$$

where $\mathbf{u} = (u_1, u_2)^T$, $\mathbf{x} = (x, y)$, $\Omega = (0, 1)^2$ and the spatial differential operator $\mathcal{L}_{\mathbf{x},\varepsilon}(t)$ is defined as

$$\mathcal{L}_{\mathbf{x},\varepsilon}(t)\mathbf{u} \equiv -\mathcal{D}_\varepsilon \Delta \mathbf{u} + \mathcal{B}_1(\mathbf{x}) \frac{\partial \mathbf{u}}{\partial x}(\mathbf{x},t) + \mathcal{B}_2(\mathbf{x}) \frac{\partial \mathbf{u}}{\partial y}(\mathbf{x},t) + \mathcal{A}(\mathbf{x},t)\mathbf{u}, \quad (2)$$

being $\mathcal{D}_\varepsilon = \text{diag}(\varepsilon_1, \varepsilon_2)$ the diffusion matrix, whose diffusion parameters ε_1 and ε_2 can be very small and very different in size; the convection matrices $\mathcal{B}_1(\mathbf{x}) = \text{diag}(b_{11}(\mathbf{x}), b_{12}(\mathbf{x}))$, $\mathcal{B}_2(\mathbf{x}) = \text{diag}(b_{21}(\mathbf{x}), b_{22}(\mathbf{x}))$ contain positive diagonal elements and the reaction matrix \mathcal{A} is an M -matrix. The solutions of (1) use to have overlapping boundary layers at the outflow boundary of the spatial domain. This fact provokes that special space discretization techniques must be implemented to capture such multiscale behavior without using meshes with a very large number of nodes. On the other hand, the use of suitable (uniformly convergent) spatial discretization techniques reduces the continuous problem (1) to a family of extremely stiff, large and complicated differential systems which require the use of suitable time integrators to solve them in a robust and efficient way. Our proposal combines the use of simple upwind schemes on appropriate piecewise uniform rectangular meshes of Shishkin type, to discretize in space, and the fractional implicit Euler method joint to a splitting of the discrete convection diffusion operator in directions and components, to integrate in time. We prove that the constructed numerical method is uniformly convergent of almost first order in space and of first order in time. Some numerical experiments will corroborate the robustness as well as the efficiency of our algorithm.

Keywords: Splitting and Alternating Directions, Singular Perturbation, Overlapping Boundary Layers, Shishkin Meshes.

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A posteriori error estimates for layer solutions: from CG to DG

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Abstract. 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 [2, 3, 4, 5], with the main focus on the recent preprints [1, 6] and the current work on the discontinuous Galerkin method.

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Numerically accurate formulation of implicit turbulent bottom stress in an ocean model with barotropic-baroclinic mode splitting

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Abstract. Bottom drag plays an important role in dissipating tides, and becomes one of the dominant forces in tidal bays and estuaries. One of such places is Galway Bay, Ireland, where tidally induced currents can reach the speed of 2.5 m/sec, posing challenges in hydrodynamic modeling, essentially due to the interference of different algorithms, which need to work in concert, but originally were not thought to be this way. Thus, the split-explicit time stepping for an oceanic model implies that the barotropic mode (vertical integrals of horizontal velocities coupled with contribution of free-surface elevation into vertical integrals of pressure-gradient terms) is solved separately from the rest of the model using smaller time step [1]. This leads to significant computational savings, because the large number of short time steps are applicable only for 2D part of the whole 3D model, but also results in more complicated code, carefully designed to avoid numerical errors and instability. At the same time, vertical processes—mixing of tracers, viscous exchange of momenta, and, recently, vertical advection (only where it is strictly unavoidable [2])—are treated implicitly, but only in a one-dimensional manner resulting in a simple and efficient solver. A final ingredient is parameterization of vertical profile of turbulent mixing coefficient along with kinematic stress bottom boundary condition, which is of the no-slip type, but nonlinear in nature due to the fact that both bottom drag coefficient and vertical viscosity profile depend on the magnitude of the current [3].

Taken separately, these three aspects are well understood at this point. However, combining them in a single computational model requires special care: the barotropic mode needs to know the bottom drag terms in advance (which can be computed only within the 3D part of the code), but when done, the result barotropic mode calculation adjusts the horizontal velocity components in the 3D mode, compromising both the no-slip boundary conditions and the consistency of bottom stress with vertical viscosity profile. The proposed remedy is to modify the barotropic mode by introducing special perturbation terms, which mimic tendencies of pending changes in 3D-mode bottom drag terms as the barotropic mode progresses. This results in smaller perturbation in bottom stress values (formally $O(\Delta t^2)$ vs. $O(\Delta t)$) during the subsequent adjustment of 3D velocities, and ultimately a more robust code allowing larger time step.

Keywords: Implicit bottom drag in time-split model; Algorithm interference, Tidal modeling

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High order bounds in time for POD-ROM methods

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Abstract. In this talk we study numerical approximations to nonlinear evolutionary equations by means of proper orthogonal decomposition (POD) methods. It is known that in case the set of snapshots is based on finite differences or time derivatives then pointwise in time error bounds can be proved. In this talk we show how to get higher order estimations in time in both cases. We show that different time steps can be applied in the full order model (FOM) and the POD method. We study the influence of the distance in time between two consecutive snapshots in the accuracy of the POD approximations.

Keywords: POD methods; High order time integrators; Pointwise error estimates.

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2D Newton Schwarz alternating method applied to the Rayleigh-Bénard convection problem

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Abstract. In this paper we present an alternate Schwarz-type domain decomposition (DD) method applied to the Rayleigh-Bénard convection problem in a 2D fluid layer. The problem is modeled with the incompressible Navier-Stokes equations together with the heat equation in a rectangular domain and the Boussinesq approximation is considered [6, 7]. The problem is numerically solved with a Legendre collocation method and the mesh used is defined by Legendre-Gauss-Lobatto collocation points [1, 2]. Since the spectral methods are ill-conditioned it is necessary to use a DD method by dividing the problem into smaller subdomains and in this way, the ill-conditioning of Legendre collocation is overcome. Then, solutions can be obtained for large aspect ratios and/or for larger Rayleigh numbers [3, 5]. The stationary problem by means of the Schwarz alternating DD method and the solutions with this method are compared to reference solutions obtained with finite elements by COMSOL Multiphysics [4].

Keywords: Turbulence; Rayleigh-Bénard convection; Legendre collocation; Domain decomposition method; Alternating Schwarz

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Adaptive Regularisation for Optimal Control

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Abstract. This talk focuses on optimal control problems for partial differential equations with rough targets. The KKT optimality conditions for PDE constrained optimisation problems can be reduced to a singularly perturbed PDE involving the, typically small, regularisation parameter. This, in conjunction with a non-smooth target, results in the formation of interior layers. We present a novel methodology to enable fast and reliable computations around this. We propose an adaptive Tikhonov-type regularisation, where the regularisation parameter is varied across the domain. We solve the problem numerically using a Galerkin finite element method. We will present some a posteriori error analysis and results using this adaptive regularisation method, and also using this method in combination with adaptive mesh refinement.

Keywords: PDE constrained optimisation; Optimal control; Interior layers; Adaptivity; Finite element method

Analysis of the behavior of a viscous fluid between two nearby moving surfaces when the distance between them tends to zero

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Abstract. In this work, we initially used the asymptotic expansion technique to investigate the behavior of an incompressible viscous fluid flowing between two very close moving surfaces (see [1]). We observe that, in this case, the fluid has two distinct behaviors, depending on the boundary conditions of the problem. If there are significant pressure differences in the open part of the domain boundary (that is, the region of the domain boundary between the two surfaces), then we derive an equation resembling a lubrication problem. If the pressure differences are small in the mentioned region of the domain boundary, then the model corresponds to a thin fluid layer problem (it can also be understood as a shallow water problem in which the depth is known).

In the second place, we justify a new two-dimensional flow model of a viscous fluid between two very close moving surfaces (see [2]), and, we confirm that when the distance between the two surfaces tends to zero, the behavior of the new model aligns with that observed in [1] for the Navier-Stokes equations.

The solutions of both the new model and the Navier-Stokes equations converge to a common limit problem, contingent on the imposed boundary conditions. If slip velocity boundary conditions are imposed on the upper and lower bound surfaces, the limit corresponds to a solution of a lubrication model, but, if tractions and friction forces are known on both bound surfaces, the limit represents a solution of a thin fluid layer model.

The proposed model has been obtained to be a valuable tool for computing viscous fluid flow between two closely spaced moving surfaces, without the need to determine beforehand whether the flow is characteristic of a lubrication or a thin fluid layer problem; and, moreover, without the enormous computational effort that would be required to solve the Navier-Stokes equations in such a thin domain.

Keywords: Fluid mechanics; Lubrication; Thin fluid layer; Asymptotic analysis.

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Application of non-uniform Haar wavelet on an adaptive mesh for singularly perturbed convection-diffusion problem with non-local boundary

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Abstract. This work presents a novel adaptive mesh method based on a non-uniform Haar wavelet for a class of singularly perturbed convection-diffusion problems with non-local boundary conditions with the perturbation parameter $0 < \varepsilon \ll 1$,

$$\begin{cases} \varepsilon \frac{d^2 u}{dx^2} + a(x) \frac{du}{dx} = f(x), & x \in G = (0, 1), \\ \frac{du}{dx}(0) = \frac{\gamma_0}{\varepsilon}, \\ \int_0^1 \xi(x) u(x) dx = \gamma_1. \end{cases} \quad (1)$$

Here, the functions a , f , and ξ and the constants γ_0 and γ_1 are known.

Firstly the concept of the non-uniform Haar wavelet was proposed by Dubeau et al. [1] in 2004. The aforesaid problem has been considered previously using non-uniform Haar wavelet on exponentially graded mesh [4]. Here we are using a similar idea of approximation of the problem using non-uniform Haar wavelet but the novelty is that we are constructing the adaptive mesh based on the equidistribution principle [2]. This mesh adjusts itself to the boundary layer via a self improving mechanism. The proposed numerical method is proved to be parameter uniformly convergent. In addition to evaluating computation efficiency and stability, numerical results are presented in various tables and plots for numerical results obtained by the implementation of the proposed method on two test examples.

Keywords: Singular perturbation problems; Adaptive mesh; Non-uniform Haar wavelet; Parameter uniform convergence

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Optimal balanced-norm error estimate of the LDG method for singularly perturbed reaction-diffusion problems

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Abstract. The solution of singularly perturbed reaction-diffusion problems in 1D and 2D using the local discontinuous Galerkin (LDG) method on Shishkin meshes is considered. We investigate error estimates in balanced norms (see [3, 4, 5, 6, 7] and their bibliographies) which are stronger than the standard energy norm associated with this class of problem. In 1D optimal-order balanced-norm convergence can be proved when the fluxes in the LDG are chosen in a symmetric way [1], but there is a difficulty in extending this analysis to the 2D case. Thus for the 2D problem we modify the choice of fluxes in a novel way [2] by using a form of upwinding even though the reaction-diffusion problem has no convective component. This innovation enables us to again prove optimal-order balanced-norm convergence for the LDG method: when tensor products of piecewise polynomials of degree k are used, it is shown that the method attains convergence of order $O((N^{-1} \ln N)^{k+1})$ in the balanced norm, where N is the number of mesh intervals in each coordinate direction. The sharpness of this result is confirmed by numerical experiments.

Keywords: Local discontinuous Galerkin (LDG) finite element method; Layer-upwind flux; Shishkin mesh; Balanced norm; Reaction-diffusion.

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A non-uniform Haar wavelet approximation of a singularly perturbed Fredholm integro-differential equation on a layer adaptive mesh

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Abstract. In this research work we are considering the following singularly perturbed Fredholm integro-differential equation [2]

$$\begin{cases} \mathcal{L}_\epsilon u := -\epsilon \frac{d^2 u}{dx^2} + a(x) \frac{du}{dx} + b(x)u + \lambda \int_0^1 \mathcal{K}(x,s)u(s) ds = f(x), & x \in (0,1), \\ u(0) = l, \quad u(1) = L, \end{cases} \quad (1)$$

where $a(x)$, $b(x)$, $f(x)$, and $\mathcal{K}(x,s)$ are known functions, and $u(x)$ is the function to be determined. Here λ is a real parameter and $0 < \epsilon \ll 1$ is called the perturbation parameter.

To tackle the multi scale characteristic of solution, we propose a novel adaptive mesh method where the adaptive mesh is generated using the equidistribution of a suitably chosen monitor function [3]. On the adaptive mesh we approximate the second derivative of the solution with the help of a non-uniform Haar wavelet basis [1] and then using its successive integrations the problem is transformed into an algebraic system of equations. Theoretical error analysis is performed to show the convergence of the proposed method. Further, the computational efficiency and stability is shown by implementing the method on two test examples.

Keywords: Singular perturbation; Fredholm integro-differential equation; Non-uniform Haar wavelet; Adaptive mesh; Parameter uniform convergence

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A balanced norm error estimate of WG-FEM for fourth-order singularly perturbed reaction-diffusion problems

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Abstract. Robust uniform convergence of WG-FEM [2] fourth in a balanced norm a layer-adapted mesh has been established for fourth order singularly perturbed reaction-diffusion problems. Since the energy norm associated with the problem is not adequate for these problems (see, e.g., [1]), we define a stronger weighted and balanced norm which reflects the boundary layers efficiently and correctly. As a result, we obtain a uniform convergence in the maximum norm. The novelty of the proposed method lies on the introduction of weak derivatives and the use of a special interpolation of the solution on the weak finite element space. Particularly, we use a special interpolation consisting in an interpolation on the finer part and a projection operator on the coarse part of the domain. The stability and the optimal error estimates of the proposed scheme are addressed in the balanced norm. Finally, we present a numerical experiment to exhibit the suitability of the stated method.

Keywords: Fourth order singularly perturbed problem; boundary layers; WG-FEM; Uniform convergence; Balanced norm;

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Structure-preserving discretisations for electrolyte continuum models

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Abstract. Electrolyte continuum models describe the transport of charged particles in the presence of a global electric field. Examples include the Poisson-Nernst-Planck (PNP) system, also known as the drift-diffusion equations (or Van Roosbroeck equations in semi-conductor literature), and its extension to the Navier-Stokes-PNP (NS-PNP) system, which includes fluidic behaviour. The variables of interest are the concentrations of different species of charged particles and the electric potential, which governs the electric field strength. In the NS-PNP case the fluid velocity and pressure are also to be found. Subject to appropriate boundary and initial conditions, each of these models possess properties at the continuous level which can be interpreted physically as conservation of mass, positivity of charge carrier density, and energy dissipation laws. Preserving these structures at the discrete level is important for physical consistency and can be beneficial for ensuring stability of the scheme. However, the presence of non-linearities provides a challenge when designing such methods. In this talk novel finite element discretisations will be presented, which linearise the problem and unconditionally preserve at the discrete level analogues of important structures inherent to the continuous system.

Keywords: Structure-preserving; Poisson-Nernst-Planck; Navier-Stokes-Poisson-Nernst-Planck; Discontinuous Galerkin; Finite element;

Physics-informed neural networks for convection-dominated convection-diffusion problems

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Abstract. In the convection-dominated regime, solutions of convection-diffusion problems usually possess layers, which are regions where the solution has a steep gradient. It is well known that many classical numerical discretization techniques face difficulties when approximating the solution to these problems. In recent years, physics-informed neural networks (PINNs) for approximating the solution to (initial-)boundary value problems received a lot of interest. PINNs are trained to minimize several residuals (loss functionals) of the problem in collocation points. In this talk, we introduce various loss functionals for PINNs that are especially designed for convection-dominated convection-diffusion problems. They are numerically tested and compared on two benchmark problems whose solutions possess different types of layers. We observed that certain special functionals reduce the $L^2(\Omega)$ error compared to the standard residual loss functional [1]. Furthermore, three types of collocation points applied to hard-constrained PINNs are compared: layer-adapted, equispaced and uniformly randomly chosen points. We observe that layer-adapted points work the best for a problem with an interior layer and the worst for a problem with boundary layers [2].

Keywords: Convection-diffusion problems; Convection-dominated regime; Physics-informed neural networks; Loss functionals; Layer-adapted collocation points

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ERRATUM

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- Acknowledgements paragraph: “PID-2021-125458NB-C21” should be replaced by “PID-2021-125485NB-C21” and include after “CIPROM/2022/13” the following sentence: “the Astrophysics and High Energy Physics program Grant No. ASFAE/2022/0003 funded by MCIN and the European Union NextGenerationEU (PRTR-C17I1)”.
- References: the authors in reference [2] should be replaced by “I. Cordero-Carrión, S. Santos-Pérez,”