XVIII CMA / XXVIII CEDYA

ABSTRACTS BOOK



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Editors: Julen Álvarez, Agurtzane Amparan, Gorka Armentia, Francisco De La Hoz, Carlos Gorria, Iker Malaina, Silvia Marcaida, Virginia Muto

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Julen Álvarez, Agurtzane Amparan, Gorka Armentia, Francisco De La Hoz, Carlos Gorria, Iker Malaina, Silvia Marcaida, Virginia Muto



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PREFACE

The Congress of Differential Equations and Applications / Congress of Applied Mathematics (CEDYA / CMA) is the biennial congress of the Spanish Society of Applied Mathematics (SëMA). The first CEDYA was celebrated in September 1978 in El Escorial (Madrid), and the first joint CEDYA / CMA took place in Málaga in 1989.

The XXVIII CEDYA / XVIII CMA was held from 24th to 28nd June 2024 at the Sciences and Technology Faculty of the University of the Basque Country (UPV/EHU) and was organized by the Department of Mathematics of the University of the Basque Country (UPV/EHU) and the BCAM Institute.

This congress attracted near 220 participants from different universities. They presented 195 lectures, nine of which were invited. The conference was structured in sixteen mini-simposia, proposed by different researchers and groups, eight special sessions and a poster session, both organized by the Local Organizing Committee. The topics of the conference covered Partial Differential Equations, Dynamical Systems and Ordinary Differential Equations, Numerical Analysis and Simulation, Numerical Linear Algebra, Optimal Control and Inverse Problems, Mathematics Applied to Industry, Artificial Intelligence Applied to Mathematics, Social Sciences and Biology, Scientific Computation, Approximation Theory and Discrete Mathematics.

These Proceedings have been published in the institutional repository of the Spanish Society of Applied MAthematics (SeMA). They contain 195 abstracts corresponding to the contributions presented at XXVII CEDYA / XVII CMA. The editors would like to thank the authors for their contributions and cooperation, without them it would have been impossible to produce these abstracts.

Finally, we thank the sponsors of the conference: Sociedad Española de Matemática Aplicada, Facultad de Ciencia y Tecnología (UPV/EHU), Departamento de Matemáticas (UPV/EHU), Basque Center for Applied Mathematics (BCAM), Departamento de Educación, Universidades e Investigación, Gobierno Vasco / Eusko Jaurlaritza and Universidad del País Vasco / Euskal Herriko Unibertsitatea (UPV/EHU). We also wish to thank the Scientific Committee, the organizes of the mini-symposia, all the conference participants, and the students collaborators, who were hugely helpful in the organization of the conference.

Spain, September 2024

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Boundary Defects in Liquid Crystals

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Abstract:

We study the effect of "weak" and "strong" boundary conditions on the location and type of defects observed in a Landau de Gennes thin-film model for liquid crystals. We study both the minimizers of the associated Ginzburg-Landau energy as well as the Gamma limit when the correlation length tends to zero. A-priori estimates in case splay and bend moduli are included in the energy will also be presented. Finally, results in the case of the 3D Landau-de Gennes model with a magnetic field will be presented. These represent joint works with S. Alama, L. van Brussel, A. Colinet, D. Louizos and D. Stantejsky.

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On compressible fluid flows driven by random data

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Abstract:

In computational fluid dynamics, stochastic collocation or the Monte Carlo methods are typically used to quantify the propagation of data uncertainty. Despite the large popularity of these methods, their rigorous convergence analysis for compressible fluid flows was missing in general.

In this talk, I will review our recent results obtained for the random compressible Euler and Navier-Stokes systems, [1]-[6]. We suppose that the initial and boundary data as well as model parameters, such as the viscosity coefficients, are random variables. Consequently, a solution of the PDE system will be a random process. The stochastic collocation or the Monte Carlo methods are combined with a suitable deterministic discretization scheme, such as a finite volume method. Since the compressible Navier– Stokes and the Euler equations are not uniquely solvable in the class of global weak solutions, we cannot apply pathwise arguments to analyze the random equations. Instead, we apply stochastic compactness arguments via the Skorokhod representation theorem and the Gyöngy–Krylov method. We study both the statistical convergence rates as well as the approximation errors.

The convergence of the deterministic Navier-Stokes or Euler system is realized via dissipative solutions [7], [8], [9]. Assuming that numerical solutions satisfy in probability suitable conditions leading to a global regular solution, we prove that the Monte Carlo finite volume method as well as the stochastic collocation finite volume method converge to a statistical strong solution. The convergence rates of the finite volume and statistical methods are discussed as well [3],[9]. Numerical experiments will illustrate theoretical results [4, 5, 6].

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Laws: Complexity, Scales and Randomness" as well as by the Sino-German project number GZ1465.

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High relative accuracy computations through Newton polynomial bases

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Abstract: The resolution of interpolation or approximation problems usually requires algebra computations related to different types of matrices. Sometimes, these matrices are notoriously ill-conditioned and so, the standard routines implementing best traditional numerical methods cannot keep numerical errors under control, providing inaccurate solutions. So, an important goal in the field of Numerical Linear Algebra is to achieve algorithms to high relative accuracy (HRA), which implies a great accuracy since the relative errors in the computations have the same order as the machine precision and this accuracy is not affected by the dimension or the conditioning of the problem to be solved.

The class of totally positive matrices has been extensively studied (see [1, 2]) and attracts much interest in several fields of mathematics and their applications, including approximation theory, combinatorics, computer-aided geometric design, or economics. Over the past years, many researchers have been concentrating on achieving accurate numerical solutions for ill-conditioned algebraic problems with totally positive matrices. In fact, many efforts have been devoted to finding a bidiagonal factorization of such matrices, since its accurate computation allows us to numerically solve relevant algebraic problems to HRA (see [3], [5], [7]).

In this presentation, we shall focus on the linear transformation between the monomial basis and the Newton basis corresponding to a sequence of interpolation nodes. The total positivity property of the matrices for the change of basis will be examined and efficient algorithms proposed for the HRA resolution of related algebraic problems.

Several interesting applications will be showcased, including the HRA calculation of the divided differences for the computation of the Newton form of the Lagrange interpolant [4]. Furthermore, Stirling matrices can be considered as particular cases of the above mentioned change of basis matrices. The algorithms for the HRA resolution of algebraic problems with

collocation and wronskian matrices of Touchard polynomial bases derived in [6] will be also shown.

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A geometric approach to characterizing Lagrangian ocean transport and exploring its environmental applications.

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Abstract:

Finding order in the apparent chaos that seems to govern transport processes in the ocean is a challenge. In this talk, I will describe a dynamical system tool referred to as Lagrangian Descriptors [1], which is able to highlight a geometric template on the ocean surface that forms a skeleton that governs underlying transport. Two selected cases will be described from this perspective. First, I will explain how this dynamical template accurately described the long-term behavior of the fuel spill subsequent to the crash of the Volcan Tamasite Ferry against the Nelson Mandela dike in La Luz Port in April 2017 [2]. Secondly, I will describe how this geometrical template, jointly supported by remote sensing imagery, helped understand the sequence of events that affected the Eastern Mediterranean and several Middle Eastern countries' shorelines in early 2021 [3]. The comparison of the performance of various datasets is discussed for both cases, and connections have been found between both the geometrical templates and uncertainty quantification [4, 5].

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Variational PINNs for solving parametric PDEs

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Abstract:

Solving inverse problems with uncertainty quantification is crucial for our society. Herein, we focus on inverse problems governed by second-order linear Partial Differential Equations (PDEs).

The most critical step for decoding inverse problems is to solve the associated parametric PDE. This step is often a bottleneck when employing classical finite element or finite difference-based methods; however, Neural Networks (NNs) show a promising avenue for solving parametric PDEs.

In this presentation, we use Robust Variational Physics Informed Neural Networks (RVPINNs) [2]. We propose to decompose the parametric PDE solution using a Proper Generalized Decomposition (PGD) [1] of the form:

$$u(x;\xi) \approx \sum_{i=1}^{N} c_i(\xi) \cdot u_i(x), \tag{1}$$

where $\{u_i(x)\}_{i=1}^N$ is a set of functions depending on the spatial variable $x \in \mathbb{R}^d$ (*d* is the space dimension), and $\{c_i(\xi)\}_{i=1}^N$ is a set of coefficients depending on the PDE parameter ξ . The key idea is to employ a NN $\mathbf{u} : \mathbb{R}^d \longrightarrow \mathbb{R}^N$ to construct the basis functions $u_i(x)$ while computing the coefficients $c_i(\xi)$ using a Least-Squares solver. The output \mathbf{u} plays the role of a set of reduced order basis, as in PGD.

Critical numerical aspects that need to be properly adjusted to ensure the proper behavior of the method include: (a) numerical integration, possibly using a high-order, stochastic, and unbiased rule; (b) a proper architecture choice possibly adapted to the regularity of the solution; and (c) an efficient implementation for the construction of the Least Squares system. We will discuss all these aspects during the presentation.

We will also illustrate the main features and limitations of the method via one- and two-dimensional numerical experiments using a specific RVPINN method known as Deep Fourier Residual [3].

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Multi-* modeling, analysis, and simulation of coupled processes in the Arctic soils.

Authors:

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Abstract: The Arctic is a complex environment which responds to, and contributes to the global climate controls at multiple spatial and time scales. In the talk we discuss multi-component models of energy, mass flow, and deformation affecting Arctic soils: these are partial differential equations involving various nonlinear non-smooth relationships and heterogeneous data. The first challenge is to define and implement robust conservative algorithms for the approximation of solutions which must respect the low regularity of solutions expected from these complex PDE systems featuring, e.g., free boundaries associated with that [1, 3, 2]. The second challenge is the data: for predictive power, the models require realistic physical data, but the empirical and field data is scarce due to the vastness of the Arctic environment; moreover, the data is rarely available for coupled processes. We approach this challenge with multi-scale techniques starting with xray images of the pore-scale applying first-principles models at the pore-scale, which we post-process with computational upscaling while respecting the non-local features and randomness [4, 6, 5].

This is joint work with the co-authors of the work listed below as well as with collaborators on current projects

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Space-time isogeometric method

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Abstract: Isogeometric analysis [1] employs splines (or NURBS, etc.) as approximating functions in space. This choice not only bridges numerical simulation with computer-aided geometric design and computer graphics, but also yields optimal approximation properties, surpassing those of continuous or discontinuous piecewise polynomial approximations used in finite elements. Then, why not approximate also the temporal dependence of the solution of evolutionary partial differential equations with splines? This approach differs from more conventional space-time methods that use discontinuous Galerkin approximation in time, and is of interest only if accompanied by an efficient, possibly parallel, solver. In [2], we proposed a class of solvers that leverage the tensor construction of spline spaces, achieving high efficiency through linear algebra tensor methods. This presentation will discuss the use, advantages, and disadvantages of space-time isogeometric analysis for parabolic and hyperbolic [3] equations.

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Resonances as a computational tool

Authors:

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Abstract:

A large toolbox of numerical schemes for dispersive equations has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever nonsmooth phenomena enter the scene such as for problems at low regularity and high oscillations. Classical schemes fail to capture the oscillatory nature of the solution, and this may lead to severe instabilities and loss of convergence. In this talk I present a new class of resonance based schemes. The key idea in the construction of the new schemes is to tackle and deeply embed the underlying nonlinear structure of resonances into the numerical discretization. As in the continuous case, these terms are central to structure preservation and offer the new schemes strong geometric properties at low regularity.

I will present the key idea behind resonances as a computational tool, their high order counterpart (via tree series inspired by singular SPDEs), their error estimates in low regularity spaces (via discrete Bourgain spaces) and numerical experiments on nonlinear dispersive quantization effects. I also want to address the fundamental question of resonance based schemes and structure preservation, i.e., central symmetries and even more so symplecticity.

Blood Rheology and Multiscale Modeling of Cardiovascular Flows

Authors:

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Abstract:

Experimental studies over many years have shown that blood flow exhibits non-Newtonian characteristics such as shear-thinning, viscoelasticity, yield stress and thixotropy. The complex rheology of blood is influenced by numerous factors including plasma viscosity, hematocrit and in particular, the ability of erythrocytes to form aggregates when at rest or at low shear rates and to deform at high shear rates, storing and releasing energy. Hemodynamic analysis of blood flow in vascular beds and prosthetic devices requires the rheological behavior of blood to be characterized by phenomenological constitutive equations relating the stress to the rate of deformation and flow.

In this talk we present a short overview of several macroscopic constitutive models that can mathematically characterize the rheology of blood and describe their known phenomenological properties. Based on numerical simulations of different blood constitutive equations under given sets of physiological flow conditions, some test cases formulated in idealized and anatomically realistic vessels will be considered to investigate the impact of the most significant non-Newtonian characteristics of blood on its flow behavior. Moreover, some approaches in multiscale modeling and simulations of blood flow problems with applications to clinical cases will also be presented.

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A high-order Lagrange–Galerkin method for compressible flows

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Abstract:

We present a novel Lagrangian–Eulerian scheme for the solution of twodimensional compressible and inviscid flows [2]. The scheme considers arbitraryorder continuous space discretizations on unstructured triangular meshes, as well as arbitrary-order implicit–explicit Runge–Kutta time marching schemes. The method preserves mass, momentum and total energy as long as the integrals in the formulation are computed exactly. The recent model proposed by Brenner [1] for viscous flows is employed to define the operators needed to stabilize the continuous Galerkin formulation. The method has been tested on several benchmark problems using a fourth-order time-marching formula and up to fifth-degree elements, showing good accuracy both for smooth and discontinuous solutions.

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Finite difference schemes for the *p*-Laplacian

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Abstract: The aim of this talk is to introduce the topic of finite difference schemes to PDEs related to the *p*-Laplacian operator

$$\Delta_p u := \nabla(|\nabla u|^{p-2} \nabla u),$$

for p > 1. In this collaboration with E. Lindgren ([1]), we first introduce monotone asymptotic expansions of the *p*-Laplacian. Based on this approximations, we propose a finite difference discretization of the operator ([2]) and apply it to study numerically the associated parabolic problem ([3])

$$\partial_t u - \Delta_p u = f.$$

We show that the explicit scheme is stable, monotone and convergent in the context of viscosity solutions. An important advantage of our approach, is that the CFL-condition makes use of the regularity provided by the scheme to reduce the computational cost. In particular, for Lipschitz data, the CFL-condition is of the same order as for the heat equation and independent of p. Finally, we will discuss extensions obtained in [4] in the context of nonlocal problems.

- del Teso, Félix; Lindgren, Erik; A mean value formula for the variational p-Laplacian. NoDEA Nonlinear Differential Equations Appl., 28 (2021), no. 3, Paper No. 27, 33 pp.
- [2] del Teso, Félix; Lindgren, Erik; A finite difference method for the variational p-Laplacian Journal of Scientific Computing, 90 (2022), Article No. 67, 31pp.
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Global bifurcation for corotating vortex pairs

Authors:

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Abstract:

The existence of a local curve of corotating vortex pairs was proven by Hmidi and Mateu via a desingularization of a pair of point vortices. In this talk, we will present a global continuation of these local curves. That is, we consider solutions which are more than a mere perturbation of trivial solutions. Indeed, while the local analysis relies on the study of the linear equation at the trivial solution, the global analysis requires on a deeper understanding of topological properties of the nonlinear problem. For our proof, we adapt the powerful analytic global bifurcation theorem due to Buffoni and Toland, to allow for the singularity at the bifurcation point. This is a collaboration with Susanna V. Haziot.

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Influence of a lower order term for the fractional Laplacian BVP in presence of the Hardy potential.

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Abstract: We study existence and regularity of solutions to a problem involving fractional Laplacian and Hardy potential:

$$\begin{cases} (-\Delta)^s u + g(x)|u|^{p-1}u = \lambda \frac{u}{|x|^{2s}} + f(x), & \text{in } \Omega, \\ u = 0, & \text{in } \mathbb{R}^N \setminus \Omega, \end{cases}$$

where $0 \in \Omega \subset \mathbb{R}^N$ (N > 2s) is a bounded domain with a smooth boundary, p > 1, $\lambda \in \mathbb{R}$, $0 < g \in L^1_{loc}(\Omega)$ and $f \in L^{\frac{p+1}{p}}_{g}(\Omega)$.

We show the regularizing effect provided by the lower order term: $g(x)|u|^{p-1}u$, as it was done for the Laplacian case, [2]. As a consequence, we improve the results obtained in absence of this lower order term, [1]. More precisely, under the following condition

$$\int_{\Omega} |x|^{\frac{2(p+1)s}{1-p}} g^{\frac{2}{1-p}} < +\infty,$$

we are able to achieve two noteworthy outcomes concerning our problem:

- 1. Existence of solutions u for every $\lambda \in \mathbb{R}$.
- 2. Increasing of the regularity, $u \in H_0^s(\Omega) \cap L_g^{pm}(\Omega)$, when $f \in L_g^m(\Omega)$, for $m \geq \frac{p+1}{p}$.

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Semilinear eigenvalue problems with an unbounded interval of bifurcation points

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Abstract:

In this work, we study the behavior of the set of solutions of the semilinear elliptic problem

$$\begin{cases} -\Delta u = \lambda f(u) & \text{ in } \Omega, \\ u = 0 & \text{ on } \partial \Omega, \end{cases}$$

where Ω is a bounded open subset of \mathbb{R}^N and f is a nonnegative continuous real function with multiple positive zeros. First, we analyze the set of the solutions whose maximum is between two consecutive positive zeros of f, arriving to the existence of an unbounded continuum of solutions with \subset shape. Then, we study the asymptotic behavior of the countable many unbounded continua in the case in which f has a sequence of positive zeros. For the model cases $f(t) = t^r (1 + \sin t)$ and $f(t) = t^r (1 + \sin \frac{1}{t})$ with $r \ge 0$, we show the surprising fact that there are some values of r for which every $\lambda > 0$ is a bifurcation point (either from infinity or from zero) that is not a branching point.

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Generalized Three Critical Point Theorem for Relativistic Equations with Applications

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Abstract: This talk presents an extension of the Pucci and Serrin three critical point theorem to convex lower semicontinuous perturbations of C^1 functionals in Banach spaces. The extension is applied to establish the existence of three solutions for a one-parameter family of relativistic problems with zero Dirichlet boundary conditions. In particular,

$$\left(\frac{q'}{\sqrt{1-|q'|^2}}\right)' = (m|q|^{m-2} - \lambda p|q|^{p-2}) \cdot q,$$
$$q(0) = q(T) = 0,$$

where p > m > 2 and T > 0.

These problems represent a simplified version of the relativistic Lorentz force equation, devoid of magnetic field influence. This extension broadens the theorem's scope to encompass relativistic scenarios, opening avenues for applications across physics and applied mathematics.

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Global effects of a saturation term in a heterogenous predatorprey model

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- Eduardo Muñoz-Hernández, UCM (eduardmu@ucm.es)

Abstract: In this talk we analyze the spatially heterogeneous predator-prey model

$$\begin{cases} \mathfrak{L}_1 u = \lambda u - a(x)u^2 - b(x)\frac{uv}{1 + \gamma m(x)u} & \text{in } \Omega, \\ \mathfrak{L}_2 v = \mu v + c(x)\frac{uv}{1 + \gamma m(x)u} - d(x)v^2 & \text{in } \Omega, \\ \mathfrak{B}_1 u = \mathfrak{B}_2 v = 0 & \text{on } \partial\Omega, \end{cases}$$
(1)

where \mathfrak{L}_1 and \mathfrak{L}_2 are second order uniformly elliptic operators, and \mathfrak{B}_1 and \mathfrak{B}_2 are general boundary operators of mixed type. In (1), $a, d > 0, b, c \ge 0$, $\gamma > 0$ and $m \ge 0$ in $\overline{\Omega}$, while $\lambda, \mu \in \mathbb{R}$ are the bifurcation parameters. The term m(x) measures the level of saturation of the predator at any particular location $x \in \Omega$ where m(x) > 0 (Holling-Tanner response), while saturation effects do not play any role if m(x) = 0 (Lotka-Volterra response).

During the talk, they will be first ascertained the regions in the plane (λ, μ) in which coexistence states exist or could exist. Then, considering a shadow system appearing when $\gamma \uparrow +\infty$, it will be provided a generic multiplicity result ensuring the existence of, at least, two coexistence states of (1) for γ large enough in the region in which one of the semitrivial positive solutions is linearly stable. Moreover, in some special cases, a S-shaped component appears implying the existence of, at least, three coexistence states. Finally, when the amplitude of m(x) is small enough, we will see that there is uniqueness in the one-dimensional counterpart of (1).

- [1] A. Casal et al., Existence and uniqueness of coexistence states for a predator-prey model with diffusion, *Diff. Int. Eqs.*, **7** (1994), 411-439.
- [2] Y. Du and Y. Lou, Some uniqueness and exact multiplicity results for a predator-prey model, Trans. Am. Math. Soc., 349 (1997), 2443-2475.
- [3] J. López-Gómez and E. Muñoz-Hernández, A spatially heterogeneous predator-prey model, DCDS-B, 26 (2021), 2085-2113.
- [4] J. López-Gómez and E. Muñoz-Hernández, A robust multiplicity result in a generalized diffusive predator-prey model, Adv. Diff. Eqs., 9 (2024), 437-476
Section: PDE

Blow-up estimates and a priori bounds for the positive solutions of a class of superlinear indefinite elliptic problems

Authors:

• Juan Carlos Sampedro, Universidad Politécnica de Madrid (juancarlos.sampedro@upm.es)

Abstract: In this talk we present some new blow-up estimates for the positive explosive solutions of a paradigmatic class of elliptic boundary value problems of superlinear indefinite type:

$$\begin{cases} \mathscr{L}u = \lambda u + a(x)u^r & \text{in } \Omega, \\ \mathscr{B}u = 0 & \text{on } \partial\Omega, \end{cases}$$
(1)

where Ω is a bounded domain of \mathbb{R}^N , $N \ge 1$, of class \mathcal{C}^2 , $\lambda \ge 0$,

$$\mathscr{L}u = -\operatorname{div}(A(x)\nabla u),$$

uniformly elliptic in Ω and \mathfrak{B} is any boundary operator of non- classical mixed type on $\partial\Omega$. These estimates are obtained by combining the scaling technique of Guidas–Spruck [2] together with a generalized De Giorgi–Moser weak Harnack inequality found, very recently, by Sirakov [4, 5]. In a further step, based on a comparison result of Amann and López-Gómez [1], we will show how these bounds provide us with some sharp a priori estimates for the classical positive solutions of (1). It turns out that this is the first general result where the decay rates of the potential a(x) do not play any role for getting a priori bounds for the positive solutions when $N \geq 3$. This is a joint work with J. López-Gómez [3].

- H. Amann and J. López-Gómez, A priori bounds and multiple solutions for superlinear indefinite elliptic problems, J. Diff. Equ. 146, (1998), 336–374.
- [2] B. Gidas and J. Spruck, A priori bounds for positive solutions of nonlinear elliptic equations, Comm. in Part. Diff. Equ. 6 (1981), 883–901.
- [3] J. López-Gómez and J. C. Sampedro, Blow-up estimates and a priori bounds for the positive solutions of a class of superlinear indefinite elliptic problems, *Submitted to J. Diff. Equ.*, ArXiv: https://arxiv.org/abs/2402.01519.
- [4] B. Sirakov, A new method of proving a priori bounds for superlinear elliptic PDE, J. Math. Pures et Appl. 141 (2020), 184–194.
- [5] B. Sirakov, Global integrability and weak Harnack estimates for elliptic PDEs in divergence form, Analysis & PDE 15 (2022), 197–216.

Semilinear Degenerate Biot-Signorini System

Authors:

• Ralph Showalter, Oregon State University (show@oregonstate.edu)

Abstract: Nonlinear extensions of the quasi-static Biot model of consolidation are studied with emphasis on boundary conditions, attainment of initial values, and parabolic regularizing effects. The local fluid content is monotone and possibly nonlinear or degenerate with respect to pressure, and the stress of the solid in the fully-saturated porous medium is strictly monotone in strain. In addition to boundary conditions of classical Dirichlet, Neumann, or Robin type, the medium may have a singular or degenerate semipermeable interface with the exterior fluid at a known pressure, and the monotone dependence of traction on boundary displacement includes unilateral constraints of Signorini type given by a variational inequality. The initial-boundary-value problem for this general system is formulated as a Cauchy problem in Hilbert space for a semilinear implicit evolution equation that is nonlinear in the time derivative, and it is shown to be well-posed with regularity of the solution dependent on the data. When the stress is the derivative of a convex strain energy function, the evolution equation is a gradient flow with corresponding *parabolic* regularizing effects on the solution.

References:

 Alireza Hosseinkhan, Ralph Showalter, "Semilinear Degenerate Biot-Signorini System", SIAM Jour. Math. Anal. 50 (2023), No. 5, pp. 5643–5665.

Asymptotic behavior of positive solutions for a degenerate logistic equation with mixed local and non-local diffusion

Authors:

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- Cristian Morales-Rodrigo, Universidad de Sevilla (cristianm@us.es)
- Antonio Suárez, Universidad de Sevilla (suarez@us.es)

Abstract: In this work, we analyze a stationary degenerate logistic equation with both local and non-local dispersion diffusion. Primarily employing bifurcation results, sub- and supersolution methods, and maximum principles, we establish results regarding the existence, non-existence, and uniqueness of positive solutions. Additionally, using appropriate large solutions, we conduct a detailed study of the asymptotic behavior of the solutions with respect to one of the equation's parameters, showing that the presence of the non-local diffusion can drastically change this point-wise behavior when compared with the local case.

References:

[1] W. Cintra, C. Morales-Rodrigo and A. Suárez. Asymptotic behavior of positive solutions for a degenerate logistic equation with mixed local and non-local diffusion. Preprint

CEDYA 2024 - Communication proposal

Section: PDE

Helmholtz decomposition based on nonlocal gradients over bounded domains

Authors:

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- Mikil Foss, University of Nebraska-Lincoln (mikil.foss@unl.edu)
- Petronela Radu, University of Nebraska-Lincoln (pradu@unl.edu)

Abstract: One of the motivations of nonlocal models is that they may able to provide a framework for more general (or singular) phenomena, since they may not need to use classical derivatives, whereas the Helmholtz decomposition is a relevant result in mathematics and fluid mechanics which states that any (sufficiently smooth) vector field can be written as the sum of curl-free vector field plus a divergence-free one. Thus, the scope of this talk aims to provide a Helmholtz decomposition based on a strongly singular nonlocal gradient. In doing so we continue further with the nonlocal calculus developed for nonlocal gradients defined as

$$D^{s}_{\delta}u(x) = c_{n,s} \int_{B(x,\delta)} \frac{u(x) - u(y)}{|x - y|} \frac{x - y}{|x - y|} \frac{w_{\delta}(x - y)}{|x - y|^{n - 1 + s}} \, dy, \quad x \in \Omega$$

for $u: \Omega \cup B(0, \delta) \to \mathbb{R}$. This operator keeps a degree of fractional differentiability while providing a framework over bounded domains. Following some previous results regarding nonlocal versions of the Fundamental Theorem of Calculus, Poincaré Sobolev inequalities, Piola identity or compact embedding concerning the operator $D^s_{\delta}u$, we develop new tools such as nonlocal Divergence and Stokes theorems, three nonlocal Green identities as well as the study of the fundamental solution of the Laplacian given by $\Delta^s_{\delta}u := \operatorname{div}^s_{\delta}D^s_{\delta}u$, for a properly defined nonlocal divergence. Most of them are employed in the path leading to the nonlocal Helmholtz decomposition.

There have been previous results on Helmholtz decompositions concerning two-points nonlocal gradients(without integration), one-point gradient with integrable kernels or the Riesz fractional one (defined over the whole space).

References:

 José C. Bellido; Javier Cueto; Mikil Foss; Petronela Radu; Nonlocal Green theorems and Helmholtz decompositions for truncated fractional gradients https://arxiv.org/pdf/2311.05465

Perturbation of the Robin eigenvalues of the *p*-Laplacian operator

Authors:

- José C. Sabina de Lis, Departamento de Análisis Matemático, Universidad de La Laguna (josabina@ull.edu.es)
- Sergio Segura de León, Departament d'Anàlisi Matemàtica, Universitat de Valéncia (sergio.segura@uv.es)

Abstract:

In this talk¹ we are concerned with the Robin eigenvalue problem for the p-Laplacian. Namely,

$$\begin{cases} -\Delta_p u = \lambda |u|^{p-2} u, & x \in \Omega \\ |\nabla u|^{p-2} \nabla u \cdot \nu + b |u|^{p-2} u = 0, & x \in \partial \Omega. \end{cases}$$

Here $\Omega \subset \mathbb{R}^N$ is a bounded smooth domain, ν stands for its unitary outward field, $-\Delta_p u = \operatorname{div} |\nabla u|^{p-2} \nabla u$ is the *p*-Laplacian operator and $b(x) \in L^{\infty}(\partial \Omega)$. Exponent p > 1 is regarded as the key parameter in our study. Some of the main features to be discussed are: i) the continuos dependence on *p* of the higher eigenvalues, ii) the existence of their limit as *p* goes to 1 and iii) the eigenvalue problem satisfied by the limit of the corresponding eigenfunctions as $p \to 1$. The so-called 1–Laplacian operator is involved in the latter problem. The reported research appears in [1] and provides the continuation of [2] to the Robin problem.

- Sabina de Lis C., Segura de León S., The limit as p → 1 of the higher eigenvalues of the p-Laplacian operator Δ_p. Indiana Univ. Math. J. **70** (2021), no. 4, 1395–1439.
- [2] Sabina de Lis C., Segura de León S., Higher Robin eigenvalues for the p-Laplacian operator as p approaches 1. Submitted for publication (2024).

¹It is going to be presented in a Mini symposium organized by Pedro Martínez Aparicio and Alexis Molino: M01, Advances in the Studies of PDE's.

Existence for quasilinear elliptic equations involving asymptotic linear growth operators

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- Sergio Segura de León, Universitat de València (sergio.segura@uv.es)

Abstract: This talk is devoted to study existence of solutions to problems

$$\begin{cases} -\operatorname{div} \left(\phi(|\nabla u|)\nabla u\right) = f(x) & \text{ in } \Omega, \\ u = 0 & \text{ on } \partial\Omega, \end{cases}$$
(1)

where $\Omega \subset \mathbb{R}^N$ is a bounded open set having Lipschitz continuous boundary, $N \geq 2$ and $f \in L^{N,\infty}(\Omega)$. Regarding the function $\phi : \mathbb{R}_+ \to \mathbb{R}_+$, it satisfies

 (ϕ_1) Function $s \mapsto \phi(s)s$ is non-decreasing in \mathbb{R}_+ ;

$$(\phi_2) \lim_{s \to +\infty} \phi(s) = 1;$$

 (ϕ_3) Function $s \mapsto \phi(s)s$ is continuous in $(0, +\infty)$.

Main examples of equations that can be writen as in (1) for suitable functions ϕ are:

- 1. When $\phi(s)s = 1$ for s > 0, the operator in (1) becomes the 1-Laplacian.
- 2. When $\phi(s)s = \frac{s}{\sqrt{1+s^2}}$, we find the prescribed mean curvature operator.

It is well-known that in both cases a smallness condition on the datum f is necessary to obtain existence of solution. Our aim is to identify, in the general case (1), the threshold on the size of the datum so that below this value there exists a solution and above it there does not.

Formally, problem (1) is the Euler-Lagrange equation of minimizing an asymptotic linear growth functional.

Doubly critical elliptic systems

Authors:

• Ángel Arroyo, Universidad de Alicante (angelrene.arroyo@ua.es)

Abstract: In this talk we show existence of positive bound and ground states of a Hardy–Sobolev type system of elliptic PDEs coupled by a singular critical Hardy–Sobolev term which reads as

$$\begin{cases} -\Delta u - \lambda_1 \frac{u}{|x|^2} - \frac{u^{2_{s_1}^* - 1}}{|x|^{s_1}} = \nu \alpha h(x) \frac{u^{\alpha - 1} v^{\beta}}{|x|^{s_3}} & \text{in } \mathbb{R}^N, \\ -\Delta v - \lambda_2 \frac{v}{|x|^2} - \frac{v^{2_{s_2}^* - 1}}{|x|^{s_2}} = \nu \beta h(x) \frac{u^{\alpha} v^{\beta - 1}}{|x|^{s_3}} & \text{in } \mathbb{R}^N. \end{cases}$$

Here h is a nonnegative function in \mathbb{R}^N , $\lambda_1, \lambda_2 > 0$, $\nu > 0$ and $\alpha, \beta > 1$ such that

$$\frac{\alpha}{2_{s_1}^*} + \frac{\beta}{2_{s_2}^*} \le 1.$$

The main novelty of this work is that the exponents $s_1, s_2, s_3 \in (0, 2)$ are not necessarily equal.

References:

 Á. Arroyo, R. López-Soriano, and A. Ortega. Existence of solutions for a system with general Hardy–Sobolev singular criticalities. Preprint, 2024. arXiv:2405.20845.

A priori estimates for quasilinear elliptic systems

Authors:

- <u>Laura Baldelli</u>, University of Granada (labaldelli@ugr.es)
- Roberta Filippucci, University of Perugia (roberta.filippucci@unipg.it)

Abstract: In this talk, based on [1], we will focus on a priori estimates of the type

$$u(x) + |Du(x)|^{\alpha_1} \le C(1 + dist^{-\alpha_2}(x, \partial\Omega)), \ x \in \Omega$$

$$v(x) + |Dv(x)|^{\beta_1} \le C(1 + dist^{-\beta_2}(x, \partial\Omega)), \ x \in \Omega,$$
(1)

where $\Omega \subseteq \mathbb{R}^N$ is an arbitrary domain, $\alpha_i, \beta_i > 0$ for i = 1, 2, for any (u, v) nonnegative solutions of an elliptic system whose prototype is

$$\begin{cases} -\Delta_p u = v^{p_1} - v^{s_1} u^{s_2} |Dv|^{\theta_1} |Du|^{\theta_2} & \text{in } \Omega, \\ -\Delta_q v = u^{q_1} - u^{r_1} v^{r_2} |Du|^{\gamma_1} |Dv|^{\gamma_2} & \text{in } \Omega, \end{cases}$$
(2)

with 1 < p, q < N, $p_1, q_1 > 1$, $s_i, r_i, \theta_i, \gamma_i > 0$ satisfying particular conditions.

Estimates of the type (1) are those that Serrin and Zou in [3] call universal a priori estimates, because they are independent of the solutions and do not need any boundary conditions.

The system (2) generalizes the celebrated Lane-Emden system, involving quasilinear operators on arbitrary domains of \mathbb{R}^N and a nonlinearity depending on the gradient. Moreover, it is a model in population dynamics used to describe the evolution of the population density of a biological species, under the effect of certain natural mechanism.

The technique used it is based on rescaling arguments combined with a key "doubling" property, which is different from the celebrated blow-up technique due to Gidas and Spruck in [2].

- L. Baldelli, R. Filippucci, A priori estimates for elliptic problems via Liouville type theorems, Discrete Contin. Dyn. Syst. Ser. S, Special Issue on the occasion of the 65th birthday of Patrizia Pucci, 13, (2020), 1883–1898.
- [2] B. Gidas, J. Spruck, A priori bounds for positive solutions of nonlinear elliptic equations, *Comm. Partial Differential Equations*, 6, (1981), 883–901.
- [3] J. Serrin, H. Zou, Cauchy-Liouville and universal boundedness theorems for quasilinear elliptic equations and inequalities, Acta Math., 189, (2002), 79–142.

A Hamilton-Jacobi approach for the evolutionary dynamics of a model with gene transfer. How to characterize monomorphic dynamics for concave fitness functions.

Authors:

- Francesco Esposito, University of Calabria (francesco.esposito@unical.it)
- Rafael López-Soriano, University of Granada (ralopezs@ugr.es)
- Berardino Sciunzi, University of Calabria (sciunzi@mat.unical.it)

Abstract: This talk will be focused on the study of a family of semilinear elliptic systems defined in \mathbb{R}^n , which is doubly critical since it involves Sobolev critical exponents and Hardy-type potentials. We aim to provide qualitative properties of positive solutions for these Gross-Pitaevskii type systems. In particular, we shall deduce that solutions are symmetric about the origin. In order to do it, we apply a suitable version of the moving planes technique for cooperative singular systems. Finally, we are able to provide a classification result for these kind of problems.

References:

 F. ESPOSITO, R. LÓPEZ SORIANO, AND B. SCIUNZI Classification of solutions to Hardy-Sobolev Doubly Critical Systems. To appear on *JMPA*. arxiv.org/pdf/2304.11066.pdf. A Hamilton-Jacobi approach for the evolutionary dynamics of a model with gene transfer. How to characterize monomorphic dynamics for concave fitness functions.

Authors:

- <u>Alejandro Gárriz</u>, Departamento de Matemática Aplicada & IMAG, <u>Universidad de G</u>ranada (alejandro.garriz@ugr.es)
- Sepideh Mirrahimi, Univ. Montpellier & CNRS (sepideh.mirrahimi@umontpellier.fr)

Abstract:

During this session we will present recent advances in the study of constrained parabolic Hamilton-Jacobi equations of the form

$$\begin{cases} \partial_t v(t,z) = |\partial_z v(t,z)|^2 + F(t,z), & t \in [0,T], z \in \mathbb{R}^d, \\ \max_{z \in \mathbb{R}} v(t,z) = 0, & t \in [0,T], \\ v(0,z) = v_0(z), & z \in \mathbb{R}^d, \end{cases}$$
(1)

paying special attention to the case where the function F is not globally concave in time and space due to the appearance of a non-local integral term. We will present the results in the frame of a problem applied to the dynamics of cell populations, modelled by the non-local equation

$$\begin{cases} \varepsilon \partial_t n_{\varepsilon}(t,z) = \varepsilon^2 \partial_{zz}^2 n_{\varepsilon}(t,z) + F(t,z) \cdot n_{\varepsilon}(t,z), \\ n_{\varepsilon}(0,z) = n_{\varepsilon,0}(z) > 0, \\ n_{\varepsilon}(t,z) > 0, \\ \rho_{\varepsilon}(t) = \int_{\mathbb{R}} n_{\varepsilon}(t,y) \, \mathrm{dy}. \end{cases}$$

$$(2)$$

The behaviour of the solutions of equation (2) as $\varepsilon \to 0$ is related to the behaviour of the solutions of (1) via the Hopf-Cole transformation

$$v(t,z) = \lim_{\varepsilon \to 0} \left(\varepsilon \cdot \ln \left(n_{\varepsilon}(t,z) \right) \right).$$
(3)

Existence results for super-Liouville systems

Authors:

- <u>Aleks Jevnikar</u>, University of Udine, Italy (aleks.jevnikar@uniud.it)
- Andrea Malchiodi, SNS Pisa, Italy (andrea.malchiodi@sns.it)
- Ruijun Wu, Beijing Institute of Technology, China (ruijun.wu@bit.edu.cn)

Abstract:

We consider super-Liouville systems on closed surfaces, which have a variational structure with a strongly-indefinite functional. We discuss existence results by means of min-max methods and bifurcation theory. Joint project with Andrea Malchiodi and Ruijun Wu.

New functional inequalities with applications to the Arctan-Fast Diffusion Equation

Authors:

- Rafael Granero-Belinchón, Universidad de Cantabria (rafael.granero@unican.es)
- Martina Magliocca, Universidad de Sevilla (mmagliocca@us.es)
- Alejandro Ortega García, UNED (alejandro.ortega@mat.uned.es)

Abstract: In this talk, we prove a couple of new nonlinear functional inequalities of Sobolev type akin to the logarithmic Sobolev inequality. In particular, one of the inequalities reads

$$\int_{\mathbb{S}^1} \arctan\left(\frac{\partial_x u}{u}\right) \partial_x u \, dx \ge \arctan\left(\|u(t)\|_{\dot{W}^{1,1}(\mathbb{S}^1)}\right) \|u(t)\|_{\dot{W}^{1,1}(\mathbb{S}^1)}.$$

Then, these inequalities are used in the study of the nonlinear *arctan*-fast diffusion equation

$$\partial_t u - \partial_x \arctan\left(\frac{\partial_x u}{u}\right) = 0.$$

For this highly nonlinear PDE we establish a number of well-posedness results and qualitative properties.

Concentrating solutions to critical competitive systems in low dimension.

Authors:

• María Medina, Universidad Autónoma de Madrid (maria.medina@uam.es)

Abstract: We will analyze the existence and the structure of different signchanging solutions to the Yamabe equation in the whole space and we will use them to find positive solutions to critical competitive systems in dimensions 3 and 4.

References:

 H. Chen, M. Medina, A. Pistoia. Segregated solutions for a critical elliptic system with a small interspecies repulsive force. Journal of Functional Analysis, Volume 284, Issue 10 (2023), 109882.

Optimal second order boundary regularity for solution to p-Laplace problems

Authors:

• Luigi Muglia, University of Calabria (luigi.muglia@unical.it)

Abstract: Solutions to *p*-Laplace problems are not, in general, of class C^2 . The study of Sobolev regularity of the second derivatives is, therefore, a crucial issue. An important contribution by Cianchi and Maz'ya shows that, if the source term is in L^2 , then the field $|Du|^{p-2}Du$ is in $W^{1,2}$. The L^2 -regularity of the source term is also a necessary condition. During the speech, we will talk about a strategy based on Fermi coordinate in order to get optimal regularity of the solutions up to the boundary.

Nonlinear Fractional Schrödinger Equations coupled by powertype nonlinearities

Authors:

- Eduardo Colorado, Universidad Carlos III de Madrid (ecolorad@math.uc3m.es)
- <u>Alejandro Ortega</u>, Universidad Nacional de Educación a Distancia (alejandro.ortega@mat.uned.es)

Abstract: In this work we study the following class of systems of coupled nonlinear fractional Schrödinger equations,

$$\begin{cases} (-\Delta)^{s} u_{1} + \lambda_{1} u_{1} = \mu_{1} |u_{1}|^{2p-2} u_{1} + \beta |u_{2}|^{p} |u_{1}|^{p-2} u_{1} & \text{in } \mathbb{R}^{N}, \\ (-\Delta)^{s} u_{2} + \lambda_{2} u_{2} = \mu_{2} |u_{2}|^{2p-2} u_{2} + \beta |u_{1}|^{p} |u_{2}|^{p-2} u_{2} & \text{in } \mathbb{R}^{N}, \end{cases}$$

where $u_1, u_2 \in W^{s,2}(\mathbb{R}^N)$, with N = 1, 2, 3; $\lambda_j, \mu_j > 0, j = 1, 2, \beta \in \mathbb{R}$, $p \geq 2$ and $\frac{p-1}{2p}N < s < 1$. We prove the existence of positive radial bound and ground state solutions provided the parameters $\beta, p, \lambda_j, \mu_j$, (j = 1, 2) satisfy appropriate conditions. We also study the previous system with *m*-equations,

$$(-\Delta)^{s} u_{j} + \lambda_{j} u_{j} = \mu_{j} |u_{j}|^{2p-2} u_{j} + \sum_{\substack{k=1\\k\neq j}}^{m} \beta_{jk} |u_{k}|^{p} |u_{j}|^{p-2} u_{j},$$

where $\lambda_j, \mu_j > 0$ for $j = 1, \ldots, m \geq 3$, the coupling parameters $\beta_{jk} = \beta_{kj} \in \mathbb{R}$ for $j, k = 1, \ldots, m, j \neq k$. We prove similar results as for m = 2, depending on the values of the parameters $p, \beta_{jk}, \lambda_j, \mu_j$.

Section: PDE

Regularity Results For The Vectorial p-Laplacian

Authors:

• <u>Domenico Vuono</u>, Università dellaCalabria (domenico.vuono@unical.it)

Abstract:

We prove some regularity results for solutions to vectorial p-Laplace equations

$$-\Delta_p \boldsymbol{u} = -\operatorname{div}(|D\boldsymbol{u}|^{p-2}D\boldsymbol{u}) = \boldsymbol{f}(x, \boldsymbol{u}) \text{ in } \Omega.$$

More precisely we address the issue of second order estimates.

References:

[1] L Montoro, L Muglia, B Sciunzi, D Vuono. *Regularity and symmetry* results for the vectorial p-Laplacian. arXiv preprint arXiv:2311.05388

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Section: PDE

Boundary value problems in magnetohydrodynamics: old and new results

Authors:

• Diego Alonso-Orán, Universidad de la Laguna (dalonsoo@ull.edu.es)

Abstract: Magnetohydrodynamics plays a crucial role in understanding the behavior of plasmas, electromagnetic fields, and fluid dynamics, providing a fundamental framework for studying phenomena in astrophysics, fusion energy, and space exploration. In this talk, we will present a short survey about the well-posedness of boundary value problems for steady ideal magnetic fluids. More precisely, we will first focus on the magneto-hydrostatic equations (in two and three dimensions) and conclude with some ongoing work related to the steady magneto-hydrodnamic equations.

Exact controllability to the trajectories of the one-phase Stefan problem

Authors:

• Jon Asier Barcena, UPV/EHU (jonasier.barcena@ehu.eus)

Abstract: In this talk we are going to study the boundary exact controllability to the trajectories of the one-phase Stefan problem in one spatial dimension. This is a free-boundary problem that models solidification and melting processes. It is assumed that the physical domain is filled by a medium whose state is liquid on the left and solid, with constant temperature equal to zero, on the right. In between we find a free-boundary (the interface that separates the liquid from the solid). In the liquid domain, a parabolic equation completed with initial and boundary conditions must be satisfied by the temperature. On the interface, an additional equality, called the Stefan condition, is imposed. We prove the local exact controllability to the (smooth) trajectories. To this purpose, we first reformulate the problem as the local null controllability of a coupled PDE-ODE system with distributed controls. Then, a new Carleman inequality for the adjoint of the linearized PDE-ODE system, coupled on the boundary through nonlocal in space and memory terms, is presented. This leads to the null controllability of an appropriate linear system. Finally, the result is obtained via local inversion, by using Liusternik-Graves' Theorem. As a byproduct of our approach, we find that some parabolic equations which contains memory terms located on the boundary are null-controllable.

Talk based on a work done in collaboration with Enrique FERNÁNDEZ-CARA and Diego A. SOUZA (see https://arxiv.org/abs/2204.04750 and https://www.sciencedirect.com/science/article/abs/pii/S0022039623005508)

On a blow-up criterion for the Navier-Stokes-Fourier system

Authors:

• <u>Danica Basarić</u>, Politecnico di Milano (danica.basaric@polimi.it)

Abstract: We consider the Navier-Stokes-Fourier system governing the motion of a compressible, viscous and heat-conducting fluid confined to a bounded domain, on the boundary of which inhomogeneous Dirichlet boundary condition for the temperature is imposed. It is well-known that the system admits solutions in the classical sense; however, their existence can be guaranteed only on a maximal time interval. We show that a blow-up will not occur as long as the density, the absolute temperature and the modulus of the fluid velocity remain bounded.

Rayleigh-Bénard convection with Navier-slip boundary conditions

Authors:

• <u>Fabian Bleitner</u>, University of Hamburg (fabian.bleitner@uni-hamburg.de)

Abstract: Rayleigh-Bénard convection describes the dynamics of a buoyancydriven fluid trapped between a hot plate on the bottom and a cold plate on top. While usually the Navier-Stokes equations are equipped with either noslip or free-slip boundary conditions, in this talk we focus on the Navier-slip conditions that interpolate between the two and, depending on the underlying system at hand, better reflect the physical behavior of the fluid. In particular, we investigate scaling laws for the vertical heat transfer with respect to the buoyancy forcing and other system parameters and analyze the role of boundary conditions in these bounds.

Existence of strong solutions for a compressible fluid-solid interaction system with Navier slip boundary conditions

Authors:

• Imène Djebour, Cergy Paris Université (imene.djebour@cyu.fr)

Abstract: We consider a fluid-structure interaction system coupling a viscous fluid governed by the compressible Navier-Stokes equations and a rigid body immersed in the fluid and modeled by the Newton's law. In this work, we consider the Navier slip boundary conditions. Our aim is to show the local in time existence and uniqueness of the strong solution to the corresponding problem. The main step of this work is that we use Lagrangian change of variables in order to handle the transport equation and to reduce the problem in the initial domain. The strategy is based on the study of the linearized system with nonhomogeneous boundary conditions and on the Banach fixed point theorem.

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Section: PDE

Dispersive equations and some of their applications

Authors:

• <u>Rafael Granero-Belinchón</u>, Universidad de Cantabria (rafael.granero@unican.es)

Abstract: In this talk we will see several applications where different dispersive equations appear as well as some new results.

Wave-structure interactions

Authors:

• <u>David Lannes</u>, CNRS & Université de Bordeaux (david.lannes@math.u-bordeaux.fr)

Abstract: The mathematical description of free surface flows through the water waves equations or simpler asymptotic models such as the nonlinear shallow water equations is well understood. This talk will focus on the mathematical analysis of wave structure interactions, in which these equations are considered in the presence of a partially immersed object. New difficulties arise such as the presence of a (possibly free) boundary for the surface of the fluid and the presence of singularities in the fluid domain.

Localization of Beltrami fields and global strong solutions of the 3d Navier-Stokes equation

Authors:

• <u>Renato Lucà</u>, BCAM & Ikerbasque (rluca@bcamath.org)

Abstract: We will describe a way to localize Beltrami fields that allows us to construct global strong solutions to the Navier-Stokes equation on \mathbb{R}^3 with initial data that are large in any critical space.

Global existence for certain fourth order evolution equations

Authors:

• Martina Magliocca, Universidad de Sevilla (mmagliocca@us.es)

Abstract: In this talk, we establish global in time results for two fourth order nonlinear parabolic equations. The first of such equations involves the Hessian and appears in epitaxial growth. For such equation we give conditions ensuring the global existence of solutions. For certain regime of the parameters, our size condition involves the norm in a critical space with respect to the scaling of the equation and improves previous existing results in the literature for this equation. The second of the equations under study is a thin film equation with a porous medium nonlinearity. For this equation we establish conditions leading to the global existence of solutions.

Time-periodic solutions for viscous fluids interacting with elastic membranes

Authors:

• <u>Claudiu Mindrila</u>, BCAM (cmindrila@bcamath.org)

Abstract: We study the interaction of viscous incompressible fluids interacting with a (non)linear membrane under time-periodic forcing. We prove the existence of at least one weak solution as long as the magnitude of the periodic forcing is sufficiently small. We also provide new, uniform in time energy estimates.

Global in time solutions for the two-phase gravity Stokes flow

Authors:

• <u>Elena Salguero</u>, Max Plank Institute Leipzig (elena.salguero@mis.mpg.de)

Abstract: The gravity-Stokes system serves as a fundamental model for understanding the dynamics of incompressible fluids in certain regimes. We focus on the scenario where two fluids of different densities interact in a two-dimensional region without mixing. The density difference together with the gravity influence induce the dynamics of the two fluids and hence the evolution of the free interface arising between them. Through a contour dynamics approach, we address questions such as the existence of global solutions for this system and their asymptotic behavior, making emphasis on the properties of the free boundary. This talk is based in joint work with F. Gancedo and R. Granero Belinchón.

On the control of some PDEs from fluid mechanics

Authors:

• Diego A. Souza, Universidad de Sevilla (desouza@us.es)

Abstract: The Navier-Stokes equations and their variants have been studied since many years and its understanding is very relevant from both mathematical and physical viewpoint. Many researchers have been concerned to solve several related major open problems. On the other hand, the control of PDEs has brought a lot of attention in the last few decades. This was motivated by its relevant role in applications. In this talk we present some recent results dealing with the control of systems of the Navier-Stokes kind.

The binormal flow and the evolution of viscous vortex filaments

Authors:

• Luis Vega, BCAM & UPV/EHU (lvega@bcamath.org)

Abstract: I'll present the so called Localized Induction Approximation that describes the dynamics of a vortex filament according to the Binormal Curvature Flow (BF). I'll give a result about the desingularization of the Biot-Savart integral proved with Marco A. Fontelos within the framework of Navier-Stokes equations. Some particular examples regarding BF obtained with Valeria Banica will be also considered. These examples allow to connect BF with the so-called Riemann non-differentiable function and the Frisch-Parisi approach to turbulence.

Nonexistence of nontrivial solutions to Dirichlet problems for the fractional Laplacian

Authors:

• <u>Carmona J.</u>, Dpto de Matemáticas, Universidad de Almería (jcarmona@ual.es)

Abstract: We prove nonexistence of nontrivial bounded solutions for the problem

$$\begin{cases} (-\Delta)^s u = f(u) & \text{in } \Omega, \\ u = 0 & \text{in } \mathbb{R}^N \setminus \Omega. \end{cases}$$
(P)

where $f : \mathbb{R} \to \mathbb{R}$ is a locally Lipschitz function with $F(t) = \int_0^t f(\tau) d\tau \leq 0$ and $\Omega \subset \mathbb{R}^N$ $(N \geq 1)$ is a bounded domain with $\mathcal{C}^{1,1}$ boundary regularity.

References:

 J. Carmona and A. Molino, Nonexistence of nontrivial solutions to Dirichlet problems for the fractional Laplacian. Electron. J. Differential Equations (2023), Paper No. 16, 10 pp.

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Section: PDE

Unexpected results for a singular elliptic problem

Authors:

• <u>Pedro J. Martínez-Aparicio</u>, Department of Mathematics, University of Almería (pedroj.ma@ual.es)

Abstract: In this lecture, I will present recent results obtained in collaboration with Daniela Giachetti (Universitá di Roma, Sapienza), Francois Murat (Sorbonne Université, París), and Francesco Petitta (Universitá di Roma, Sapienza), for the one-dimensional singular boundary value problem

$$-\frac{d}{dx}\left(a(x)\frac{du(x)}{dx}\right) = -\frac{d\phi(u(x))}{dx} - \frac{dg(x)}{dx} \text{ in } (0,L), \quad u(0) = u(L) = 0,$$

where the model for the singular function ϕ is $\phi(s) = \frac{1}{|s|^{\gamma}}$ with $\gamma > 0$.

This singular problem presents a number of unexpected phenomena: nonexistence of solutions under certain assumptions, existence of an infinite number of solutions under other assumptions, and non-continuity of the solution with respect to the data.

Section: PDE

Neumann problem for a class of doubly equations for the 1–Laplacian

Authors:

• <u>Alexis Molino</u>, Dpto de Matemáticas, Universidad de Almería (amolino@ual.es)

Abstract: This talk is concerned with the Neumann problem for a class of doubly nonlinear equations for the 1-Laplacian,

$$\frac{\partial v}{\partial t} - \Delta_1 u \ni 0 \text{ in } (0, \infty) \times \Omega, \quad v \in \gamma(u),$$

and initial data in $L^1(\Omega)$, where Ω is a bounded smooth domain in \mathbb{R}^N and γ is a maximal monotone graph in $\mathbb{R} \times \mathbb{R}$. We prove that, under certain assumptions on the graph γ , there is existence and uniqueness of solutions. Moreover, we proof that these solutions coincide with the ones of the Neumann problem for the total variational flow. We show that such assumptions are necessary.

References:

[1] J. Mazón, A. Molino and J. Toledo; Doubly nonlinear equations for the 1–Laplacian, *Journal of Evolution Equations* (2023)

Section: PDE

Lower bounds for Dirichlet energy of entire stable solutions

Authors:

• <u>Salvador Villegas</u>, Dpto de Análisis Matemático, Universidad de Granada (svillega@ugr.es)

Abstract: We provide some lower bounds on $\int_{B_R} |\nabla u|^2$, as a function of the radious R > 0, where u is a nonconstant stable solution of the equation $-\Delta u = f(u)$ in \mathbb{R}^N , being $f \in C^1(\mathbb{R})$ a general function.

These bounds are optimal for dimensions $N \ge 10$ and $N \le 3$. This optimal lowest growing of $\int_{B_R} |\nabla u|^2$ is attained in radial solutions if $N \ge 10$. It is also shown that radial solutions cannot give

A quaternion approach to determine the angle between adjacent sides in the evolution of regular polygons under the vortex filament equation

Authors:

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- <u>Francisco de la Hoz</u>, University of the Basque Country UPV/EHU (francisco.delahoz@ehu.eus)

Abstract:

In this talk, using a quaternion formalism, we give a sketch of the proof [1] for the expression of the angle between adjacent sides in the skew polygons appearing at rational times in the evolution of regular polygons of M sides under the vortex filament equation [2, 3, 4],

$$\mathbf{X}_t = \mathbf{X}_s \wedge \mathbf{X}_{ss},$$

where \wedge is the cross product.

More precisely, after transforming the rotation matrices that characterize those skew polygons into quaternions, we show that the products of those matrices can be expressed in terms of products of quaternions in a compact form, which enables us to reduce the problem of determining the angle into another one of proving that some trigonometric sums are purely imaginary.

Acknowledgments:

Fernando Chamizo is partially supported by the PID2020-113350GB-I00 grant of the MICIU (Spain) and by "Severo Ochoa Programme for Centres of Excellence in R&D" (CEX2019-000904-S). Francisco de la Hoz is partially supported by the research group grant IT1615-22 funded by the Basque Government, and by the project PID2021-126813NB-I00 funded by MICIU/AEI/10.13039/501100011033 and by "ERDF A way of making Europe".

- Fernando Chamizo and Francisco de la Hoz. A quaternion-based obtention of the angle between adjacent sides in the evolution of regular polygons of M sides under the vortex filament equation. arXiv:2403.17758v1, pages 1–21, 2024. Preprint.
- [2] Francisco de la Hoz and Luis Vega. Vortex filament equation for a regular polygon. Nonlinearity, 27(12):3031–3057, 2014.

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- [3] Francisco de la Hoz and Luis Vega. The Vortex Filament Equation as a Pseudorandom Generator. Acta Appl. Math., 138(1):135–151, 2015.
- [4] Francisco de la Hoz and Luis Vega. On the Relationship Between the One-Corner Problem and the M-Corner Problem for the Vortex Filament Equation. *Journal of Nonlinear Science*, 28:2275–2327, 2018.

On the regularity of solutions to a slightly subcritical Neumann problem

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- Rosa Maria Pardo San Gil, Universidad Complutense de Madrid (rpardo@ucm.es)

Abstract: We consider the following Neumann problem

$$\begin{cases} -\Delta u + u &= f(x, u), \quad x \in \Omega, \\ \frac{\partial u}{\partial \eta} &= 0, \quad x \in \partial\Omega, \end{cases}$$
(1)

where $\Omega \subset \mathbb{R}^N$ (N > 2) is a bounded, open domain, with $C^{2,\alpha}$ $(0 < \alpha < 1)$ boundary $\partial\Omega$, $\partial/\partial\eta := \eta(x) \cdot \nabla$ denotes the outer normal dervative on $\partial\Omega$, and the nonlinear reaction term $f : \Omega \times \mathbb{R} \longrightarrow \mathbb{R}$ is a *slightly subcritical* Carathéodory function.

Through a De Giorgi-Nash-Moser iteration scheme, it is known that weak solutions to (1) with critical growth are in $L^{\infty}(\Omega)$.

Our contribution is to provide an explicit $L^{\infty}(\Omega)$ -estimate of weak solutions with slightly subcritical growth, in terms of powers of $H^1(\Omega)$ -norms, by combining the elliptic regularity of weak solutions with Gagliardo–Nirenberg interpolation inequality.

Keywords: De Giorgi-Nash-Moser estimate; Sobolev embedding; Hölder inequality.

- [1] Rosa Pardo. $L^{\infty}(\Omega)$ a priori estimates for subcritical semilinear elliptic equation with Catathéodory non-lineality. J. Fixed Point Theory Appl. (2023)25:44
- [2] Rosa Pardo. L[∞] a priori estimates for subcritical p-laplacian equations with Catathéodory non-lineality.Rev. Real Acad. Cienc. Exactas Fis. Nat. Ser. A-Mart (2024)118 : 66
Total positivity and symmetric functions

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- Beatriz Rubio, Departamento de Matemática Aplicada. Universidad de Zaragoza (brubio@unizar.es)

Abstract: When a basis of functions is totally positive, the entries of the bidiagonal decomposition of its collocation matrices at increasing sequences of nodes on the domain can be expressed in terms of symmetric functions of the nodes. This idea relies on two important facts. On the one hand, the elements of the bidiagonal decomposition of a nonsingular and totally positive matrix can be expressed as quotients of some particular minors of it (cf. [1]). On the other hand, the structure of the collocation matrix is such that any of its minors is an antisymmetric function of its nodes. For polynomial bases, an explicit realization of this result can be found in [2], allowing to derive criteria for the total positivity of the class of polynomial bases.

In this talk, we shall exploit the link between totally positive bases and symmetric functions to present novel formulae to compute the elements of the bidiagonal decomposition of collocation matrices. Besides, we will show that these results naturally extend to other interesting algebraic objects related to bases of functions, such as Gram and Wronskian matrices.

Aknowledgement

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- [2] P. Diaz, E. Mainar, B. Rubio, Polynomial total positivity and high relative accuracy through Schur polynomials, J. Sci. Comput. 97 (2023) no.1, 10.

A GENERIC guided approach to learning entropy-based constitutive equations for polymeric liquids using PINNs

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- Pep Español, Fundamental Physics, UNED, Madrid, Spain (pep@fisfun.uned.es)
- Marco Ellero, Basque Center for Applied Mathematics BCAM, Bilbao, Spain (mellero@bcamath.org)

Abstract: We present a GENERIC guided approach using PINNs to determine the entropy leading to the constitutive equation for the stress in rheological models. Our methodology uses the eigenvalue decomposition of the evolution equation of the conformation tensor to instill physical knowledge into a neural network approximation of the real function. Despite the PINNs model is trained on the steady-state line, its safe extrapolation limits are studied in complex flows away from the model steady-state line. We thus evaluate the error in the model predictions of the entropy and the stress in the region covered by simulations of complex flow around a cylinder at moderate Wi numbers, by comparing the results with traditional rheological models.

Modeling orbital dynamics around irregular elongated asteroids

Authors:

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Abstract: This work studies the dynamics of non-uniform elongated asteroids through two approaches. The first one, the dipole-segment model, consist of a massive segment joined to point masses at its extrema. In the second one, the asteroid is modeled as a segment with variable linear density. The qualitative behaviour of the periodic orbits is studied using numerical techniques for both models. Several families of periodic orbits have been found through continuation of planar orbits and out-of-plane bifurcation processes, obtaining results in agreement with previous studies about the dynamics around irregular asteroids. This highlights the relevance of simple mathematical models in studying asteroid dynamics and the importance of accounting for density and geometric properties. Alhough the families of periodic orbits studied in this work are not comprehensively sampled, they constitute an example of the variety of orbits that can be followed by a particle orbiting the asteroid, helping us to better understand the dynamics around these elongated bodies.

- X. Zeng, Y. Zhang, Y. Yu, and X. Liu, *The Dipole Segment Model for Axisymmetrical Elongated Asteroids*, The Astronomical Journal, 155, 85-102, 2018.
- [2] A. Elipe, A. Abad, M. Arribas, A. F. S. Ferreira, and R. V. de Moraes, Symmetric Periodic Orbits in the Dipole-segment Problem for Two Equal Masses, The Astronomical Journal, 161, 274-287, 2021.

How higher-order interactions modify the synchronization transition

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Abstract: Synchronization is a ubiquitous phenomenon wherein multiple units behave in unison, ensuring coherence across a wide range of systems. To understand the mechanisms underlying synchronization, the Kuramoto model was introduced in the 1970s. This simple yet effective model elucidates the synchronization transition in weakly interacting units. However, most studies have traditionally focused on pairwise interactions. In recent years, it has become evident that higher-order (multibody) interactions are pivotal for accurately describing dynamics.

Given the limited understanding of synchronization influenced by higherorder interactions, we propose the simplest extension of the Kuramoto model incorporating three-body interactions. Our model's simplicity facilitates a comprehensive analysis of its dynamics, revealing novel transitions to synchrony. Notably, under certain parameters, synchronization arises amidst significant multistability or from two-cluster states. Moreover, our extended Kuramoto model, since it is derived from phase reduction, represents a generic scenario applicable to systems of coupled units. We hope this work expands our understanding of synchronization in complex systems, highlighting the role of multibody interactions.

The Plutonian Moons and its dynamics

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Abstract:

The former planet Pluto has five main moons. Charon, the biggest of the moons has a considerable mass compared with the planetoid (approximately one tenth). In addition, it rotates in an almost circular orbit around Pluto. The other four moons (Nix, Styx, Cerberus and Hydra) rotate in the Charon's orbital plane. However, [1] provided numerical evidences of the non-keplerian motion of the small moons. Due to the properties of the system, i.e. the coplanarity of all the bodies and the circular motion of the primary objects, the Circular Restricted Three Body Problem (CR3BP) is a good model. The mass ration between the primaries is high enough to be above the Routh's μ . Therefore, the equilateral fixed points are no longer fixed.

In this talk, we will revisit previous results on the motion of the smaller moons and present a suitable family of periodic orbits in the CR3BP which mimics the position of the moons. We will analyse the stability of this family of periodic orbits and discuss whether it enables a possible transport from the primaries to the smaller moons.

References:

 J. M. Y. Woo and M. H. Lee. A numerical method for determining the elements of circumbinary orbits and its application to circumbi- nary planets and the satellites of pluto-charon. *The Astronomical Journal*, 159:277, 5 2020.

Semi-Analytical Solutions for Systems with Slowly Varying Parameters

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Abstract: The central equation in the analysis of vibratory systems in engineering is

$$M\ddot{\mathbf{x}} + C\dot{\mathbf{x}} + K\mathbf{x} = F.$$

A large body of literature has been developed around the approximation that the mass M, damping C, and stiffness K matrices are constants, which makes the analysis more tractable.

This approximation is untenable for many processes in industrial environments, and their study mainly relies on numerical simulations, which may not only obscure the structure of the solutions but could also misrepresent the system. In particular, when there are two processes, one fast and another slow — for example, a turning process with a beam rotating at high speed and slowly varying length — it may occur that at bifurcation points, the approximated solution computed by traditional numerical schemes, like the Runge–Kutta methods, is highly inaccurate due to the computer's inability to faithfully represents numbers like $1 + 10^{-100}$, which leads to significant divergences from the real solution in a short period of time [2].

We propose a semi-analytical method for solving scalar systems, but its theoretical correctness hangs upon a conjecture that we call the Existence of Steady State Conjecture [1]. We explain the reason for the strong instability of these systems, and why we believe that a delayed loss of stability observed in other numerical studies [3] will not play any role in real-world systems.

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Generalized extrapolation methods based on compositions of a basic 2nd-order scheme

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- <u>Luke Shaw</u>, Departament de Matemátiques, Universitat Jaume I, Castellón (shaw@uji.es)

Abstract: We propose new linear combinations of compositions of a basic second-order scheme with appropriately chosen coefficients to construct higher order numerical integrators for differential equations. They can be considered as a generalization of extrapolation methods and multi-product expansions. A general analysis is provided and new methods up to order 8 are built and tested. The new approach is shown to reduce the latency problem when implemented in a parallel environment and leads to schemes that are significantly more efficient than standard extrapolation when the linear combination is delayed by a number of steps.

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Integrability criteria for nonlinear oscillators and suprintegrable geodesic flows

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Abstract:

We consider a family of cubic, with respect to the first derivative, secondorder differential equations. This family of equations is a projection of equations for the geodesics of a two-dimensional Riemannian manifold and, therefore, these equations are often called projective.

The family of projective equations is closed with respect to nonlocal transformations. This allow one to study equivalence problems for this family and its integrable members, for example linear or Painlevé-type equations. We demonstrate that solutions to these equivalence problems lead to new integrability criteria for the projective equations [1, 2, 3]. For each member of such equivalence classes, it is possible to obtain a first integral and integrating factor, and, in the case of autonomous equations and transformations, invariant curves.

First integrals of projective equations can be lifted to the first integrals of the corresponding Hamiltonian systems for geodesics, if a certain projective equation corresponds to a metric. We propose an approach to construct superintegrable metrics using non-autonomous first integrals of autonomous projective equations [4]. We suppose that the Hamiltonian system for geodesics admits a linear with respect to momentum first integral and classify all autonomous projective equations that correspond to such a metric. We demonstrate that all these equations either can be linearized by nonlocal transformation or trivially integrable.

We use this approach to connect several applied nonlinear oscillators with superintegrable Riemannian metrics and explicitly construct their additional first integrals, which can be polynomial, rational and transcendental function in momenta. As examples of nonlinear oscillators we consider the anharmonic oscillator, the cubic Liénard oscillator with linear damping, the Kolmogorov system and cubic oscillators with biological applications.

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Data-assimilation meets automatic differentiation for identification of dynamical systems from irregularly-sampled, noisy data

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Abstract:

We present advances on leveraging automatic differentiation —computerbased evaluations, via repeated application of the chain rule, of partial derivatives of software defined functions— for learning and predicting continuous (dynamics), discrete (observation) dynamical systems that underpin real-world messy time-series data.

We study (unknown) stochastic dynamical systems $\dot{x} = f(x,t) + L(x,t)\dot{w}$, where $x \in \mathbb{R}^{d_x}$, $x(0) = x_0 \sim \mathcal{N}(\mu_0, \Sigma_0)$, f is a state and/or time-dependent drift function, L a possibly state and/or time-dependent diffusion coefficient, and \dot{w} the derivative of a d_x -dimensional Brownian motion with covariance Q. Data are observed at arbitrary times $\{t_k\}_{k=1}^K$ collected via a noisy measurement process $y(t) = h(x(t)) + \eta(t)$, where $h : \mathbb{R}^{d_x} \mapsto \mathbb{R}^{d_y}$ and $\eta(t) \sim \mathcal{N}(0, \Sigma_\eta)$. We denote the collection of all parameters as $\theta = \{f, L, \mu_0, \Sigma_0, Q, h, \Sigma_\eta\}$. Given a sequence of irregularly sampled and noisy observations $Y_K = [y(t_1), \ldots, y(t_K)]$, we wish to (i) filter estimate $p(x(t_K)|Y_K, \theta)$, (ii) smooth —estimate $p(\{x(t)\}_t|Y_K, \theta)$ (iii) predict —estimate $p(x(t > t_K)|Y_K, \theta)$, and (iv) infer parameters —estimate $p(\theta|Y_K)$, for systems with linear and non-linear unknown functions f and h.

We merge machine learning tools (i.e., automatic differentiation) with state-of-the-art data-assimilation to solve all these interconnected Bayesian inference problems [1]. We devise a framework that allows for differentiation through filtering/smoothing algorithms [2] and the SDE solver. By virtue of this novel synergy, we enable usage of modern optimization and inference techniques (e.g., stochastic gradient descent, Hamiltonian Monte Carlo) for learning and parameter inference of continuous-time dynamics. Our work opens up novel research directions on uncertainty quantification and the combination of mechanistic and machine-learning models for improved dynamical system identification from irregularly-sampled, noisy data.

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On the structure of the sets of heteroclinic connections between libration points and some applications

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Abstract: Heteroclinic connections in the spatial circular restricted threebody problem are well recognized for their significance role in astrodynamics. These connections, which occur at the intersections between hyperbolic manifolds of invariant sets, offer zero-propellant transfer opportunities, making them crucial not only for mission design but also for understanding the system's global dynamical behavior. Some previous work in computing systematically these solutions for the spatial problem can be found in [1, 2].

Our work is based on the results presented in [3], where heteroclinic connections between the center manifolds of the libration points L_1 and L_2 are computed using a semianalytical strategy. These connections, when intersected with a surface of section, are found to be a two-sphere topologically. Our work focuses on assessing the accessibility of these spheres from the tori of the center manifolds of both libration points. We provide results on the specific connectivity of each torus and show global connection diagrams of the isoenergetic slices of the center manifolds. Sample connections performing inclination changes of quasi-periodic orbits around L_2 are also provided.

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About non-local reaction-diffusion equations

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Abstract:

Let consider the problem of finding a function u(t, x) such that

$$\frac{\partial u}{\partial t} - a(\int_{\Omega} u(t, x) dx) \frac{\partial^2 u}{\partial x^2} = g(t, u) \tag{1}$$

In such equation, u could describe the density of a population subject to spreading. The diffusion coefficient a is then supposed to depend on the entire population in the domain rather than on the local density.

It is possible to distinguish two basic cases of (1).

If we consider the non-local equation

$$\frac{\partial u}{\partial t} - a(\|u\|_{H_0^1}^2) \frac{\partial^2 u}{\partial x^2} = \lambda f(u)$$
(2)

with Dirichlet boundary conditions, then it is possible to define a suitable Lypaunov functional. In [1] it is shown that regular and strong solutions generate (possibly) multivalued semiflows having a global attractor. In the case where the function f is odd and equation (2) generates a continuous semigroup the existence of fixed points of the type given in the Chafee-Infante problem was established in [2]. Moreover, if a is non-decreasing, then they coincide with the ones in the Chafee-Infante problem. In this work we extend these results for a more general function f.

If we consider $l \in (L^2(\Omega))'$ a functional acting on u over the whole domain, we obtain results similar to the previous ones about fixed points of the following problem

$$\frac{\partial u}{\partial t} - a(l(u))\frac{\partial^2 u}{\partial x^2} = \lambda f(u)$$

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Nonautonomous mathematical modeling of the Allee effect: from bifurcations to critical transitions.

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Abstract: This talk explores mathematical models of critical transitions in nonautonomous scalar differential equations depicting the dynamics of single species populations influenced by the Allee effect. Specifically, we focus on equations where population growth rate exhibits concave derivative with respect to the population size, as seen in several models of this kind. Drawing from the framework of [1], we introduce intrinsic time dependence in both past and future equations. The nonautonomous nature of the model allows for the consideration of phenomena like Earth's rotation or seasonal alternation, potentially impacting species evolution laws. Different types of mechanisms that can produce a critical transition are studied and incorporated into the equation as parametric variations. The critical transition is typically triggered by a saddle-node bifurcation of hyperbolic solutions by varying the parameter. Notably, we examine rate-induced tracking, and illustrate how finite-time Lyapunov exponents can serve as early warning signals for such transitions. This is joint work with I.P. Longo, C. Núñez and R. Obaya.

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- [2] J. Dueñas, I.P. Longo, R. Obaya. Rate-induced tracking for concave or d-concave transitions in a time-dependent environment with application in ecology. Chaos 33, 123113 (2023).
- [3] J. Dueñas, C. Núñez, R. Obaya. Critical transitions in d-concave nonautonomous scalar ordinary differential equations appearing in population dynamics. SIAM J. Appl. Dyn. Syst. 22 (4), 2649-2692 (2023).
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Collision leading to chaos in the Restricted Planar Circular 3-Body Problem

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Abstract:

We consider the restricted planar circular three body problem (RPC3BP), which describes the motion of a massless body under the attraction of other two bodies, the primaries, which describe circular orbits around their common center of mass located at the origin.

In a suitable system of coordinates, this system is Hamiltonian with two degrees of freedom, whose conserved energy is usually called the Jacobi constant. In such system, we are interested in solutions of the RPC3BP called ejection-collision orbits, i.e., solutions that depart from the big primary at some time t_0 and collide with it at some time t_1 .

In this talk, I will explain how to construct arbitrarily large ejectioncollision orbits for small values of the mass ratio. To this end, we show that, for small values of the mass ratio and the Jacobi constant, there exist transverse intersections between the stable (unstable) manifold of infinity and the unstable (stable) manifold of collision.

Close to such transverse intersections, we prove the existence of a sequence of ejection-collision orbits that travel arbitrarily far away. Moreover, using a similar argument, we prove the existence of a sequence of forward and backward periodic parabolic orbits that travel close to collision too. Finally, we also prove the existence of periodic orbits that travel close to collision and arbitrarily far away.

Heteroclinic connections around double resonances in an Arnold model

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Abstract: In his seminal paper (see [1]), Arnold introduced the concept of Arnold diffusion for nearly integrable systems: the existence of trajectories presenting an arbitrarily large drift in the space of actions due to the accumulated effect of an arbitrarily small perturbation over a large period of time. He designed a very particular model where he could prove its existence and raised the question of whether it occurs generally in nearly integrable systems.

An important technical difficulty when trying to answer this question is the appearance of exponentially small phenomena. Arnold dealt with it by introducing two independent perturbative parameters, one of which was exponentially small with respect to the other. This is convenient to illustrate the existence of diffusion, but it creates a very artificial setting that does not include the physically relevant nearly integrable systems. Hence, this technique does not provide a satisfactory answer.

In this work we analyze a generalized Arnold model in the more natural setting where both parameters are of the same order. This means that we need to apply techniques of analysis of exponentially small phenomena. We prove the existence of heteroclinic connections of order $\mathcal{O}(|\mu|\sqrt{\varepsilon}) - \mu$ and ε are the two parameters in the system—, although we cannot chain them to obtain global diffusion. Our approach involves averaging the system around double resonances and studying separately the averaged and the complete systems. We find that the averaged system presents heteroclinic connections which persist in the complete system.

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Analysis of some periodic problems via topological methods

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Abstract: In this talk we study a general class of planar periodic nonautonomous Hamiltonian systems trough the use of different topological methods such as bifurcation theory, the Poincaré–Birkhoff theorem and topological horseshoe theory.

As a result of this analysis, it will be first shown the existence and multiplicity of subharmonic solutions for any configuration of the periodic weights. Secondly, as long as the system exhibits twist and stretching dynamics, it will be possible to prove the existence of chaos in a general sense implying the most common chaotic dynamics definitions.

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Dynamical study of a family of asteroids

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Abstract: Many families of asteroids describe very specific motions. The aim of this talk is to dynamically study one of this families, the Hilda family, constituted by more than 5,000 asteroids located beyond the main asteroid belt but within Jupiter's orbit. These asteroids exhibit a 3:2 orbital resonance with Jupiter and follow orbits that sequentially approach three Lagrangian Points (L_3 , L_4 , and L_5) in the Sun-Jupiter system. Our objective is to analyze their orbits within the Sun-Jupiter Circular Restricted Three Body Problem (CRTBP) and the Elliptical Restricted Three Body Problem (ERTBP), both in the planar case. One of our goals is to investigate the impact of Jupiter's eccentricity on this phenomenon.

To achieve this, we first select Hilda asteroids from the JPL database based on their orbital elements. The database provides coordinates in an inertial ecliptical reference frame, centered at the solar system's mass center. To transform these coordinates into the CRTBP or ERTBP Sun-Jupiter systems, we perform a non-trivial change of coordinates using the instantaneous orbital elements of the Sun and Jupiter.

Subsequently, we numerically compute periodic and quasi-periodic orbits for the Hilda asteroids within our simplified models. We employ temporal or spatial Poincaré sections to identify families of invariant objects governing these asteroids motion.

Exponential small splitting of separatrices in a molecular model

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Abstract:

In this presentation, we will study the dynamics of the hydrogen atom interacting with a circularly polarized microwave field. This problem can be effectively modeled as a perturbed Kepler problem, which, upon suitable transformations of coordinates and time, manifests as a Hamiltonian system with two degrees of freedom, dependent on a single parameter (K > 0). Its formulations is given by

$$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) - xp_y + yp_x - \frac{1}{r} + Kx.$$
 (1)

Despite the simplicity of the model, which can be seen as the simplest perturbation of the Kepler problem, its dynamics exhibit great complexity. The system of ordinary differential equations associated with the Hamiltonian H has properties of interest for our study. In particular, it has two equilibrium points, L_i , located at $(x_{L_i}, 0)$, i = 1, 2 with $x_{L_1} < 0$ and $x_{L_2} > 0$. L_1 is a center-saddle for any K > 0 and L_2 is a center-center for $K \leq K_{crit}$ and a complex saddle for $K > K_{crit}$ where $K_{crit} = 3^{-4/3}/2$. In this talk, we will mainly focus on the behavior of the invariant manifolds associated with the equilibrium point L_1 .

Critical transitions in complex systems: the role of timescales and unstable states

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Abstract:

Many systems in nature exhibit the coexistence of different stable states for a given set of environmental parameters and external forcing. Examples for such behaviour can be found in different fields of science ranging from mechanical or chemical systems to ecosystem and climate dynamics. As a consequence of the coexistence of a multitude of stable states, the final state of the system depends strongly on the initial condition. The set of initial conditions which all converge to the same stable state is called the basin of attraction. In autonomous systems, the boundaries of these basins are made up by the stable manifolds of saddle invariant sets, e.g. saddle fixed points, saddle periodic orbits or chaotic saddles. We analyse systems experiencing a parameter drift during which bifurcations are crossed that lead to the emergence of new attractors including their basins of attraction. Using an ensemble of trajectories, we study the role of the relative size of the nonautonomous basins of attraction and the location of their boundaries in ratedependent tipping. We demonstrate that the decision whether a trajectory tips or tracks the moving stable state depends crucially on the changes in the non-autonomous basins of attraction, in particular on their boundaries, that also move in state space under a time-dependent variation of a parameter. Our ensemble approach reveals that such bifurcations occurring during the parameter drift might be masked because the relative size of the newly formed non-autonomous basins of attractions goes to zero the slower the rate of the parameter drift. As a consequence, the whole ensemble of initial conditions evolving under parameter drift is not signalling the bifurcation. This phenomenon can be observed for smooth basin boundaries as well as for fractal ones. We show that the relationship between the timescale of the parameter drift and the intrinsic dissipative timescale is responsible for this behaviour.

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Transition between forward attractors for a non-autonomous Lotka-Volterra system

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Abstract:

The autonomous Lotka-Volterra model is used to study the evolution of species population from an ecosystem, and the full characterization of the asymptotic behavior of their solutions is well known. In particular, it is possible to give conditions on the coefficients which guarantee the existence of a globally asymptotically stable equilibrium point, and construct the full structure of the global attractor associated through the heteroclinics connections between equilibrium points [1].

Based on the works of Lazer and Ahmad [2], [3], we provide a full characterization of the structure of attractors for a planar non-autonomous Lotka– Volterra cooperative system. We show sufficient conditions for the existence of forward attractors and give a full description of them by proving the existence of such bounded global solutions that all bounded global solutions join them, i.e. converge towards them when time tends to plus and minus infinity.

Furthermore, we obtain sufficient conditions on the problem parameters for different structures of attractors which leads to understanding different paths of the solutions towards the globally stable one. This change of the structure of the attractor will be determined at the value of the averages of the intrinsic growth rate vector a, seeing that depending on the sign of these averages the semistable solutions $(u_1^*, 0)$ and $(0, u_2^*)$ exist or not.

This is a joing work with José Antonio Langa and Piotr Kalita.

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Critical transitions in asymptotically slow-fast systems

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Abstract: We discuss a geometric approach to the study of bifurcation and rate induced transitions in a class of asymptotically slow-fast systems, which are in some sense 'intermediate' between the (smaller resp. larger) classes of asymptotically autonomous and non-autonomous systems. After showing that the relevant systems can be viewed as singular perturbations of a limiting system with a discontinuity in time, we consider an analytical framework for their analysis based on geometric blow-up techniques. Using this approach, we provide sufficient conditions for the occurrence of bifurcation and rate induced transitions in low dimensions, as well as sufficient conditions for tracking in arbitrary (finite) dimensions, i.e. the persistence of an attracting and normally hyperbolic manifold through the transitionary regime. The proofs rely on geometric blow-up, a variant of the Melnikov method which applies on non-compact domains, and general invariant manifold theory. We conclude by applying these results to a low-dimensional problem with forward and backward attractors that feature slow but nonconstant dependence on time.

References:

 S. Jelbart. Rate and bifurcation induced transitions in asymptotically slow-fast systems. To appear in SIAM Journal on Applied Dynamical Systems, (2024). arXiv:2401.08482.

Global bifurcations of homoclinic solutions for nonautonomous ordinary differential equations

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Abstract: We establish an alternative classification of the shape of global bifurcating branches of bounded solutions to Carathéodory ordinary differential equations. Our approach is based on the parity associated to a path of index 0 Fredholm operators and the Evans function as a recent tool in nonautonomous bifurcation theory. Similarly to the classical Rabinowitz alternative, we establish that a bifurcating branch of bounded solutions either returns to a given branch, or it fails to be compact. Under further assumptions on the Carathéodory equation (and the known solution branch) one can even establish that the bifurcating branch is unbounded.

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Critical transitions for asymptotically concave ordinary differential equations

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Abstract:

The occurrence of tracking or tipping situations for a transition equation $x' = f(t, x, \Gamma(t, x))$ is analyzed under the assumption on concavity in x of the maps giving rise to the asymptotic equations $x' = f(t, x, \Gamma_{\pm}(t, x))$, but without assuming this condition on the transition equation itself. The approaching condition is just $\lim_{t\to\pm\infty}(\Gamma(t, x) - \Gamma_{\pm}(t, x)) = 0$ uniformly on compact real sets, and so there is no restriction to the dependence on time of the limit equations. The analysis provides a powerful tool to analyze the occurrence of critical transitions for one-parametric families $x' = f(t, x, \Gamma_{\pm}^{c}(t, x))$. The new approach significatively widens the field of application of the results, since the evolution law of the transition equation can be essentially different from those of the limit equations. As an application, a scalar population dynamics model subject to non trivial predation and migration terms is analyzed.

This is a joint work with Jesús Dueñas and Rafael Obaya (Universidad de Valladolid).

Tracking nonautonomous attractors in slow-fast systems of ODEs with dependence on the fast time

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Abstract: Coupled slow and fast motions generated by ODEs are considered, with dependence on the fast time:

$$\begin{cases} \dot{x} = f(x, y), \\ \varepsilon \, \dot{y} = g\left(x, y, \frac{t}{\varepsilon}\right) \end{cases}$$

where $\varepsilon > 0$ is a small parameter. The autonomous case has received a lot of attention since the works by Tikhonov in the 1950s (see [4]), but a nonautonomous variation of the fast dynamics with respect to the fast time has not been introduced until the work by Artstein [1], with information on the asymptotical behaviour of the fast motion as $\varepsilon \to 0^+$ given in terms of statistical convergence. In this talk we present a new dynamical interpretation of the limit behaviour of the fast motion, by using the theory of nonautonomous attractors (see, e.g., [2]). Some simulations are presented to illustrate the results.

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Existence of strange non-chaotic attractors in a quasi-periodically forced piecewise-linear map

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Abstract: We consider the following family of one-dimensional quasiperiodically forced maps:

$$F_{a,b}(x,\theta) = (f_{a,b}(x,\theta), \theta + \omega \mod 2\pi),$$

where x is real, and θ is an angle. We assume that the second component of the map is an irrational rotation and

$$f_{a,b}(x,\theta) = h_a(x) + b\sin\theta,$$

where $h_a(x) = ax$ if $x \in [-\pi/(2a), \pi/(2a)]$, $h_a(x) = -\pi/2$ if $x \leq \pi/(2a)$ and $h_a(x) = \pi/2$ The dynamics depends on two parameters: b is real and a > 0. For this family we can prove the existence of both smooth and nonsmooth pitchfork bifurcations. As what happens for a smooth pitchfork bifurcation, for a > 1 there exists $b = b_a(a)$ such that for $b < b_0(a) f_{a,b}$ has two continuous attracting invariant curves and one continuous repelling invariant curve, and for $b > b_0(a)$ there is only one continuous attracting invariant curve. But for $b = b_0$ the situation is different: we have two noncontinuous attracting invariant curves and one continuous repelling invariant curve such that the attracting invariant curves intersect the repelling one in a zero-Lebesgue mesure set of angles. We can say that in this case we have a non-chaotic strange attractor, consisting on the closure of the three invariant curves (see [1]).

It is remarkable that this family is a simplification of the smooth family $G_{a,b}(x,\theta) = (\arctan(ax) + b\sin(\theta), \theta + \omega)$ for which there is numerical evidence of existence of non-smooth pitchfork bifurcations (see [2]).

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Rational methods for abstract evolution problems without order reduction

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Abstract: We are concerned with the numerical time integration of abstract, linear, non-homogeneous IVPs of the form

$$\begin{cases} u'(t) = Au(t) + f(t), & 0 \le t \le T, \\ u(0) = u_0, \end{cases}$$

where $A: D(A) \subset X \to X$ is the infinitesimal generator of a \mathcal{C}_0 semigroup of linear and bounded operators in a complex Banach space X. This abstract framework covers a wide variety of situations of practical interest, including both parabolic and hyperbolic problems.

It is well known that a Runge-Kutta method of order p applied to one of these IVPs suffers from the so called order reduction phenomenon: it occurs that the method, applied in the context of a solution $u \in \mathcal{C}^{(p+1)}([0,T],X)$, exhibits an order of convergence $\mu \leq p$ which is related to the stage order of the method, rather than to p itself.

To overcome this issue, we part from an A-stable rational approximation r(z) to e^z of order p (typically, the stability function of a RK method) and propose a new family of stable methods that recover the order p for every solution $u \in C^{(p+1)}([0,T],X)$, thus avoiding order reduction. These methods have a similar computational cost than the original RK ones in terms of linear systems required to solve per time step. In addition, only evaluations of the source term and not of its derivatives are required.

Finally, a strategy to extend the methods to semilinear IVPs of the form

$$\begin{cases} u'(t) = Au(t) + f(t, u(t)), & 0 \le t \le T, \\ u(0) = u_0, \end{cases}$$

with A sectorial, is also presented.

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Intrinsic Proper Generalized Decomposition modes of parametric symmetric elliptic problems on Grassmann manifolds.

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Abstract:

In this work, we introduce an iterative optimization algorithm to obtain the intrinsic Proper Generalized Decomposition modes of elliptic partial differential equations. The main idea behind this procedure is to adapt the general Gradient Descent algorithm to the algebraic version of the intrinsic Proper Generalized Decomposition framework, and then to couple a onedimensional case of the algorithm with a deflation algorithm in order to keep enriching the solution by computing further intrinsic Proper Generalized Decomposition modes. For this novel iterative optimization procedure, we present some numerical tests based on physical parametric problems, in which we obtain very promising results in comparison with the ones already presented in the literature. This support the use of this procedure in order to obtain the intrinsic PGD modes of parametric symmetric problems.

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Analysis of a Mathematical Model Arising in Plant Disease Epidemiology

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Abstract: Xylella fastidiosa (Xf) is a bacteria originating from the Americas, identified in Europe during the last decade when the Italian authorities reported the first outbreak of Xf in the south of the Apulia region in 2013. Several important crop diseases can be associated with Xylella fastidiosa, such as the Pierce's disease of grapevine, the plum leaf scald, the Citrus varie gated chlorosis, the phony peach disease, and as confirmed in Italy, Xf is the cause of olive quick decline syndrome, which dramatically brought the Apulia olive growing sector to its knees. So, we can see the importance of the knowledge on the dynamics of Xylella fastidiosa infection which is an essential element for the effective management of new foci.

In this communication, we study from the mathematical and numerical point of view a problem arising in vector-borne plant diseases. The model is written as a nonlinear system composed of a parabolic partial differential equation for the vector abundance function and a first-order ordinary differential equation for the plant health function. An existence and uniqueness result is proved using backward finite differences, and the regularity of the solution is also obtained ([1]). Using the finite element method and the implicit Euler scheme, fully discrete approximations are introduced. A discrete stability property and a main a priori error estimates result are proved. Finally, some numerical results, in one and two dimensions, are presented to demonstrate the accuracy of the approximation and the behaviour of the solution.

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Combining BEM-FEM and CQ Techniques for Wave Propagation Simulation

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Abstract:

In this work, we introduce a non-overlapping Boundary and Finite Element Method (BEM-FEM in what follows) approach to simulating wave propagation in unbounded and heterogeneous media via Multistep Convolution Quadrature (CQ) techniques. Initially proposed in [3], the CQ approach to our problem reduces the evolution problem into a sequence of stationary wave problems, with complex wave-numbers, in the full plane/space. We show how these problems can be solved efficiently in parallel using the BEM-FEM method, as introduced in [2]. This method exploits the strengths of both algorithms in space discretization: the FEM's flexibility in dealing with heterogeneities and the BEM's fast convergence for smooth solutions and the natural handling of the behavior at infinity

Furthermore, we present numerical experiments to demonstrate the effectiveness of our algorithm.

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- [3] Lubich, C. Convolution quadrature and discretized operational calculus. *I.Numer. Math.* 52 (1988), no.2, 129-145.

Numerical analysis of a thermoelastic problem of Moore-Gibson-Thompson type with history dependence

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Abstract:

In this talk, we will consider, from the numerical point of view, a thermoelastic problem where the heat conduction is described by a history dependent version of the Moore-Gibson-Thompson equation [2]. The analytical results were obtained recently in [1]. First, we will study the thermal problem (without mechanical components), introducing a fully discrete approximation by means of the finite element method and the implicit Euler scheme. The discrete stability of its solution will be proved, and an a priori error analysis will be provided, which will lead to the linear convergence under suitable regularity conditions. Secondly, we will consider the natural extension to the thermoelastic case. Following the analysis of the thermal problem, similar results will be shown. Finally, we will present some onedimensional numerical simulations for both problems which will demonstrate the accuracy of the approximations and the behavior of the discrete energy.

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CEDYA 2024 - Communication proposal

Section: NAS

Residual-based a posteriori error indicator for a dual-mixed method for the Darcy-Forchheimer model

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Abstract: The Darcy-Forchheimer model is used to describe fluid flow through porous media when the fluid velocity is moderate or high. In this talk, we consider the dual-mixed finite element method proposed by Pan and Rui [1] to numerically solve the Darcy-Forchheimer model. The pair velocity-pressure is approximated by Raviart-Thomas elements. We develop a novel a posteriori error analysis and derive a reliable a posteriori error indicator of residual type. Moreover, we provide a numerical study that supports its use in practice.

References:

 H. Pan and H. Rui, Mixed element method for two-dimensional Darcy-Forchheimer model, J. Sci. Comput. 52 (2012) 563–587.

A Partition of Unity Finite Element Method for acoustic wave propagation problems in layered media

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Abstract:

Among the methods which mitigate the numerical pollution, the Partition of the Unity Finite Element Method (introduced by Babŭska and Ihlenburg in 1995 [1]) has been used recently to deal with the time-harmonic wave propagation in stratified fluid (see [2]). The FEM discretization space is modified by enriching the basis functions with plane waves, and so inserting free-space solutions of the homogeneous model into the standard local polynomial basis. To guarantee the continuity of the approximated solution, Lagrange multipliers are used to enforce the coupling conditions on the boundary between media of different nature.

In this work, the time-harmonic acoustic model is numerically solved by means of a PUFEM method which uses a new enrichment procedure. Instead of using simple plane wave solutions of a constant-coefficient partial differential equation, the proposed method is based on local solutions of the variable coefficient model. Some numerical experiments are carried out to illustrate the performance of this PUFEM procedure.

- J. M. Melenk, I. Babŭska, The Partition of Unity Finite Element Method: Basic Theory and Applications, Computer Methods in Applied Mechanics and Engineering 139 (1996), 289–314.
- [2] O. Laghrouche, P. Bettess, E. Perrey-Debain, J. Trevelyan, Wave interpolation finite elements for Helmholtz problems with jumps in the wave speed, Computer Methods in Applied Mechanics and Engineering 194 (2005), 367–381.
- [3] L. Hervella-Nieto, P.M. López-Pérez, A. Prieto, Robustness and dispersion analysis of the Partition of Unity Finite Element Method applied to the Helmholtz equation, Computers and Mathematics with Applications 79 (2020), 2426–2446.

WENO scheme on characteristics for the equilibrium dispersive model of chromatography with generalized Langmuir isotherms

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Abstract: Column chromatography is a laboratory and industrial technique used to separate different substances mixed in a solution. Mathematically, it can be modeled using non-linear partial differential equations whose main ingredients are the adsorption isotherms, which are non-linear functions modeling the affinity between the different substances in the solution and the solid stationary phase filling the column.

In this talk, we consider multicomponent adsorption isotherms which are generalizations of the multicomponent *Langmuir* isotherms. Following the techniques in [1], we will prove that, for this family of functions, there is a smooth bijection between the concentrations of the solutes in the liquid phase and the conserved variables that allows us to write the model as a well-posed system of conservation laws with diffusive corrections. We will show that this correspondence allows us to numerically recover the characteristic information of the Jacobian matrix of the convective fluxes and use it to design an implicit-explicit scheme that uses characteristic-based numerical fluxes for the fifth-order WENO reconstruction technique. Finally, some numerical examples will be displayed to reinforce that the proposed numerical technique is a reliable and robust tool for numerically solving this model [2].

- R. Donat, F. Guerrero, P. Mulet, Implicit-explicit WENO scheme for the equilibrium dispersive model of chromatography, Appl. Numer. Math. 123 (2018) 22-42.
- [2] R. Donat, M.C. Martí, P. Mulet, WENO scheme on characteristics for the equilibrium dispersive model of chromatography with generalized Langmuir isotherms, Appl. Numer. Math. 201 (2024) 247–264.

A numerical method to solve Maxwell's equations in singular 3D geometry

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Abstract: We propose a variational method to compute the three-dimensional Maxwell equations in an axisymmetric singular domain generated by the rotation of a singular polygon around one of its sides, which contains reentrant corner or edges. Due to the axisymmetric assumption, the singular computational domain reduces to a subset of R^2 . However, the electromagnetic field and other vector quantities still belong to R^3 .

Taking advantage of the fact that the domain becomes two-dimensional, through Fourier analysis in the third dimension, one arrives to a sequence of singular problems set in a 2D domain, depending on the Fourier variable k. Under these conditions, the 3D solution is solved by addressing several 2D problems, each dependent on k.

Furthermore, for each mode k, we can show that the solution can be decomposed into a regular and a singular part. Therefore, the regular part can be computed using a classical finite element method. The singular part belongs to a finite-dimensional subspace, its dimension being equal to the number of reentrant corners and edges of the 2D polygon that generates the 3D domain.

We first compute this singular part using an *ad hoc* numerical method only for $k = 0, \pm 1, 2$, where the mode k = 2 appearing as a "stabilization" mode for all other k. Then, the total solution will be computed based on a non-stationary variational formulation. Numerical examples will be presented to illustrate that the proposed method can capture the singular part of the solution. This approach can also be viewed as the generalization of the Singular Complement Method to time-dependent three-dimensional axisymmetric problem [1], [2].

- F. Assous, I. Raichik, Numerical solution to the 3D static Maxwell equations in axisymmetric singular domains with Arbitrary Data, J. Comput. Meths. Appl. Maths, 20-3, 419-435 (2020).
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RK integrators for the DG discretization of linear Friedrichs systems

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Abstract: Symmetric Friedrichs systems include a broad category of linear hyperbolic systems that cover various mathematical models for linear wave propagation phenomena. The discontinuous Galerkin method stands out as a favored technique for spatial discretization in these models, offering greater versatility compared other methods such as finite elements. By employing off-centered numerical fluxes, it introduces artificial dissipation, which proves useful in controlling spurious oscillations observed with centered fluxes, particularly when modeling convection phenomena.

In time-dependent simulations, the temporal discretization of the semidiscrete problem derived from the discontinuous Galerkin method, in both conservative and dissipative scenarios, is crucial. For large-scale simulations, explicit schemes are preferred, raising concerns about their stability.

In our presentation, we will discuss various results regarding the stability of RK schemes by means of the energy method continuing and (in some aspects) extending the works in [1,2].

- E. Burman and A. Ern and M. A. Fernández. Explicit Runge-Kutta schemes and finite elements with symmetric stabilization for firstorder linear PDE systems. SIAM Journal on Numerical Analysis, 48(6):2019–2042, 2010.
- [2] D. Levy and E. Tadmor. From semi-discrete to fully discrete: Stability of Runge–Kutta schemes by the energy method, SIAM Review,40:40–73, 1998.

Numerical Methods of Second Order for Stochastic Differential Equations

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Abstract: Ordinary differential equations and their numerical analysis aim to model numerous real-world phenomena. While numerical analysis is wellestablished in the deterministic context, the introduction of stochastic terms allows us to capture the inherent randomness present in natural processes, unlocking characteristics unattainable in deterministic problems.

The numerical resolution of the stochastic systems required tailored development of methods, along with a comprehensive understanding of error analysis, convergence rates, and other related concepts. This approach is crucial for comprehending the stochasticity and can be supported by the extensive literature devoted to numerical analysis in the deterministic case.

In this talk, our focus is the development and numerical examination of the stochastic version of the TR-BDF2 method. We delve into its performance characteristics, focusing on preserving the second-order accuracy of the deterministic counterpart and conduct stability analysis in the presence of stochastic terms. Additionally, we present validation tests in academic scenarios to assess the practical applicability of the theoretical results obtained.

Numerical approximation of PGD modes to parameterized elliptic problems

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Abstract: The Proper Generalized Decomposition (PGD) is a reduced order method to solve parameterized differential equations. This method compute approximations of the solution under the form of a low-rank tensorized decomposition and so that, these approximations are constructed without any information on the solution, but only on the differential equation to be solved.

This work focus on the analysis of the approximation of the PGD expansion modes for the parameterized solutions of elliptic equations. The modes are obtained by alternated Galerkin problems in a Lebesgue space of the parameter set and the space in which lives the solution of the equation. In practice, both problems have to be discretized to be resolved and so, the computation of the modes requires a double discretization. On one hand, we approximate the integral on the parameter set by means of composed quadrature formulas based upon finite element approximations of the integrands with respect to the parameter. On the other hand, the framework space for the solution is approximated by a finite-dimensional subspace. In this context, we prove that the discrete PGD modes converge to the continuous ones in the mean quadratic norm associated to the parametric elliptic operator. For that, we are based on the casting of the modes PGD as solutions of a calculus of variations problem on optimal subspaces of finite dimension that minimize the residual in this mean quadratic norm. We have also performed some numerical experiments to asses the convergence of the PGD modes and to provide some indications on the rate of convergence. The results show an spectral or algebraic convergence according to the regularity of the solution. Moreover, in all the cases we have observed a spectral convergence of the truncated PGD series in the parametric L^2 norm.
A Trefftz discontinuous Galerkin method for the acoustic scattering in a waveguide

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Abstract: We simulate the propagation of time-harmonic waves along an unbounded tubular waveguide by means of a Trefftz Discontinuous Galerkin (TDG) formulation which we discretize with the superposition of Plane Waves (PWDG).

We first rewrite the problem on a bounded computational domain by using the Neumann-to-Dirichlet map on the truncation walls. We formulate variationally this problem in a DG way, in the sense that the interelement continuity is imposed weakly within the variational formulation by introducing suitable numerical fluxes: Indeed, we make use of standard numerical fluxes except for facets on the truncation boundary, for which we use some more exotic numerical fluxes. We then get a consistent and coercive formulation which achieves quasi-optimal convergence when discretized with e.g. plane waves.

For the PWDG formulation in two dimensions, we verify and illustrate the behavior of the numerical solutions and their order of convergence with numerical experiments obtained with a Python code that we have developed from scratch. In particular, we investigate the role of the choice of the flux parameters, as well as the instability and ill-conditioning inherent in this kind of methods.

- R. Hiptmair, A. Moiola, I. Perugia, A survey of Trefftz methods for the Helmholtz equation, In: Building Bridges: Connections and Challenges in Modern Approaches to Numerical Partial Differential Equations, Springer Lect. Notes Comput. Sci. Eng., edited by G.R. Barrenechea, F. Brezzi, A. Cangiani, E.H. Georgoulis, 2016, pp. 237–278
- [2] S. Kapita, P. Monk, V. Selgas, A Trefftz Discontinuous Galerkin method for time-harmonic waves with a generalized impedance boundary condition, Applicable Analysis 99(3), 2020, pp. 379–40

Semi-implicit fully exactly well-balanced schemes for shallow flows

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Abstract:

This study focuses on the development of semi-implicit schemes for onedimensional shallow flows, with a primary emphasis on preserving all steady states, rather than just water-at-rest ones. Drawing inspiration from prior research (see [1] and [2]), the authors employ splitting and relaxation techniques to avoid the nonlinearities associated with pressure terms. The proposed methodologies exhibit better performance compared to conventional explicit schemes, particularly in the low Froude regime, characterized by celerity larger than the fluid velocity. This advantage minimizes the necessity for many iterations over large time intervals. The performance of the scheme is further demonstrated through different numerical simulations.

- C. Caballero-Cárdenas, M. J. Castro, T. Morales de Luna, and M. L. Muñoz-Ruiz, "Implicit and implicit-explicit Lagrange-Projection finite volume schemes exactly well balanced for 1d shallow water system", *Applied Mathematics and Computation*, 443, 2023, p. 127784, https://doi.org/https://doi.org/10.1016/j.amc.2022.127784.
- [2] C. Caballero-Cárdenas, M. J. Castro, C. Chalons, T. Morales de Luna, and M. L. Muñoz-Ruiz, "A semi-implicit fully exactly well-balanced relaxation scheme for shallow water system", *SIAM Journal on Scientific Computing*, submitted, 2023.

Robustness and entropy inequalities through artificial viscosity

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Abstract:

In the present work, we consider the numerical approximation of the weak solutions of first order system of hyperbolic PDEs supplemented with entropy inequalities. Here we propose a general procedure to ensure the robustness and the entropy stability of any first order finite volume numerical scheme by introducing a suitable artificial numerical viscosity.

In order to obtain the required properties, first a reformulation of any given first order finite volume solver is performed in terms of a judicious approximate Riemann solver. Next, we show that choosing a proper numerical viscosity, and setting a suitable CFL condition, both robustness and the discrete entropy inequalities are recovered. Finally, we show numerical approximations of the solutions of the isentropic gas dynamic model and the one and two-layer shallow water systems. We show the ability of the here designed technique to stabilize entropy violating schemes.

The main results of this talk have been published on [1]

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References:

 Berthon, C., Castro Díaz, M.J., Duran, A., Morales de Luna, T., Saleh, K. Artificial Viscosity to Get Both Robustness and Discrete Entropy Inequalities. J Sci Comput 97, 65 (2023).

A hierarchy of debris flows models with dilatancy effects

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Abstract: In this work, first we present here a modification of the two-layer model for grain-fluid flows with dilatancy effects derived in [1]. This model solves the depth-averaged mass and momentum conservation equations for both a grain-fluid layer and an upper fluid layer as well as the exchange of mass and momentum between these layers. In this model the fluid can be expelled from the mixture during contraction and to be sucked into the mixture during dilation thanks to the presence of a thin fluid layer on top of the mixture layer. It appears a non-hydrostatic contribution in the solid and fluid pressures in the mixture, defined by a dilatancy closure equation. Secondly, a hierarchy of models is presented, in terms of several simplifications and the relationship with other models in the bibliography (see [2]). Finally, several numerical tests are presented.

- F. Bouchut, E.D. Fernández-Nieto, A. Mangeney, G. Narbona-Reina. A two-phase two-layer model for fluidized granular flows with dilatancy effects. Journal of Fluid Mechanics (801):166–221, 2016.
- [2] R. M. Iverson, D. L. George. A depth-averaged debris-flow model that includes the effects of evolving dilatancy. I. Physical basis. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences (470): 2170, 2014

Quasi-conservative discontinuous Galerkin schemes for hyperbolic systems in non-conservative variables with subcell finite volume corrections

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Abstract: We present a novel quasi-conservative arbitrary high order accurate ADER discontinuous Galerkin (DG) method allowing to efficiently use a non-conservative form of the considered PDE system, so that it can be modeled directly in the most physically relevant set of variables. This is useful for multi-material flows with moving interfaces and strong contact discontinuities, as well as in presence of very non-linear thermodynamics. Regrettably, the non-conservative formulation introduces a conservation error which would normally lead to a wrong approximation of shock waves. Hence, we start by giving a formal definition of the conservation defect of non-conservative schemes and we analyze it providing a local quasiconservation condition, which allows us to prove a modified Lax-Wendroff theorem. Then, to numerically deal with shock waves, we exploit the framework of the so-called a posteriori subcell finite volume (FV) limiter, so that, in shocktriggered troubled cells appropriately detected, we can incorporate a local conservation correction. Our corrected FV update entirely removes the local conservation defect allowing to fit in the hypotheses of the proposed modified Lax-Wendroff theorem. To prove the capabilities of our novel approach, first, we show that we are able to recover the same results given by conservative schemes on classical benchmarks for the single-fluid Euler equations. We then conclude the presentation by showing the improved reliability of our scheme on the multi-fluid Euler system on examples like the interaction of a shock with a helium bubble for which we are able to avoid the development of any spurious oscillations, see the figure here below.

E. Gaburro gratefully acknowledges the support received from the European Union with the ERC Starting Grant ALcHyMiA (grant agreement No. 101114995).

Well-balanced reduced order models based on POD for hyperbolic systems of balance laws

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Abstract: Let us consider a general one-dimensional hyperbolic system of balance laws of the form

$$W_t + F(W)_x = S(W)H_x + R(W), \quad x \in I, \ t > 0,$$
 (1)

which describe a great number of relevant phenomena in fluid dynamics, such as shallow water models, multiphase flow models, gas dynamic, etc. Systems of balance laws of the form (1), which admit non-trivial stationary solutions satisfying

$$F(W)_x = S(W)H_x + R(W), \tag{2}$$

have been widely applied in simulation of the waves generated by small perturbations of stationary solutions: think, for instance, of tsunami waves in the ocean. The design of well-balanced numerical schemes is a very active line of research. We will consider reduced order models (ROMs) based on Proper Orthogonal Decomposition (POD), which are extensively employed to reduce computational costs in contrast to standard numerical methods. In this work we will prove that, if a standard first-order well-balanced full order model (FOM) of the form

$$W_i^{n+1} = W_i^n - \frac{\Delta t}{\Delta x} \mathcal{L}\left(W_{i-1}^n, W_i^n, W_{i+1}^n\right).$$
(3)

is considered, the corresponding reduced order method will be also wellbalanced. Moreover, predictions for parameter-dependent systems will be also considered. In particular, the source terms depend on a physical parameter μ . Our interest is to quickly obtain good approximations when considering variations of the parameter μ .

Submarine avalanches modelling with two coordinates multilayer system.

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Abstract:

Submarine avalanches models usually have to choose between two systems of coordinates: horizontal or parallel to the slope or both with a change of coordinates at the interface between fluid and avalanche, but this can limit the range of modeled avalanches profile. We aim to develop a model based on the 2-coordinates systems option but with an interstitial water layer in local coordinates so that the change of coordinates happens at an unmoving water-water interface.

We will present the model derivation from Euler's equation, the layeraveraging and preliminary simulation results, as well as the expected advantages of this model.

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A high order ImEx method for the shallow water model

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Abstract: This talk is devoted to the development and analysis of a robust and efficient high order numerical scheme for the shallow water flows in the low Froude number limit. We focus on ocean and coastal simulations at different scales, in particular, on the variation of the Froude number that goes from 1 at the coastline to two or three orders less offshore. In order to propose an efficient method in such regime, a part of the system has to be considered implicitly, leading to an ImEx (Implicit Explicit) scheme. In order to limit the size and number of linear systems to be solved, the CPR scheme [1] is a good first order candidate. The CPR approach is a fully diagonal segregated method which only relies on the implicit treatment of the water height and hybrid mass fluxes using explicit velocities. Concerning the high order in time integration, several Runge-Kutta schemes can be found in the literature [2] in the context of ImEx schemes, however to limit the number of linear systems to solve, we focus on Crank Nicolson schemes. For the space discretization, a classical second order MUSCL reconstruction is used. We finally show, thanks to one-and two-dimensional test cases, that the developed scheme achieves the theoretical second-order rate of convergence. Furthermore, we conduct a comparative analysis of CPU times between the ImEx and explicit schemes, revealing important computational savings with the ImEx scheme particularly under the low Froude regime.

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CEDYA 2024 - Communication proposal

Layer-averaged models for bedload and suspension sediment transport with erosion and deposition effects

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Abstract: Understanding the dynamics of bedload and suspesion sediment movement in a variety of natural and ingeneered systems is crucial for sediment transport and erotion modeling. Based on a multilayer Shallow Water system approach [1], we introduce in this work in progress a novel model that incorporates erosion and deposition of sediment in suspension. We also consider non-hydrostatic pressures to better capture dispersive effects.

Moreover, we discuss the application of non-equilibrium bedload transport models [2], particularly in scenarios involving erosive dam breaches in 2D, employing a finite volume approach on rectangular meshes [3].

Through this approach, our work seeks to advance in sediment transport modelling by improving the understanding of this phenomena and practical implications in real-world applications.

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Numerical schemes for the compressible Cahn-Hilliard-Navier-Stokes equations

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Abstract: In [4] a spinodal decomposition, governed by the Cahn-Hilliard equation [2], is conjectured as the underlying mechanism that explains the layered sedimentations of monodisperse colloidal particles.

Since the Cahn-Hilliard equation cannot explain this phenomenon by itself, the gravitational force is introduced into the model by means of conservation of mass and momentum, which, together with conservation of individual species and ignoring temperature changes, yields a system of equation, the isentropic compressible Navier-Stokes-Cahn-Hilliard equations [3, 1], which are a system of fourth-order partial differential equations that model the evolution of mixtures of binary fluids under gravitational effects.

Although incompressible models for these equations might be more suitable for explaining the cited layering phenomenon, we consider the compressible case for the evolution of, e.g. foams, solidification processes, fluid-gas interface.

The goal of this contribution is the design of implicit-explicit timestepping schemes to avoid the severe restriction posed by the high order terms for the efficient numerical solution of boundary-initial problems with these equations.

We show some two-dimensional experiments to assess the possibilities of obtaining efficient algorithms.

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High-order fully well-balanced numerical methods for one-dimensional blood flow with discontinuous properties and friction. Application to networks.

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Abstract:

We are interested in the numerical study of the one-dimensional blood flow model with discontinuous mechanical and geometrical properties and friction. We present the mathematical model together with its nondimensional form. The investigation of all its stationary solutions will be the main point of this talk since they are not given in a explicit or implicit form so numerical techniques proposed in [1] will be used. Following the numerical study done in [2] we propose high-order fully well-balanced numerical methods that are able to preserve all the discrete stationary solutions. These schemes are given as a combination of the Generalized Hydrostatic Reconstruction and well-balanced reconstruction operators. Moreover these methods are able to deal with more than one discontinuous parameter. Some numerical tests are shown to prove its well-balanced and high-order properties, and its convergence to the exact solutions. We will also show results applied to blood flow networks.

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Invariant domain preserving method for solving Lagrangian Hydrodynamics equations

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Abstract: In this talk I am going to describe a new explicit approximation technique for the Lagrangian hydrodynamics equations equipped with an arbitrary equation of state. The approximation of the state variable is done with piecewise constant finite elements and the approximation of the mesh motion is done with higher-order continuous finite elements. This method is invariant domain preserving and exactly mass conserving. I will illustrate numerically the robustness of our method on various benchmark problems.

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POD-based reduced-order modelling applied to parametrized hyperbolic problems

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Abstract: Reduced-order models (ROMs) based on the proper orthogonal decomposition (POD) are widely used to reduce computational costs when compared to standard numerical methods, also called full-order models (FOMs). The ROM strategy consists of two parts: the off-line part, in which the ROM is trained by applying the snapshot method (cf. [1]]) to the solutions of the FOM computed up to the training time; and the on-line part, in which the ROM is solved up to the same training time. One of the most important limitations of POD-based ROMs is the prediction of solutions beyond the training set considering hyperbolic problems. It is very interesting to explore the ability of ROMs to work on parameterised problems and to see if they are able to obtain satisfactory results by modifying the value of the training parameters. In this work we study this possibility applied to hyperbolic transport problems such as the shallow water equations [2].

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Geometric multigrid for local space-time FEM to 3d Navier–Stokes and dynamic Biot systems

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Abstract: Space-time finite element methods (STFEMs) allow the natural construction of higher order discretizations to systems of flow and multiphysics [1, 3]. They offer the potential to achieve accurate results on computationally feasible grids with a minimum of numerical costs. However, constructing higher order numerical methods maintaining stability and inheriting most of the rich structure of the continuous problem becomes increasingly difficult. Further, to realize higher order schemes that require less CPU time for achieving comparable accuracy, also solvers of optimal complexity, are necessary. Ideally, the approach should also offer robustness with respect to the physical (model) and discretization parameters. We present corresponding solution techniques for the Navier–Stokes equations of incompressible viscous flow and the coupled hyperbolic-parabolic Biot system of dynamic poroelasticity with applications in geophysical and bio-medical engineering. To solve the algebraic systems, geometric multigrid (GMG) preconditioning with local Vanka-type smoother of GMRES iterations is suggested. The performance of the combined STFEM and GMG approach is investigated for challenging three-dimensional test problems [1, 2].

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Parallel Nonlinear Schwarz Domain Decomposition Solvers for Two-Phase Flow in Porous Media

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Abstract: In the context of the storage of radioactive waste, the need for advanced parallel nonlinear solvers becomes evident in simulating the neighboring geological environment. These models for two-phase flow equations in porous media are highly nonlinear and are solved over timeframes that could reach millions of years, presenting a significant challenge. Addressing this requirement, innovative nonlinear solvers have been developed and applied, showcasing their effectiveness in handling complex environmental simulations [1]. These solvers stand out due to their use of nonlinear domain decomposition methods, which not only enable efficient parallelization but also significantly improve both nonlinear and linear convergence rates [2, 3]. This is achieved by partitioning the problem into subdomains and solving a smaller subproblem within each. Thanks to an implementation using petsc4py [4], the solvers capabilities were validated through their application to an international benchmark that models the injection of hydrogen into an initially saturated porous medium. This application highlighted the solver's robustness and rapid convergence, essential qualities for the simulation of geological environments. Moreover, the challenge of communication slowdown, which becomes apparent when dealing with a large number of subdomains and negatively affects the linear inner loops, is effectively mitigated. A second-level strategy employing a nonlinear multigrid approach, specifically the Full Approximation Scheme (FAS), addresses this issue. The FAS approach stabilizes the number of inner loops regardless of the number of subdomains, ensuring scalable efficiency suitable for extensive parallel computing applications. Furthermore, the sequence in which operations of the first and second level are applied plays a significant role in enhancing overall performance and convergence. Properly ordering these operations is critical, as it impacts both the effectiveness and efficiency of the method.

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Section: NAS

Second-order space-time parallel methods for diffusion-dominated problems and extension to reaction-diffusion problems

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Abstract: The existing limits of sequential computing have led the community to adopt new strategies to improve the speedup of numerical simulations. Among them, parallelization has gained popularity in recent years. In the context of evolutionary parabolic problems, space-time parallel solvers are integrators of great interest on the grounds of their optimal use of the processors available.

In this work, we present a new family of space-time parallel methods based on the combination of the parallel-in-time parareal algorithm (cf. [2]) and suitable splitting techniques that permit us to perform space parallelization. In particular, the elliptic operator is partitioned into simpler suboperators, using either dimensional or domain decomposition splittings (cf. [3]). Then, second-order splitting time integrators are considered as the propagators of the parareal algorithm to solve the split problem (see [1] for a comprehensive study).

A theoretical analysis of convergence is performed for diffusion-dominated problems, and the methods are further extended in order to solve reactiondiffusion problems. In that regard, numerical experiments are shown so as to confirm the potential of the proposed solvers.

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Efficient, robust and accurate method for simulating a tumor growth model

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Abstract: In Sciences and Engineering, there is a diversity of problems to be studied in the area of Computational Fluid Dynamics, which include relevant applications in Biomedicine. For the solution of these problems, numerical methods are employed regardless of complexity, geometry, physical parameters, boundary and initial conditions. However, one of the main disadvantages of numerical methods concerns the determination of computational errors associated with their use, in which numerical solutions can be affected by truncation, iteration and rounding errors. Although numerical errors cannot be completely eliminated, it is essential that they are controlled or minimized. Among the sources of numerical error, discretization error is considered the most significant, requiring careful analysis. Therefore, in this work, we examine the effectiveness of Richardson's Extrapolation as an alternative to decrease and estimate discretization error in the numerical solution of a two-dimensional mathematical model of tumor growth described by a system of four partial differential equations in transient regime, where two of the equations are nonlinear [1]. The numerical approach adopted involves the use of the finite difference method, with central differences for the spatial discretization and the Crank-Nicolson method for the discretizationin time. Linearization is performed by applying Taylor Series expansion, while the solution of the resulting system of linear equations is addressed with a Gauss-Seidel solver together with the multigrid method to accelerate the convergence of the iterative process. Numerical tests were conducted with satisfactory results both for convergence acceleration and for reduction and estimation of discretization error for a problem with a known analytical solution, verifying the robustness and effectiveness of the multigrid method and the accuracy of the used error estimators. Subsequently, numerical tests were conducted with satisfactory results for a realistic problem, ensuring the reliability and accuracy of the results.

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Parallel performance of preconditioners for mechanics with a second gradient regularization problems

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Abstract: The modeling of a deep geological disposal facility built in a clay-based host rock is of interest to us. To avoid problems with the loss of uniqueness of a solution and, more importantly, problems of localization which are often encountered in soil computations, we consider non-locally regularized equations based on a second gradient theory [1]. The objective of this work is the development of a scalable solution technique for the linearized equation. There has been research on models involving second gradient regularization, but linear solvers have not been in the focus of these works [2]. We will present a block preconditioner for the mechanics equilibrium equations with a regularization via a second gradient of dilation. Our proposed preconditioner is based on the theory of block preconditioners for saddle point problems [3]. We use a block Jacobi approach, where we precondition with an algebraic multigrid the blocks corresponding to the finite element discretization of the displacement and micro volume changes, whereas the Lagrange multipliers block is preconditioned with a mass matrix. The method is implemented in code_aster [4]. Numerical results reflect the good performance of the proposed preconditioner that shows to be weakly scalable until more than 2000 cores. Furthermore, the iteration count of the iterative solver is independent of the mesh size.

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Section: NAS

Iterative coupling solution of a novel stabilization scheme for Biot's model

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Abstract: The coupling of fluid flow and mechanical deformation within a porous media is studied by Biot's model [1]. For the numerical simulation of this poroelastic problem, there are mainly two ways to deal with the solution of the large sparse systems arising after discretization of the system. Namely, fully coupled or monolithic methods and iterative coupling methods. In this talk, we present a decoupled method falling in this latter group. The proposed iterative scheme naturally appears by iterating between the flow and mechanics problems from a new stabilized discretization of the model. We demonstrate the parameter-robust convergence of the proposed iterative coupling method, and show the optimality of this method for one-dimensional problems and their good behavior in higher dimensions.

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Multipoint Flux Finite Element Methods for the Dual-Porosity Darcy Flow Model and Their Efficient Multigrid Solution

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Abstract: The aim of this work is two-fold. On the one hand, we formulate multipoint flux mixed finite element approximation schemes for the single-phase Darcy flow model in dual-porosity rigid porous media. Two classes of methods are derived for quadrilateral elements, depending on the type of meshes (namely, smooth or distorted) under consideration. These are based on the application of symmetric and non-symmetric variants of certain quadrature rules, which were introduced in [1] and [2], respectively, for the single-porosity case.

On the other hand, we focus on the efficient solution of the algebraic systems that arise when considering the aforementioned discretization. Such a task is a crucial part of the numerical simulation process, since it consumes a considerable amount of time in practical applications. The proposed solver is a cell-centered geometric multigrid method [3] on logically rectangular meshes. Remarkably, these meshes take advantage of recent computer architectures that achieve their best performance when structured data are used.

We present a series of numerical experiments that illustrate the convergence behaviour of the approximation schemes, and show the robust performance of the multigrid solver with respect to the permeability tensor coefficient, the mesh size and several families of quadrilateral meshes considered in this work.

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Matrix Factorizations With Newton's Method

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Abstract:

We present a general group-theoretic framework to derive efficient Newtonlike iterations for the computation and certificate of various matrix decompositions, assuming that a suitable condition is known. We illustrate the approach on a list of applications, such as LU-decomposition, QRdecomposition, eigen decomposition, singular value decomposition. This framework generalize the contents of the paper [1]

References:

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Combined matrix of diagonally dominant matrices

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Abstract: Let A be an $n \times n$ diagonally matrix. In this talk, properties of nonsingular matrices that are doubly diagonally dominant are considered [4]. In addition, other kinds of diagonally dominance as strictict or equipotent are revised [1]. Finally, properties of the combined matrix of A, [2, 3], in function of the dominance character of A are studied, in particular, when the dominance is strictly and when the matrix A is irreducible and equipotent.

Joint work with Cristino Castillo, Randy Leonardo and Máximo Santana of Universidad Autónoma de Santo Domingo (Dominican Republic), and María T. Gassó of Universitat Politècnica de València (Spain).

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Well-distributed points on the sphere and the real projective plane

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Abstract:

In the last decades, the problem of evenly distributing points on manifolds like spheres and projective spaces has attracted the attention of the mathematical community due to its theoretical interest and its numerous practical applications, constituting nowadays a very active field of research. One of the main open problems in the area is Smale's 7th problem, which asks for a collection of spherical points with very low logarithmic energy, in some precise sense. This problem dates back to 1993, when Michael Shub and Stephen Smale [2] discovered an astounding fact: if the logarithmic energy of a set of N points on the sphere is very close to the minimum, then the monic polynomial associated to the stereographic projection of these points has small condition number.

In this talk, I will tackle the problem of distributing points on the usual two-dimensional sphere and on the real projective plane. More precisely, I will present a generalization of a family of spherical points, the Diamond ensemble [1], containing collections of N points on the sphere with low logarithmic energy for any natural number N. In addition, I will also show how the ideas for distributing points on the sphere can be extended to the real projective plane, thereby obtaining lower and upper bounds for the Green and logarithmic energies which constitute the best results in that regard thus far [3].

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Randomized V-AISM preconditioner

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Abstract: In this work we consider the application of randomized approximate inverse LU preconditioners for solving iteratively linear systems of the form Ax = b where $A \in \mathbb{R}^{n \times n}$ is a large nonsymmetric and sparse nonsingular matrix. We solve the system using Krylov subspaces methods.

The preconditioner is a randomized version of the V–AISM preconditioner introduced in [2] which is a variant of the AISM preconditioner [1]. In this new approach the matrix products used to compute the preconditioner are approximated as the product of some randomly selected rows and columns of the matrices to be multiplied.

Acknowledgements Supported by Conselleria de Innovació, Universitats, Ciència i Societat Digital, Generalitat Valenciana (CIAICO/2021/162).

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Approximate Inverse LU preconditioning applied to least squares problems

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Abstract:

In this work we consider the application of approximate inverse LU preconditioners to compute preconditioners for the iterative solution of sparse least squares problems of the form

$$\min \|b - Ax\|_2,\tag{1}$$

where $A \in \mathbb{R}^{m \times n}$ $(m \ge n)$ is a large and sparse matrix with full column rank. We consider the solution of (1) with the preconditioned CGLS method, [3] which implicitly applies the conjugate gradient method to the normal equations

In this work we apply the V–AISM preconditioner introduced in [2] which is a variant of the AISM preconditioner [1]. The main difference is that the Sherman-Morrison formula is applied multiplicatively that allows for a compact representation of the partial factors. The results of numerical experiments show that this new preconditioner is efficient compared with other approximate inverse preconditioners that appear in the bibliography.

Acknowledgements Supported by Conselleria de Innovació, Universitats, Ciència i Societat Digital, Generalitat Valenciana (CIAICO/2021/162).

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Section: NLA

Accurate computations with matrices associated to q-Jacobi polynomials

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Abstract: A matrix is totally positive if all its minors are nonnegative [1]. A remarkable property of nonsingular totally positive matrices is that they can be factorized as a product of nonnegative bidiagonal matrices. This representation is known as bidiagonal decomposition and, if it is known accurately, it can be used as a parameterization to solve many common problems in numerical linear algebra with high relative accuracy [2, 3]. This has been possible for some collocation matrices of important bases of polynomials such as Bernstein polynomials or the monomials, as well as families of orthogonal polynomials like Laguerre polynomials, Bessel polynomials or Jacobi polynomials.

In this talk, we will consider the case of the little *q*-Jacobi polynomials, which extends some of the families of orthogonal polynomials previously mentioned. We will show under which circumstances it is possible to achieve accurate computations with their collocation matrices.

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Section: NLA

The discrete-time para-Hermitian rational eigenvalue problem

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Abstract:

Strongly minimal linearizations of rational matrices [1] are linear polynomial system matrices of the form: $L(z) := \begin{bmatrix} zA_1 - A_0 & zB_1 - B_0 \\ -zC_1 + C_0 & zD_1 - D_0 \end{bmatrix}$, where $zA_1 - A_0$ is regular, and the pencils $\begin{bmatrix} zA_1 - A_0 & zB_1 - B_0 \end{bmatrix}$ and $\begin{bmatrix} zA_1 - A_0 \\ -zC_1 + C_0 \end{bmatrix}$ have no finite or infinite eigenvalues. Strongly minimal linearizations contain the complete information about the zeros, poles and minimal indices of the corresponding rational matrix R(z) and allow to recover very easily its eigenvectors and minimal bases. Therefore, they can be combined with algorithms for the generalized eigenvalue problem for computing the complete spectral information of R(z).

Rational matrices play a fundamental role in systems and control theory [2], and in some important applications they can have a particular selfconjugate structure. In [1] it is shown how to construct strongly minimal linearizations that preserve it for Hermitian and skew-Hermitian rational matrices, with respect to the real line, and for para-Hermitian and paraskew-Hermitian rational matrices, with respect to the imaginary axis. In this talk we describe the solution for discrete-time para-Hermitian rational matrices. These are rational matrices that are para-Hermitian on the unit circle. However, a linearization can not be discrete-time para-Hermitian. Therefore, given a discrete-time para-Hermitian rational matrix R(z), we instead construct a palindromic linearization for (1 + z)R(z), whose eigenvalues that are not on the unit circle preserve the symmetries of the zeros and poles of R(z). This can be solved via Möbius transformations. We also give a constructive method that is based on an additive decomposition into the stable and anti-stable parts of R(z).

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Bidiagonal decompositions of totally positive Gram matrices and applications

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Abstract:

Finding classes of matrices with relevant applications, for which linear algebraic computations can be efficiently performed to high relative accuracy, is an important research topic. Bidiagonal decompositions of totally positive matrices, by means of Neville elimination, have become an instrumental tool to parameterize and perform accurate computations involving these matrices.

Gram matrices are implicit in many diverse applications, such as the finite element method, the model fitting of the covariance structure, machine learning (see [1], [2], [3]) and some of the fundamental problems of interpolation and approximation which lead to interesting related linear algebra computations. Unfortunately, Gram matrices are often ill-conditioned and, therefore, computations with these matrices can lose accuracy as the dimension of the problem increases.

Hilbert matrices $H_n = (1/(i+j-1))_{1 \le i,j,\le n+1}$ are well-known notoriously ill-conditioned Gram matrices corresponding to monomial polynomial bases with respect to the usual inner product

$$< f,g >= \int_0^1 f(t)g(t) \, dt$$

In [4, 5], it is shown that these matrices are strictly totally positive and a bidiagonal decomposition to Hilbert matrices is obtained providing matrix computations to high relative accuracy.

In this talk new contributions to this field will be presented (see [6, 7, 8, 9]). In particular, some examples of Gram matrices of totally positive polynomial bases with respect to several inner products will be considered. Their total positivity will be analyzed and a bidiagonal decomposition of the considered matrices will be derived. Furthermore, using the proposed representations, it will be shown the numerical resolution of linear algebra problems with these matrices is achieved to high relative accuracy.

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Sparse recovery of an electrical network

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Abstract:

We study the problem of recovering the edges and weights of an electrical network from power and voltage data at all vertices.

This problem consists in fitting both an algebraic variety and a graph and it is often ill-posed. In case there are multiple electrical networks which fit the data up to a given tolerance, we seek a solution in which the graph and therefore the algebraic equations associated with the electrical network are sparse, i.e. with few edges and terms.

We propose an algorithm to obtain a sparse solution based on original theoretical results (see [1]). It combines in an iterative procedure the resolution of convex optimization problems and techniques of spectral graph sparsification. We show experimental results of its application.

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Model identification in diathermy based on skin temperature

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Abstract: The knowledge of the distribution of temperatures inside the human body allows to assess the effect of a physical therapy on the internal tissues. There are different mathematical models to know this distribution, generally called bioheat equation [1]. They have parameters that represent the different physical processes involved. Usually, simulations are carried out, based on typical values obtained from databases or theoretical calculations [2]. These values show great variability, so that the results obtained are not reliable enough. In order to find better values, temperature measurements can be made on the skin. Thermographic cameras, which are well suited for these measurements, are available. Moreover, their image analysis software allows recording curves of temperature evolution over time. This is the data to be analyzed. The first step is to find the solution of the mathematical model based on given values of the parameters. In some simple cases, as 1D problems, it is possible to find analytical solutions [3]. Electromagnetic theory is necessary to model the heating of tissues by Joule effect [4]. More complicated cases are solved using numerical methods. It is common to use hybrid methods, where two methods are combined. First, the geometric coordinate are discretized and the problem is converted into a system of ODEs [5] [7]. From this solution, the temperature at the surface is selected, which must be compared with the actual data. To be able to perform this comparison and tune parameters, it is necessary to define a loss function and its sensitivity with respect to the parameters. Adjoint method is the most suitable for these computations[8]. Different methods of performing this optimization have been applied to bioheat equation. Some of them are based on the gradient concept [6]. Other methods are based on the randomness, such as Monte Carlo methods [9] or evolutionary algorithms [10], which have greater robustness in ill-conditioned problems[11]. Several methods are considered: Hamiltonian Monte Carlo [12], Evolucionary Centers Algorithm [13] and BFGS[14]. Artificial datasets have been created, simulating the system and adding Gaussian noise. The original values of the parameters and their estimates have a very good agreement.

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Section: OC-IP

Observability and control of parabolic equations on networks with loops

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Abstract: Network theory can be useful for studying complex systems such as those that arise, for example, in physical sciences, engineering, economics and sociology. In this communication, we prove the observability of parabolic equations on networks with loops. By using a novel Carleman inequality, we find that the observability of the entire network can be achieved under certain hypothesis about the position of the observation domain. The main difficulty we tackle, due to the existence of loops, is to avoid entering into a circular fallacy, notably in the construction of the auxiliary function for the Carleman inequality. The difficulty is overcome with a careful treatment of the boundary terms on the junctions. Finally, we use the observability to prove the null controllability of the network and to obtain the Lipschitz stability for an inverse problem consisting on retrieving a stationary potential in the parabolic equation from measurements on the observation domain. This communication is based on the paper [1].

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Stochastic control with state constraints of a photovoltaic plant with batteries.

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Abstract:

The ongoing clean energy transition suffers from geopolitical tensions and volatile energy markets. This issue, together with the rising demand for energy, makes necessary the employment of affordable and reliable energy supplies, [1], [2]. In order to achieve the desired transition, both renewable energies and storage have become key factors. In particular, the combination of solar photovoltaic sources with batteries provides a short-term flexible solution for electricity markets despite the uncertain nature of the renewable resource.

In this work, we develop a technique for electricity producers to determine optimal offers in day-ahead electricity market auctions and to control the renewable power plant in real time. For these purposes, we make use of mathematical modelling and stochastic control theory. Specifically, a system of stochastic differential equations is presented for the modelling of a photovoltaic power plant with storage in conjunction with the price of electricity, [4], [6]. Later, a stochastic optimal control problem with state constraints is introduced. Then, we make use of the Fokker-Planck equation, [7], which allows us to equivalently formulate the optimal control problem for stochastic ordinary differential equations as an optimal control problem for deterministic partial differential equations. Finally, the optimality conditions are deduced, which involve the Hamilton-Jacobi-Bellman equation, [8], [3]. A similar work for a wind power plant has been recently published in [5].

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Testing multi-frequency linear sampling indicators on experimental data.

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Abstract: The Linear Sampling Method (devised by Colton and Kirsh in [2]) is a qualitative method for solving inverse scattering problems in the resonance region. This is a non-iterative method which does not require any a priori information on the nature of the scatterer.

The method only requires to approximately solve a small linear system on each (sampling) point in the domain to be inspected. The size of these systems does not grow with the number of sampling points (that, is, with the resolution) and the matrix does not change between points.

This method has been applied on problems modelled by the Helmholtz equation in acoustics, electromagnetism and vibrations as well as on the Maxwell equations.

In this communication we will show part of the results obtained in [4] were we study a database collected by the Institut Fresnel de Marseille and made available in [1]. This database contains multi-static and multi-frequency measurements of the scattered electric field when several dielectric and conducting targets are irradiated.

In particular, we test two multi-frequency indicators developed in [3], as well as a new one. We also show a very fast adaptative implementation which allows to greatly reduce the number of sampling points, further reducing the computational cost of the method.

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Application of topological derivative methods to non-destructive inspection of metallic plates

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Abstract:

In this work, we apply topological derivative tecniques for the detection of small defects of different shapes and sizes in aluminium plates, using Lamb wave excitation signals in a wide range of frequencies. We propose a general framework which adapts to different experimental setups of practical interest. Numerical experiments illustrating the capabilities of the method will be presented.

Combining dynamic modes and topological sensitivities for active thermographic inspection

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Abstract: In this work we propose a new data processing tool for active thermographic inspection of metallic plates based on the combination of the higher order dynamic mode decomposition (HODMD) and the topological sensitivity. HODMD will first be used to clean up experimental noise and identify the thermographic modes. Then, the topological sensitivity of a cost functional defined in terms of those modes will used to diagnose defects inside the plate. The performance of the method will be evaluated for a database of experimental thermographic images.

Lie brackets and optimal feedback regulation of stochastic control problems and differential games

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Abstract:

We consider stochastic optimal control problems and differential games of fixed duration and prove that the optimal feedback solutions satisfy a system of quasilinear partial differential equations (PDEs henceforth). Under suitable assumptions about the dimension of the state space, the number of controls and the number of independent Brownian motions, we show that the system is of second order. The system of PDEs is obtained by computing the Ito differential(s) of the stochastic Hamiltonian and applying the maximum principle, so that Lie brackets of the vector fields defining the problem appear quite naturally. The system of PDEs is obtained by elimination of the adjoint variables of first and second order. The method is easily implementable in symbolic calculus packages. The new system is especially useful to study questions where it is crucial a direct knowledge of the optimal controls, without resorting to the value function(s). For instance, in the so called certainty equivalence problem, about determining whether the optimal solution or the Nash equilibrium of a given stochastic model is also the solution to a companion deterministic problem. Also, it provides a suitable framework to find model structures such that feedback especial controls (linear, open loop, Markov stationary, etc.) are optimal solutions. The method is applied to some important models in economics and finance. In particular, we study a differential game of exploitation of a productive asset subject to random shocks and a model of Merton of choosing optimal portfolios and consumption.

Numerical Solution for Ventilated Facade Heat Transfer in Building Energy Analysis

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Abstract: This project aims to integrate a custom heat transfer model for ventilated facades into a building energy simulation software called EnergyPlus [2]. The primary focus is to formulate the equations describing the temperature variation along the ventilated facade, considering atmospheric conditions, wall temperature, facade geometry and materials. The system of nonlinear equations posed is solved along with the heat conduction transfer equations using Conduction Transfer Functions (CTFs) [1].

Subsequently, the thermal behaviour is modeled within the ventilated channel, incorporating the influence of the air mass flow due to wind and natural convection. This was accomplished through an energy balance analysis between the internal and external conditions of the channel, including conduction, convection and radiation as well as a mass balance analysis within the cavity of the ventilated facade. The core challenge lies in the interdependencies among variables, requiring a systematic approach to solve the system of equations. A nested loop strategy, combining two additional numerical methods tailored to problem requirements, was implemented: successive approximations and the bisection method. As a result, the three combined and tuned numerical methods proved to be highly effective and convergent, enabling a robust numerical framework to simulate energy transfer in buildings with ventilated facades using EnergyPlus [3].

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A Model for the Economic Impact of Healthcare Facilities During a Pandemic

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Abstract:

This work deals with the economic implications of epidemics, in particular with those related with the implementation of healthcare infrastructure and facilities. It is evident that insufficient medical resources imply costs both in terms of human lives and economic burdens stemming from longer hospitalization stays and absenteeism due to sick leaves. An increase of medical resources is likely to have a positive impact on the mitigation of its consequences, primarily by reducing mortality rates, but it represents an economic cost to be assumed by the society. Also, beyond a certain point, additional medical resources do not necessarily imply a significant improvement in health care quality. The goal of this work is to establish a mathematical model to describe such a situation that might help in the decision-making to find a balance between the different costs involved in the health care system in the case of a pandemic.

Our proposal considers a continuous compartmental model for the evolution of the pandemic that separates hospitalized and ICU hospitalized individuals, and is linked to a cost functional that describes the economic cost derived from the different agents implied in the model, resulting in an optimization problem whose parameters are the number of hospital and ICU beds.

Section: AMI

An updated proper orthogonal decomposition to approximate the time-dependent neutron diffusion equation

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Abstract: Accurate and fast simulations in nuclear reactors depend on obtaining efficient approximations to the neutron transport equation. The prohibitive cost of its resolution has recently led to the application of Reduced Order Model (ROM) especially for the neutron diffusion equation [1]. These algorithms approximate high-dimensional systems by low-dimensional ones, which are much faster to solve and have, as far as possible, the accuracy of the full model [2]. In this context, this work proposes a ROM method for the time-dependent multigroup neutron diffusion equation based on the Proper Orthogonal Decomposition (POD) approach.

This projection-based method consists of two steps. In the offline step, a reduced space has to be built from previously known data, called 'snapshots', and singular value decompositions. Several types of sampling techniques are tested to obtain efficient methods for a given reactor transient. A strategy for selecting the dimension of the basis of the snapshots is also investigated. In the online step, the reduced model is solved on the reduced space, which requires much less computational time than the original problem. Additionally, this work investigates the updating of the reduced space along the transient to improve the reduced model with a moderate number of snapshots. The accuracy and computational time of the proposed POD method are verified in several benchmark problems. The numerical results are compared with the full order model.

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Mesoscale Modelling of Thrombus Formation using smoothed Dissipative Particle Dynamics

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Abstract:

Mathematical modeling and numerical analysis are fundamental allies in medical applications, such as understanding thrombus formation dynamics and exploring therapeutic interventions for clotting disorders. We propose a computational scheme for modeling blood coagulation using Advection-Diffusion-Reaction (ADR) equations.

Our computational scheme employs a particle-based representation, adapting the smoothed Dissipative Particle Dynamics (sDPD) method to capture fluid momentum transport at mesoscales. Additionally, we account for diffusion and reaction phenomena among multiple coagulation species through compositional-field variables associated with each particle. Notably, our model faithfully reproduces concentration profiles observed in blood experiments reported previously [1, 2], validating its accuracy.

Our approach facilitates the exploration of diverse scenarios, spanning from homogeneous to heterogeneous conditions, both static and dynamic. Particularly in dynamic scenarios, we explore the impact of the Peclet number on species concentration distribution across the domain. This analysis offers promising prospects for applications in in-vivo and in-vitro systems, as well as in multiscale models involving medical devices.

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Convergence of a IMEX time scheme to weak solutions of a chemotaxis model in 3D domains.

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Abstract: The purpose of this work is to prove the existence of weak solutions of the parabolic–parabolic chemotaxis system

$$\begin{array}{l} u_t = \Delta u - \nabla \cdot (u \nabla v) + u - u^2 & \text{in } \Omega \times (0, +\infty), \\ v_t = \Delta v - v + u & \text{in } \Omega \times (0, +\infty), \\ \partial_n u = 0, \quad \partial_n v = 0 & \text{on } \partial\Omega \times (0, +\infty), \\ u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x) & \text{in } \Omega, \end{array} \right\}$$
(1)

being $\Omega \subset \mathbb{R}^3$ a bounded domain with regular enough boundary. This problem describes the density of cells $u(x,t) \geq 0$ with logistic growth term and attractive chemotaxis towards a chemical signal $v(x,t) \geq 0$.

Chemotaxis is the essential phenomenon in which bacteria and other cells of unicellular or multicellular organisms direct their movements based on the concentration of a chemical signal in their environment. This effect is modeled by the term $\nabla \cdot (u\nabla v)$.

To attain our goal an implicit-explicit time discrete scheme (IMEX scheme) is set up as approximations of problem (1). The numerical behaviour of the nonnegative solutions (u^n, v^n) , of this scheme is analyzed in detail in order to pass to the limit and deduce our objective.

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Analysis of the effect of a therapeutic treatment in a SIC model

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Abstract: A Susceptible-Infections-Contaminant (SIC) epidemic model is a mathematical model that fits the evolution of a disease through indirect transmission. In this model, in addition to the variables of susceptible and infected individuals, we incorporate the variable that measures the amount of contaminants or bacteria found in the environment. In our case, this contaminant has been produced by infected individuals. We start from a discrete-time SIC epidemic model that describes the spread of an infectious disease. Several control strategies can be considered: vaccination, quarantine, therapy, [1, 2]. As a control strategy, we incorporate a medical treatment for infectious individuals. This treatment decreases, among other things, the production of bacteria that affects the infection (this is the effect that we are going to analyze). In particular, we are interested in knowing how the percentage of individuals to whom the treatment is applied affects the eradication of the disease. To do this, we analyze the significance of the effectiveness of the treatment, the percentage of individuals who are treated, and the regimen used to reduce bacterial production. Once a strategy is defined, this analysis can precisely indicate the steps to be followed to combat the disease. Our numerical simulation also suggests under which conditions the treatment is effective.

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Enhancing N-PERT Solar Cells under the Atacama Desert Solar Spectrum

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Abstract: In the Atacama Desert, solar radiation deviates from the global standard, boasting high irradiation levels with intense ultraviolet content. Given the spectral dependence of photovoltaic (PV) technologies, optimizing PV devices mandates consideration of local conditions and technology type. Solar cells are typically optimized for standard conditions, but our study focused on adapting them for Atacama's unique spectrum. We optimized an n-type bifacial passivated emitter and rear totally diffused solar cell (n-PERT) by adjusting geometrical and doping parameters using a hybrid genetic algorithm. Six parameters—cell and emitter thicknesses, back surface field thickness, and doping concentrations—were optimized for both Atacama spectrum (AM 1.08) and standard conditions (AM 1.5). Validating our model, we found the computed and experimental efficiencies to differ by less than 1% under standard conditions, affirming accuracy. Our optimization revealed the necessity of tailored configurations and doping for Atacama deployment. Reducing layer thicknesses and increasing doping led to a 5.4% efficiency boost under AM 1.08. Finally, we emphasize the potential impact of metallization and the feasibility of thinning the emitter and back surface field, opening avenues for enhanced PV technology in extreme environments.

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Identifiability and observability for a class of epidemiological models

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Abstract: Mathematical modelling is widely used for the study of epidemics. Some of the most famous models are the so-called compartmental models, which separate the population in different disjoint groups attending to their health state: for example, the broadly known Susceptible, Infectious and Recovered compartments. These models are usually systems of ODEs, which are the ones we are going to address.

A typical methodology to apply these models to a real epidemic is the following: setting a model considering the main known features of the disease, looking for the parameters that are available in the literature, and recollecting real data series to calibrate the remaining parameters and (if necessary) initial conditions. However, before doing such a calibration, one can wonder the following: given the known data, can we recover the unknowns univocally? This question is addressed by the theories of *identifiability* and *observability*.

Both identifiability and observability theories have been widely used in different fields, such as bioreactors, navigation, or electronics. However, it is not that common in epidemics (see [1] and the references therein). In [2], we present a class of systems such that, under some hypotheses, we can identify and observe them. Moreover, we provide a constructive way to recover both the initial conditions and the parameters. Many epidemiological models are included in this class of systems; in particular, we will illustrate this theory through some basic examples.

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Numerical modelling of Enveloped Virus Hydrodynamics

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Abstract: Since 2019, the virus SARS-CoV-2 has been a critical issue worldwide because of its massive health impact. Here, we investigate the diffusion of SARS-CoV-2 virions using computational simulations. Due to the morphological features, virions can be modelled as decorated nanoparticles and characterized according to their translational and rotational diffusivity. Since they lack an active motion mechanism we used the Rigid Multi-Blob (RMB) [1] methodology and Smoothed Dissipative Particle Dynamics (SDPD) [2] to simulate the effect of the spike proteins on the virions transport. Using RMB, we construct virion models by discretizing the structures as rigidly connected spherical beads; later, we compute their mobility tensor to determine the diffusion. The results revealed the effect of spike arrangement, number, density, and morphology on virion transport and paves the way to look at possible effects on viral infectivity [3]. Moreover, using a similar blob discretization of RMB, we conduct SDPD simulations, treating the envelope and spikes as separate rigid bodies to introduce flexibility in the spikes. This approach allowed us to characterize the effects of flexible spikes and their effect on the rotational diffusivity of the virion. We identify that passive microrheology provide relevant information about viruses.

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Investigation on the disaggregation mechanisms of red-blood-cells

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Abstract: The aggregation and disaggregation of red blood cells (RBCs) play a crucial role in biological processes and the characterization of pathological conditions. Currently, various mechanisms have been identified for RBC interactions, primarily involving either depletion or bridge formation between proteins at the cell membrane[1]. Recent experimental evidence suggests that these interactions may occur concurrently, leading to intricate disaggregation phenomena.

In this study, we present a numerical model that leverages highly-resolved triangulated RBC membranes[2] to capture both depletion and bridge formation. Notably, our model also accounts for the formation of mobile bridges. By comparing our results on RBC disaggregation with existing experimental evidence[3], we observe an initial dependence of the force on the depletion interaction, followed by an increase in force just before cell separation due to bridge migration. Interestingly, when bridges are not allowed to diffuse, the characteristic disaggregation behavior deviates from experimental observations.

Furthermore, we propose a reduced spring-dashpot model that effectively describes the observed disaggregation mechanism. Our findings contribute valuable insights to understanding RBC dynamics and hold promise for applications in biomedical research and clinical contexts.

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Population Dynamics Model with Age Structure

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Abstract: When studying the behavior of a population, understanding what factors inherent to the population influence the decisions of the individuals that make it up, its age structure is of particular importance. Typical phenomena such as the Allee effect, interspecific competition (between individuals of different species) and intraspecific competition (between individuals of the same species but of different ages or qualities), logistic effect (the latter addressed in the model presented), must be considered at the moment. to model said dynamics.

The studied model, conditions for the existence of equilibria and description of said equilibria are presented. In addition, a brief historical review of the main publications on this topic is made, and connections with other branches of science are presented.

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An ETD-based numerical methods for multidimensional nonlinear pricing models

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Abstract: We introduce an approach for pricing American options within multidimensional nonlinear pricing models. One key aspect of our approach is the efficient elimination of cross-derivative terms through appropriate transformations[1], ensuring precise pricing in multidimensional scenarios. Our method is designed to tackle the complexities of pricing multi-asset options, employing a finite difference scheme combined with the exponential time differencing (ETD) technique[2]. By combining these methodologies, we achieve not only accuracy and efficiency but also streamlined implementation. Through exhaustive numerical experiments encompassing diverse option models, such as those with jumps and vulnerable options[3], we address as well the specific challenges inherent in pricing American options, such as early-exercise opportunities tackled by the penalty method. The proposed numerical algorithm is shown to be both accurate and efficient through numerical experiments, which also compare the results with existing methods and analyse the numerical stability and convergence rate.

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Option pricing with Chebyshev-Expanded Artificial Neural Networks

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Abstract: Pricing different types of options is a subject of interest in finance. Classical numerical methods such as finite difference, finite elements or spectral methods, have been successfully applied to solve pricing problems in low-dimensional cases. However, the mentioned numerical methods suffer from the curse of dimensionality. When working in high-dimensional spaces, or with several underlying stocks, they become inefficient, as the computational cost grows exponentially. Artificial Neural Networks are a good solution to overcome the limitations of the previous methods. In particular, the purpose of this work is to combine the benefits of Artificial Neural Networks with Chebyshev polynomial approximation properties. We will see that applying a Chebyshev polynomial expansion can improve convergence rates of Artificial Neural Networks, providing an interesting framework for option pricing.

Pricing American options with endogeneous negative rates under Heston model.

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Abstract: Some decision-making problems in finance can be formulated as American options with endogeneous negative interest rates. Recently, in [1], the authors proved that such problems involve the presence of a double continuation region when there is only one underlying stochastic factor following a geometric Brownian motion. Indeed, a continuation region appears when the option is not enough in the money (standard case for endogeneous positive rates), but also when the option is too deep in the money (non standard case). This properties are theoretically obtained for the call and put American option. As real options applications, the case of a gold loan and a capital investment are considered.

In the present work, specially motivated by the case of the gold loan, we extend the modelling approach proposed in [1] by considering a stochastic volatility model for the underlying asset, so that not only the gold price but also its volatility are stochastic, which is more realistic that a constant volatility. Thus, for American options with endogeneous negative rates we pose the pricing problem in terms of partial differential equations under the Heston model [2]. Numerical methods allow to obtain the behaviour of the continuation region and compare the results with the ones in [1]. Also the pricing of the gold loan is addressed in this more realistic modelling approach.

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Two-productive sector equilibrium problems with heterogeneous agents under jump-diffusion models

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Abstract: In this talk, we assume rational expectations to pose general equilibrium models with heterogeneous firms, which can enter or exit the industry. We consider a jump-diffusion process for two different productivity dynamics corresponding to two sectors, thus extending our previous work [2]. Obstacle-type problems associated with Hamilton-Jacobi-Bellman (HJB) partial integro-differential equations (PIDEs) model the endogenous decision of firms to remain or leave each productive sector. Moreover, the probability density function of firms in each productive sector satisfies a Kolmogorov-Fokker-Planck (KFP) PIDE with a source term. Equilibrium models are completed with household problem formulations and feasibility conditions. For the numerical solution, we propose a Crank-Nicolson method for time discretization and the Adams-Bashforth scheme for the explicit treatment of integral terms. Moreover, we use augmented Lagrangian active set (ALAS) methods for solving the unilateral and bilateral obstacle problems [1], jointly with finite difference discretizations for the HJB formulations. Also, appropriate finite difference discretizations for the KFP problems are considered. For the global nonlinear equilibrium problem, we propose a Steffensen algorithm. Finally, numerical examples illustrate the performance of proposed numerical methodologies as well as the expected behaviour of economic variables.

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Models and numerical methods for XVA pricing in multicurrency derivatives.

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Abstract: In this work, we propose appropriate models to compute the total valuation adjustments (XVA) in a multicurrency setting by means of dynamic hedging methodologies. In this way, we extend previous works in the single currency setting (see [1] and the references therein). Besides the stochastic evolution of the assets in different currencies, the presence of stochastic intensities of default and the consideration of constant or stochastic exchange rates are assumed when computing the XVA associated to European options contracts. These models can be formulated in terms of (non)linear parabolic partial differential equations (PDEs) or in terms of expectations.

When the number of stochastic factors is not greater than two, we propose a Lagrange-Galerkin scheme for solving the PDEs, combined with fixed point techniques for the nonlinear problems [2]. For problems that include more than two underlying stochastic factors (assets, intensities of default, and/or stochastic FX rates), we propose the use of Monte Carlo simulations applied to the formulations based on expectations, combined with a Picard method and the more efficient Multilevel Picard iteration (MPI) scheme for the nonlinear cases [3]. We apply these techniques to different European style option.

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Tuning porosity to improve efficiency of adsorption columns

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Abstract: Assessing and improving the performance of adsorption columns is crucial for various applications. To this end, several mathematical models have been developed over recent years to describe the adsorption process using a set of partial differential equations. These equations capture the evolution of contaminant concentration in the fluid traveling along the filter and the amount of contaminant captured by the adsorbent (see, for instance, [1], [2]).

Traditionally, adsorbents are manufactured using pellets of similar sizes, resulting in a media with roughly constant porosity. However, both experimental and analytical evidence suggest that using porosity-graded adsorbent media can enhance performance. In this talk, we will explore the impact of porosity gradients on breakthrough curves, which describe the time evolution of contaminant concentration at the outlet and serve as the industry-standard measure of adsorption performance.

We will begin by deriving the governing equations under the assumption of axial porosity gradients, corresponding to columns where grains of different sizes are arranged in layers. We will then demonstrate how various porosity functions influence the profiles of the breakthrough curves.

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Removal of multiple contaminants using column sorption

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Abstract: We develop a mathematical model to describe an adsorption process where two contaminants are simultaneously removed from a gas mixture as it flows through a packed column. Both species compete to occupy the available sites, including displacing previously attached molecules. The system is described by mass balances for the two species coupled to an attachment model. A numerical solution is first developed. The results show that, after making certain assumptions concerning the system parameters, the column may be split into a region where competition dominates the adsorption process, and a second region where the weaker contaminant is able to be adsorbed without being displaced. In both regions, it is possible to find travelling waves which may be used to construct an analytical expression for the breakthrough curves of both contaminants. The model results are verified by experiments on the competitive adsorption of the siloxanes D4 and L2 on activated carbon. Extensions for larger number of components are explored.

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3D simulations of gas transport in porous media with adsorption and comparison to 1D models

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Abstract: Fluid flow and mass transport in porous media involving mass transfer between the fluid phase and the solid matrix occurs in a great variety of applications. One such application is capturing a contaminant from a carrier fluid forced through a porous adsorbing bed. Describing this process in realistic 3D porous geometries is complex. A standard approach involves reducing the governing equations describing the process to one spatial dimension via averaging procedures [1, 2]. These models can be solved analytically in some limiting cases. The obtained solutions can be implemented in optimisation routines to find unknown parameters of the process such as the adsorption rate [3]. However, the details of the 3D microstructure are difficult (or impossible) to capture in 1D models and they are often lost in the averaging procedure. This makes it difficult to analyse the possible effects of the microstructure in the adsorption process. In this talk, we will formulate and solve a 3D mathematical model of contaminant capture by adsorption in 3D idealised porous media. The results of the simulations will be compared with the solutions of averaged 1D models. We will show how structure-related features such as porosity and structure homogeneity affect the adsorption process

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Modelling and experiments on hydrogen storage in metal hydrides

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Abstract: Storing hydrogen in an efficient and safe manner is a pivotal area of research due to its potential applications as a green energy vector. In this talk, I will summarize the modeling of hydrogen storage in a metal hydride tank. The model is supported by a microscopic description of the hydrogen-metal hydride reaction, which generalizes prior approaches based on a rate-controlling step. At the macroscopic level, the model can be effectively approximated by a compartmental, 0-dimensional system. Through this approach, we can accurately estimate the evolution of pressure inside the tank over time, which allows to compare the results of our model with pressure measurements in typical experimental set ups.

On the removal of large quantities of contaminant via column sorption

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Abstract:

Column sorption is a practical method for removing a contaminant from a fluid. It has uses in environmental applications such as greenhouse gas capture, groundwater remediation and biogas cleansing as well as industrial uses such as the purification of biopharmaceutical products, the cleansing of flue gases, biofuel purification and many more. It is one of the most widely used methods for the removal of environmental contaminants and is regarded as an essential component in achieving the UN Sustainable Goals and EU Green Deal. Mathematical models for sorption are equivalent to those describing the storage of hydrogen in a metal hydride matrix, so providing further motivation for its study.

Standard mathematical models of the process describe the capture of trace amounts of contaminant, however these are not appropriate for the cleansing of flue gases where the contaminants may be the main component (up to around 70% of the fluid) or hydrogen storage (100% of the fluid). In this talk we describe a new mathematical model for the adsorption of an arbitrary amount of contaminant. The model consists of a coupled PDE/ODE system describing the evolution of the contaminant concentration, the fluid velocity and pressure and the rate of contaminant adsorption. An approximate travelling wave solution is developed and shown to reduce to previous results in the limit of small amounts of contaminant. Both numerical and analytical solutions are shown to compare well against experimental data for the capture of CO_2 .

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 Modelling large mass removal in adsorption columns TG Myers, M Calvo-Schwarzwalder, F Font, A Valverde. Submitted to Int. Comm. Heat and Mass Transfer, Apr. 2024. ArXiv preprint:2404.02939 Optimisation of adsorption column processes: the role of adsorbent microstructure and its packing arrangement.

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Abstract: In adsorption column processes, the design of the adsorbent microstructure and its packing arrangement is key to define the optimal conditions for the process to take place. The relation between the void region, the radius of the adsorbent particles and the size of the pores determine the adsorption capacity of the column, as well as the energetic cost of the process. The pollutant is captured in the adsorbent micropores, which can be accessible either directly through the external surface in contact with the fluid flow, or through the internal surface of the pellets. To reach this region, an intraparticle diffusion phenomenon drives the contaminant molecules through mesopores and macropores to the inside of the adsorbent. These wider pores distribute the pollutant to the micropores located in the inner regions of the adsorbent, where they are finally captured. In this talk, we describe a new mathematical model that considers a representative cell accounting for the dimensions of the column void region and the pellet structure. The advection-diffusion-reaction equation is coupled with the momentum equation to describe the motion of the pollutant through the fluid flow and through the mesopores and macropores. The effect of the variation of the parameters defined in these equations is not trivial, since the mechanisms present in the model are inter-related. The behaviour of the model under certain changes is explained, and the optimal dimensions of the adsorbent particles to obtain the maximum removal efficiency after a certain time are provided. Energetic considerations are also taken into account, defining a trade-off between outlet concentration levels and energetic cost. The final aim is to show the potential of this new model, which can be useful when designing new adsorption materials for the filtering of pollutants.

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 The role of adsorbent microstructure and its packing arrangement in optimising the performance of an adsorption column. A Valverde, IM Griffiths. Submitted to Discover Chemical Engineering, Apr. 2024. https://doi.org/10.21203/rs.3.rs-3951770/v1

Analyzing pedestrian density at football stadium entrances

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Abstract: Massive events require a precise management of pedestrian crowds in order to control high-density scenarios and avoid the accidents that have dramatically increased over the last decades. The simulation of the access of fans to stadiums is an important area that needs to be addressed, as certain crowd-related tragedies have occurred during this process. In this contribution, we study the access of football fans to San Mamés stadium in Bilbao using empirical data provided by the Athletic Club.

We introduce a novel technique to define the desired velocity fields for pedestrians both outside and inside the stadium using OpenFOAM, a tool frequently employed in computational fluid dynamics. By introducing a single additional parameter to control the inflow of people through turnstiles, we reproduce the empirical access rate of people in 15 matches and calculate the time evolution of the maximum local density. We use our macroscopically calibrated version of the Social Force Model for pedestrian simulations and consider three different settings of the agents, varying in them their initial position in the geometry and their sizes. Finally, we evaluate the impact of the total number of attendees and the time distribution of their arrival on maximum local densities. We create multiple virtual scenarios in which a varying number of agents N arrive at the stadium at different rates characterized by logistic distributions with standard deviations σ [1].

References:

 A. García, D. Hernández-Delfin, B. González, G. Garitaonaindia, D.-J. Lee, M. Ellero, Analysis of local density during football stadium access: Integrating pedestrian flow simulations and empirical data, Physica A 638, 129635 (2024).

Temperature optimization in a gas reactor for the synthesis of carbon nanofibers: a numerical approach

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Abstract: Carbon nanotubes (CNT) and Carbon nanofibers (CNF) have become materials with a great variety of applications: Information and Communication Technologies (ICT)[1], construction industry [2], medicine [3], among others.

The temperature at which the CNF synthesis process is carried out determines the final structure of the carbon nanofiber. At 873.15K the formation of the fishbone structure is favored, which is the most interesting industrially and the one with the best process performance [4].

In this work we address the modeling and numerical simulation of flow and temperature for a mixture of gases in a reactor to optimize the temperature inside it using COMSOL Multiphysics [5]. The study is focused on determining appropriate temperatures at the reactor shell, to assure optimal temperatures at the catalyst support device where the reaction of formation of CNF takes place. Different locations of the support device are considered.

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High-quality smooth finishing of blade-like geometries via G^1 multipass 5-axis flank CNC machining using conical cutting tools

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Abstract: Existing multi-pass planning methods often result in undesirable gaps or overlaps between adjacent paths of a cutter. These gaps and/or overlaps in the path-planning stage cause artifacts in the physical machining and these locations must be polished as a post-process using either a tiny ball-end cutter and/or by hand-polishing. While highly curved or convex geometries are impossible to be flank CNC-machined with conical tools, certain hyperbolic geometries, like blades of blisks, admit a new path-planning strategies that aim at smooth surface finish by joining neighboring flank paths of the tool with G^1 continuity.

In this paper, we further develop the approach of flank milling with conical tools such that the surface finish is as smooth as possible in terms of the continuity of the neighboring paths, verify the effectiveness of the method by physical machining of a blade geometry, and show that our machining paths reduce the machining error by up to 85% while maintaining the same machining time when compared to a state-of-the-art commercial software. Moreover, in the vicinity of the boundaries of the paths, the proposed approach basically eliminates the approximation error caused by the transition from one path to another, providing smooth surface finish, and consequently avoiding the necessity of post-process polishing.

We introduce a novel technique to define the desired velocity fields for pedestrians both outside and inside the stadium using OpenFOAM, a tool frequently employed in computational fluid dynamics. By introducing a single additional parameter to control the inflow of people through turnstiles, we reproduce the empirical access rate of people in 15 matches and calculate the time evolution of the maximum local density. We use our macroscopically calibrated version of the Social Force Model for pedestrian simulations and consider three different settings of the agents, varying in them their initial position in the geometry and their sizes. Finally, we evaluate the impact of the total number of attendees and the time distribution of their arrival on maximum local densities. We create multiple virtual scenarios in which a varying number of agents N arrive at the stadium at different rates characterized by logistic distributions with standard deviations σ [1].

References:

 A. García, D. Hernández-Delfin, B. González, G. Garitaonaindia, D.-J. Lee, M. Ellero, Analysis of local density during football stadium access: Integrating pedestrian flow simulations and empirical data, Physica A 638, 129635 (2024).

Hybrid RANS turbulence Reduced Order Models for Heat Transfer Fluid

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Abstract: We present a Reduced Order Method (ROM) approach using hybrid RANS turbulence model to the heat exchange in a fluid of cylindrical irradiated pipes of a simulated 3D cavity of CSP tower receivers. These simulations often entail a very high computational cost thus, to drastically reduce it, we have developed a ROM for this industrial application. We validate the proposed method in a 2D Boussinesq model problem for natural convection monitoring temperature, pressure and velocity for different values of the Rayleigh number. For the 3D forced convection problem of Heat Transfer Fluid (HTF) running through the irradiated pipes, we compute the snapshots with Ansys Fluent in a realistic model of a pipe flow in a solar receiver, with the mass flow inlet as varying parameter. The ROM is developed using the open-source software FreeFEM. The reduction in computational time can be up to three orders of magnitude with relative errors of 10^{-3} .

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Modelling, numerical simulation, and optimization of new technologies related to hydrogen production (Zeppelin project)

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Abstract:

The rising global energy demand, due to population growth, highlights the urgency for sustainable alternatives to fossil fuels. Hence, green Hydrogen (Green H2) is considered as a key energy solution for its ability to produce electricity, mechanical, and thermal energy without CO2 emissions. However, producing hydrogen from fossil fuels harms the environment, so we need to use circular economy ideas and manage waste better to minimize the impact and encourage industries to work together. Four types of technologies are considered for this purpose: catalytic technologies (bioethanol and biogas reforming reactors [1]), microbiological technologies (dark fermentation [2] and microbial electrolysis cell [4] reactors), thermochemical technologies (fluidized and fixed bed gasification reactors [5]), and storage technologies (inside porous materials [6] and in the form of ammonium [7]).

Each individual technology or a network of technologies is modelled by a system of Differential Algebraic Equations (DAEs). In addition, to simulate and optimize it, a direct transcription approach is considered where the DAEs are discretized in a system of algebraical equations. This model is able to make decisions to turn on and off some of interconnected technologies by minimizing a cost function (and/or maximizing the hydrogen production). The final product of this research is a Python simulation and optimization package which can be used for designing and optimizing a network of hydrogen production and storage technologies based on minimizing the production and storage costs. Finally, some specific cases are solved and the results are discussed.

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In-silico simulation of RNA viruses

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Abstract:

In vivo virology research faces constraints like security, cost, and time. Not all labs can study all viruses, and generating synthetic RNA is expensive and time-consuming. We present an approach to study disease evolution at the microscopic level, simulating RNA replication for any virus quickly. This method uses a probabilistic model for mutations, a dynamic population model, and a diffusion model for disease propagation. As a result, we can efficiently compute these processes, enabling studies on virus evolution, propagation, and potential treatments.

Understanding Drug-Target Dynamics through Mathematical Formalism

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Abstract:

Evidence suggests G protein-coupled receptors heteromerize in both Central Nervous System and non-Central Nervous System regions, providing a framework for drug combination therapies. This study presents a heterodimer model using differential equations to represent the binding dynamics of two ligands (A and B) to a receptor heterodimer (R1R2). We prove the existence of a unique, biologically plausible equilibrium within a broad parameter space of rate constants, ensuring feasible pharmacological scenarios. The time dynamics of the biological response vary with the efficacies of the four heterodimeric species, aiding in the exploration of drug combinations.

Modelling Marine Ecosystems for Biodiversity Protection: the case of Øresund strait

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Abstract:

Currently, over 17,000 marine protected areas (MPAs) cover nearly 9% of the oceans, but only 23% have clear management plans, and just 1% have evaluated their management effectiveness. Effective plans are crucial but face financial and infrastructural challenges. Existing guidelines lack systematic approaches for balancing biodiversity targets with socio-economic impacts, and none provide adaptive plans for necessary transformative change. This gap is critical because socio-ecological systems are complex and unpredictable, leading to rapid ecosystem degradation. In this talk, we will discuss a trophic chain model using ordinary differential equations to study the population dynamics of shallow marine ecosystems in the Oresund strait, focusing on the role of cod in controlling various trophic levels, including mesopredators, mesoherbivores, filamentous algae, and eelgrass meadows.
Theoretical Logistics: Distributing Perishable Goods over Long Distances

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Abstract:

In the world of grocery transport, companies face the tough task of managing deliveries while dealing with various constraints. Each pickup and delivery problem is unique, making universal solutions hard to find, thus necessitating optimization. This study focuses on a specific scenario involving multi-commodity pickups and long-distance deliveries, inspired by a real company situation. We propose a mathematical approach to tackle these challenges and discuss different suitable algorithms. Our goal is to develop a strategy that efficiently assigns products to vehicles, minimizing transportation costs and meeting all time and resource constraints.

Automatic Heart Disease Recognition in Limited Databases of Echocardiograms Improved with Higher Order Dynamic Mode Decomposition and Vision Transformers

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Abstract: Heart diseases are the main cause of human mortality in the world (around 18 million deaths per year [1]). Also considering the increase of available medical data, much pressure is therefore put on the health industry to develop systems for early and accurate heart disease recognition. The several deep learning frameworks currently available handle echocardiography data. Most of them resort to Convolutional Neural Network (CNN) technology. However, these systems are typically specialized on a single disease, or a closely related family of them [2]. In this contribution, we describe a system for automatic heart disease recognition, based on a novel deep learning framework, which analyses echocardiography videos in real time. The system comprises two stages. The first one creates a large database from different sources of echocardiography videos. This allows to train any machine learning-based framework, and especially deep learning algorithms. This also includes the use of the Higher Order Dynamic Mode Decomposition (HODMD) algorithm [3], for the first time to the authors' knowledge in the medical field [4] for both data augmentation and feature extraction. The second stage is aimed to build and train a Vision Transformer (ViT), adapted to be effectively trained from scratch, even with small databases. This designed ViT analyses the images from an echocardiography video to automatically estimate the heart state. The results demonstrate that the proposed system is superior and the HODMD algorithm effective in the recognition of different heart conditions, outperforming several CNNs.

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Enhancing prognostic precision in Acute Lymphoblastic Leukemia: a synergy of Topological Data Analysis and Artificial Intelligence

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Abstract: Despite advancements in treatment, a subset of patients with acute lymphoblastic leukaemia (ALL) faces relapse, highlighting the need for improved prognostic tools. Traditional risk assessment methods rely on manual interpretation of flow cytometry data, which may overlook subtle but significant patterns. In this talk, we present a novel approach integrating topological data analysis (TDA) and machine learning (ML) to analyze pre-treatment ALL datasets [1]. By quantifying shapes, including empty spaces, in the high-dimensional flow cytometry data, our method accurately predicts the risk of relapse, particularly in patients previously classified as 'low risk'. Additionally, we validate the predictive power of specific biomarkers such as CD10, CD20, CD38, and CD45. We propose three prognostic pipelines of increasing complexity, offering tailored approaches depending on technical availability. Our findings extend beyond ALL, demonstrating the potential of TDA and ML in enhancing risk stratification in haematological malignancies.

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A POD-Neural Network model for a molten glass flow inside a furnace

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Abstract: In this work, we present a non-intrusive POD model of a molten glass flow inside of a furnace, based on Artificial Neural Networks. The impossibility of observing the real flow of the molten glass inside of a furnace, makes interesting the construction of a CFD model that could be of big interest for the glass industry. With the CFD simulation, we can better understand how the molten glass behaves, letting the glass industry to optimize the process of glass production. We first present the CFD model, for the molten glass flow, based on industrial data. Moreover, since this model may depend on several parameters, we present a non-intrusive POD model, based on Artificial Neural Networks, that let us to compute numerical solutions for different parameter values in real time. This non-intrusive POD model is constructed for helping the glass industry in the decisions adopted for the quality improvement in the glass production. We present numerical results for both the CFD and the non-intrusive POD model.

CEDYA 2024 - Communication proposal

Section: ML

Trajectory Classification through Topological Data Analysis: A Study on Simulated and Real-World Datasets

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Abstract: This study introduces Topological Data Analysis (TDA) as a novel method for classifying trajectories, incorporating machine learning techniques to enhance the understanding and interpretation of complex spatial movement patterns. By applying TDA, we leverage the power of machine learning to investigate the structures and relationships within trajectory datasets, offering a new angle on classification methodologies. This research examines how TDA techniques, augmented with machine learning algorithms, can be seamlessly integrated into trajectory analysis to capture spatial features that traditional methods might overlook. Our machine learning-enhanced approach is tested on both simulated data trajectories and real-world datasets from vehicles and ships, illustrating TDA's versatility and effectiveness across various transportation modes. The use of simulated trajectories allows for a controlled evaluation of TDA and machine learning techniques together. Findings from this study highlight the significant potential of TDA, combined with machine learning, to transform trajectory analysis by uncovering intricate spatial patterns and relationships that conventional analytics might miss. Through detailed computational experiments and analysis of real-world data, we demonstrate how the integration of machine learning with TDA can enhance our ability to analyze and interpret trajectory data, opening up new possibilities for research and practical applications in numerous fields.

Some applications of neural networks in the resolution of partial differential equations

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Abstract:

This work has been motivated by the study of a fluid flow model, with applications in solar power generation. Concentrated solar power (CSP) receivers consist of dozens of tubes with a very high aspect ratio, where a turbulent heat-receiving fluid flows at high temperatures (about 800° C). The optimisation of CSP receivers to provide the highest energy concentration capacity depends on the number of tubes, their dimensions and the inlet flow rate. Due to the complexity of the geometry of CSP receivers, this optimisation is beyond the scope of standard turbulence models. This requires the development of techniques that allow resolution in reasonable time and with sufficient accuracy.

We will present a combined technique of domain decomposition, reduced order methods and neural networks for the resolution of the heat flux at the outlet of CSP receivers. In the offline phase, the parametric heat flux inside the tubes is modelled in terms of reduced boundary conditions. The reduction process is based on a POD approximation of the varieties of the traces at the subdomain boundaries, while the mapping between the traces at the different subdomain boundaries is constructed using deep neural networks. In the online phase, this will allow to replace the calculation of the flow within a large part of the pipes by a reduced mapping between the flow traces at the inlet and outlet boundaries. We will present some applications to realistic situations.

Reducing the Spatial Discretization Error in Coarse CFD Simulations Employing Deep Learning

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Abstract: Many Computational Fluid Dynamics (CFD) applications that employ the Finite Volume Method (FVM) require fine spatial discretisations, which are often computationally prohibitive. In these cases, Deep Learning (DL) has emerged as a key technology to enhance traditional algorithms. In this work, we reduce the spatial discretisation error on coarse meshes by learning from fine-mesh data, following a super-resolution approach. Specifically, we embedded a feed-forward neural network in the workflow of a traditional FVM solver to interpolate face velocities from cell centre values. Thus, we obtain a solver-in-the-loop [1] model, whose physics needs to be differentiable to be correctly trained. For that, we use the open-source CFD code OpenFOAM and its discrete adjoint version [2] for the differentiation process. We also developed a fast communication method between Tensor-Flow (Python) and OpenFOAM (c++) to speed up the training process. We applied the model to the flow past a square cylinder problem, reducing the error to about 50% for simulations outside the training distribution compared to the traditional solver in the x- and y-velocity components using an 8x coarser mesh. The training is affordable in terms of time and data samples since the architecture exploits the local features of the physics while generating stable predictions for mid-term simulations.

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Neural Network based Finite Volume Methods for hyperbolic conservation laws

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Abstract:

The rapid evolution of Physics Informed Neural Networks (PINNs) [1] and Variational PINNs (VPINNs) [2] signifies a transformative shift in the field of computational mathematics, particularly in solving complex non-linear partial differential equations (PDEs). These methodologies efficiently encode physical laws into the architecture of neural networks, allowing the numerical approximation of PDEs.

In this context, we propose to combine PINNs and the traditional finite volume methods (FVM), which are widely used for numerical approximations of hyperbolic conservation laws. First, we consider the integral form of the hyperbolic conservation law and a suitable partition of our computational mesh into cells. Next, we will use neural networks in each cell as a reconstruction operator in the FVM framework. The advantage of using neural networks is to be able to consider implicit methods without increasing the complexity, which allows us to increase stability and to be able to use larger time steps. The neural network performs the crucial task of reconstructing intercell fluxes. The way the method is assembled will allow us to construct well-balanced methods in this framework [3], or to make use of entropy-conservative numerical fluxes.

Moreover, the efficiency of the proposed method will be demonstrated through its application to a variety of hyperbolic conservation laws, including Burgers' equations, shallow water equations, and the compressible Euler equations.

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Data-driven characterization of viscoelastic materials using timeharmonic hydroacoustic measurements

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Abstract: Predictive numerical tools in computational mechanics require choosing an adequate model to capture the material's physical behaviour under consideration. The most common assumptions regarding linear wave propagation in a viscoelastic material are the standard linear solid model, (generalized) Maxwell, Kelvin-Voigt models [1] or the most recent fractional derivative models [2]. Usually, once the frequency-dependent constitutive law is fixed, the intrinsic parameters of the mathematical model are estimated to fit the available experimental data with the mechanical response of that model. This modelling methodology potentially suffers from the epistemic uncertainty of an inadequate a priori model selection. However, in this work, the mathematical modelling of linear viscoelastic materials and the choice of their frequency-dependent constitutive laws is performed based only on the available experimental measurements without imposing any functional frequency dependence [3]. This data-driven approach requires the numerical solution of an inverse problem for each frequency. The acoustic response of a viscoelastic material due to the time-harmonic excitations has been calculated numerically. In these numerical simulations, the transducer's non-planar directivity pattern has been considered. Experimental measurements of insertion loss and fractional power dissipation in underwater acoustics have been used to illustrate the data-driven methodology that avoids selecting a parametric viscoelastic model.

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Spanish Tsunami Early Warning System: Enhancing Maximum Wave Height Predictions via Neural Networks

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Abstract:

Tsunami Early Warning Systems (TEWS) are crucial for mitigation and highly reducing the impact of tsunamis on coastal communities worldwide. In the NEAM region (North-East Atlantic, the Mediterranean, and connected Seas), historical approaches involve using Decision Matrices and precomputed databases due to the short time between tsunami generation and coastal impact. Overcoming real-time simulation challenges, the EDANYA group at the University of Málaga developed Tsunami-HySEA, a GPU code enabling Faster Than Real Time (FTRT) tsunami simulations [1].

A first approach using neural networks (NN) for maximum wave height and arrival time was done in [2]. In collaboration with the National Geographic Institute of Spain, we are extending that work for several faults and multiple coastal locations on the Spanish coast. The main importance of this work is that the models developed can be implemented in the Spanish TEWS producing estimations of the tsunami impact in seconds.

Tsunami-HySEA numerical model is used to generate the data to train the NN models. Around 300,000 simulations have been executed to account for various fault scenarios in the Atlantic Ocean, underlining the substantial demand for High-Performance Computing (HPC) resources.

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Machine learning techniques for inverse problems on brain cell migration in neurogenesis

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Abstract: Neurogenesis is the process of formation of new neurons in the brain from precursor cells called neuroblasts. This process, where new born neuroblasts migrate in the adult brain before maturng into neurons, has been widely described in the literature. However, few models have been developed for that, and as far as we know, the only one in realistic meshes of the brain is the one proposed in [1]. In this model, the route of migration is determined by PDEs that depend on several parameters and describe the chemoattraction forces and the heterogeneous mobility of neuroblasts in different regions of the rodent brain.

In our current study, we delve into the use of Physics-Informed Neural Networks [2] for neurogenesis modeling. Our primary objective is, above all, to refine the parameters of the governing PDEs that dictate the migration pathways of neuroblasts. The target is to improve the accuracy of the predictions with respect to the experimental data from real rodent brains provided by our collaborating neurobiology researchers. Through a series of tests, we compare the efficacy of our Physics-Informed Neural Network approach with other L-BFGS-B minimizing techniques.

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Section: ML

Optimizing Variational Physics-Informed Neural Networks Using Least Squares

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Abstract: Variational Physics-Informed Neural Networks (VPINNs) [1, 2] often suffer from convergence problems when using gradient-descent-based (GD-based) optimizers. By introducing a Least Squares solver for the weights of the last layer of the neural network [3], we improve the convergence of the loss during training in most practical scenarios. This presentation analyzes the computational cost of the resulting hybrid Least-Squares/Gradient-Descent (LS/GD) optimizer and explains how to implement it efficiently. In particular, we show that a traditional implementation based on backward-mode automatic differentiation leads to a prohibitively expensive algorithm. To remedy this, we propose using either forward-mode automatic differentiation or an ultraweak-type scheme that avoids the differentiation of trial functions in the discrete weak formulation. The proposed alternatives are up to 1,000 times faster than the traditional one, recovering a computational cost-per-iteration similar to that of a conventional GD-based optimizer alone. We derive computational estimates and conduct numerical experiments in one- and two-dimensional problems to support our analysis, monitoring the accuracy and computational cost during training.

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An open MRI defacing algorithm based on object detection and deep learning algorithms

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Abstract:

The development of mechanistic mathematical models and artificial intelligence (AI) algorithms in neuro-oncology requires the use of medical images that allow us to quantify the size and other morphological characteristics of lesions, their temporal evolution and their response to treatments. This is fundamental both for studies of brain metastases (which occur in approximately 30% of all oncology patients) and primary brain tumors (which account for 3% of all cancer deaths, approximately 3200 in Spain).

High volumes of data, if possible publicly available, are needed to develop mathematical and AI models. However, head images present the problem that patients are recognizable by their facial features, which raises ethical and data protection issues for their sharing, thus slowing down the development of predictive techniques that can be of enormous value for patients.

This talk will present an artificial intelligence algorithm developed to solve this problem, ensuring complete anonymization of the images, with quality results while keeping intact the anatomical brain structures and with calculation times that allow real-time execution of the algorithms. The resulting algorithm improves on all existing packages, which have different limitations. Open mathematical problems related to this technical development and some information on datasets that have been released with this methodology will also be presented. The result is of great interest because it transcends neuro-oncology and can be extended to other types of diseases where head imaging is used such as neuro-degenerative diseases.

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Imposition of boundary conditions for PINNs in high-dimensional nonlinear parabolic PDEs and applications

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Abstract: One of the main drawbacks in the use of neural networks to solve PDEs via PINNs methodology is the difficulty in imposing the boundary conditions. The standard approach consists of adding them as penalty terms in the training loss function. We propose a novel methodology that allows us to get rid of the heuristic choice of the associated penalty weights. It is based on defining the losses associated to the boundaries by means of the PDEs that arise from substituting the related conditions into the model equation itself. This approach is applied to challenging problems appearing in quantitative finance, namely, in counterparty credit risk management.

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On an Approximate Analytical Solution to a Problem of Radzievskij

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Abstract: In [1] we considered a problem of Celestial Mechanics posed by Radzievskij [2], namely, the problem of motion of two point masses within a homogeneous spherical cloud, supposing that the mutual interaction between these point bodies and between the bodies and the particles of the cloud is described by their Newtonian gravitational attraction. The constant density of the cloud is assumed to be sufficiently small so that the resistance of the medium to the motion of the two point masses can be neglected.

After these simplifying hypotheses, the problem of relative motion of one of the bodies with respect to the other can be recast as a perturbed Keplerian system, in which the perturbing effects are due to an attractive, conservative central force (RADZIEVSKIJ, [2]), and the constant density of the cloud can be taken as (proportional to) a small perturbation parameter.

In [1] we took different analytical approaches to the formulation and solution of this perturbed Keplerian system. In particular ([1], §7), we established the so-called *Planetary Equations in Gaussian Form* (a system of six first-order ordinary differential equations governing the time variations of the classical Keplerian orbital elements under perturbations), and obtained a first-order analytical solution, in closed form, in terms of the eccentric anomaly E as the independent variable. Such a solution allows us to identify the *first-order secular and periodic variations* undergone by the set of elliptic orbital elements at issue due to the effect of the perturbing force.

In this contributed paper we derive an alternative set of Gauss Planetary Equations, on this occasion using the true anomaly f as the independent variable, and develop the corresponding first-order solution in terms of f.

AMS 2020 Mathematics Subject Classification: 70 F 15, 70 F 05, 70 M 20.

Keywords: Celestial Mechanics, perturbed Keplerian systems, central force, Gauss Planetary Equations, true anomaly, first–order perturbations.

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Subdivision schemes based on robust regression

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Abstract: In the last years, Subdivision Schemes have been used to design curves and surfaces. Typically, they are based on two rules of refinement to obtain a regular curve or surface from some control points. The goal of this talk is to construct a new subdivision scheme using robust regression, in particular, minimizing a weighted local polynomial regression problem in ℓ^1 -norm. The result is a non-linear method with appropriate characteristics when the data presents an isolated discontinuity. Some properties as order of accuracy and stability are studied. Also, some numerical tests are performed comparing the new method with known linear and non-linear subdivision schemes.

Graph diffusion for improving nodal feature classification

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Abstract: We propose a novel approach for optimizing the topology of graph neural networks using non-linear partial differential equations based on forward-backward diffusion mechanisms [1, 3]. Our approach introduces a natural technique for node feature classification, which improves efficient construction of proximity graphs in large, high-dimensional datasets [2, 4], substantially enhancing the accuracy of k-nearest neighbor searches. To address forward-backward diffusion equations on networks, implicit-explicit schemes are explored. Forward diffusion prompts the attraction between neighbor nodes, while backward diffusion fosters repulsion among distant nodes, leading to an effective data clustering method.

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Non-linear Moving Least Squares method and applications

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Abstract: The approximation of noisy data is a long-standing challenge in various fields, including computer-aided geometric design, solving partial differential equations numerically, and designing curves and surfaces. Existing methods work well for continuous data, and moving least squares, a popular technique in statistics and applied mathematics, is a successful example. However, these methods can suffer from unwanted effects like the Gibbs phenomenon when discontinuities are present in the data.

This talk proposes a novel approach that combines moving least squares with the well-established WENO (Weighted Essentially Non-Oscillatory) scheme. This hybrid method aims to create a non-linear operator that delivers improved approximations near discontinuities while maintaining accuracy in smooth regions. We will explore its properties in multiple dimensions and validate the theoretical findings through numerical experiments

Non-linear Partition of Unity method

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Abstract: Kernel-based schemes are used in many applications, such as machine learning or regression. One of their principal advantages is their easy implementation in several dimensions. However, these methods present some problems due to their computational cost when a large number of data is used. In order to solve this disadvantage, Partition of Unity method is presented, see e.g. [1], as an efficient solution. It consists in dividing the domain in some patches and solving a small interpolation problem for each of those subdomains. Finally, a convex combination of these solutions is applied. In this work, we modify the last part of this algorithm introducing a non-linear procedure based on the well-known WENO method, see e.g. [2]. The result is a non-linear interpolation technique with accurate results when the data presents isolated discontinuities or strong gradients. Some numerical experiments are performed to check the theoretical properties.

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