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Contents

Plenaries

Plenary Talk

Mathematical Analysis of Stratified Fluids

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Under appropriate averaging, most of the Earth's ocean can be considered a stably stratified fluid, whose dynamics are described by fluctuations around a mean background density profile which increases with depth (stable stratification). Stably stratified fluids are an approximation of non-homogeneous density flows that is simple enough to allow the application of mathematical analysis and PDE theory, and at the same time rich enough to capture the underlying physics in several contexts. We will be interested in the analysis of a system of PDEs modeling continuously stratified fluids under the influence of gravity.
I will present some mathematical results related to (in)stability and long-time dynamics.

Aggregation-Diffusion Equations for collective behaviour in the sciences

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Many phenomena in the life sciences, ranging from the microscopic to macroscopic level, exhibit surprisingly similar structures. Behaviour at the microscopic level, including ion channel transport, chemotaxis, and angiogenesis, and behaviour at the macroscopic level, including herding of animal populations, motion of human crowds, and bacteria orientation, are both largely driven by long-range attractive forces, due to electrical, chemical or social interactions, and short-range repulsion, due to dissipation or finite size effects.

Various modelling approaches at the agent-based level, from cellular automata to Brownian particles, have been used to describe these phenomena. An alternative way to pass from microscopic models to continuum descriptions requires the analysis of the mean-field limit, as the number of agents becomes large. All these approaches lead to a continuum kinematic equation for the evolution of the density of individuals known as the aggregation-diffusion equation. This equation models the evolution of the density of individuals of a population, that move driven by the balances of forces: on one hand, the diffusive term due to spreading of the population, where individuals escape high concentration of individuals, and on the other hand, the aggregation forces due to the drifts modelling attraction/repulsion at a distance.

The aggregation-diffusion equation can also be understood as the steepest-descent curve (gradient flow) of free energies coming from statistical physics. Significant effort has been devoted to the subtle mechanism of balance between aggregation and diffusion. In some extreme cases, the minimisation of the free energy leads to partial concentration of the mass.

Aggregation-diffusion equations are present in a wealth of applications across science and engineering. Of particular relevance is mathematical biology, with an emphasis on cell population models. The aggregation terms, either in scalar or in system form, is often used to model the motion of cells as they concentrate or separate from a target or interact through chemical cues. The diffusion effects described above are consistent with population pressure effects, whereby groups of cells naturally spread away from areas of high concentration.

This talk will give an overview of the state of the art in the understanding of aggregation-diffusion equations, and their applications in mathematical biology.

Large Scale Computational Systems Biology in Cancer Genomics and Onco-Immunology

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The availability of high throughput technologies in the life sciences, particularly molecular biology, allows pursuing significant biomedical discoveries by associating molecular features to biological status and phenotypes such as stage and type of diseases, prognosis, and response to therapies, and others. The research in Computational Biology plays a fundamental role in this contest. In particular, the development of novel computational algorithms and the recent technological advances in statistical machine learning methods can be considered the main game-changers for better understanding diseases and leveraging large-scale datasets' availability. The bioinformatics research workflow aims to develop novel data analysis strategies and tools that allow identifying of novel candidate hypotheses, such as drivers of tumor progression, main mediators of cancer states, markers of response to therapies etc. which guide the selection of validation experiments. The results of experiments, on the other hand, guide the selection of suitable profiling platforms and analysis tools that can be used to validate in independent external datasets, the results obtained in-house. I will focus on recent computational approaches to dissect the immunological features of tumors that can be used to predict response to immune therapies and to understand the role of the interaction between tumor cells [1] and their microenvironment [2] using single cell data.

References

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Plenary Talk

Meshfree Approximation: from Interpolation to ML/AI Applications

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Over the last years meshfree methods have been gaining more and more importance and recognition from applied mathematicians and engineers since they are powerful and effective numerical tools that enable us to solve various types of problems in approximation theory and in the field of integral and differential equations. In particular, meshfree methods involving the use of radial kernels have constantly being studied and developed to effectively model science and engineering problems. Such methods can indeed be easily implemented even in high dimensions and with complex domain geometries, and can also get high convergence orders. Moreover, the Partition of Unity Method, performed with local radial kernel approximants, has been proved to be an effective tool for solving large scattered data interpolation problems and it is nowadays a popular technique for solving partial differential equations [2]. In this talk some recents results about efficiency and accuracy of the method will be reviewed and new applications to AI/ML will be proposed [1].

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Reduced Order Modelling in Computational Fluid Dynamics: state of the art, challenges and perspectives

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We do provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD).
Recent developments involve a better integration of emerging topics with model reduction, such as high performance computing (HPC), uncertainty quantification (UQ), data science (DS), machine learning (ML) in a data driven perspective, in order to allow a better exploitation of digital twins.
All the previous aspects are quite relevant – and often challenging — when well integrated also in CFD problems, including turbulence, to focus on real time simulations for complex parametric industrial, environmental and biomedical flows, or even in a flow control/inverse problems setting with data assimilation.
Crucial aspects to be addressed are related with uniqueness, stability, accuracy, as well as reliability of solutions. Some model problems will be illustrated by focusing on few benchmark study cases, for example on fluid-structure interaction problems and/or on shape optimisation, applied to some industrial and applied science problems of interest.

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[1] G. Rozza, G. Stabile, F. Ballarin, Eds. *Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics*, CSE series, Vol. 27, 2022, SIAM Press, Philadelphia, US: 20 Chapters co-authored with SISSA mathLab researchers and collaborators.

Plenary Talk

Some results on morphoelastic evolution

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Growth is a fundamental process that occurs not only in biological systems but also finds relevance in various technological applications, such as additive manufacturing. The interaction between growth and mechanics in deformable bodies gives rise to a wealth of mathematical questions.

In my talk, I will provide an brief overview of the fundamental concepts of morphoelasticity, namely, the theory of elastic deformations in growing bodies. In contrast to classical mechanical systems, the reference state of a growing body evolves over time in response to external stimuli and stress. In some cases, this calls for a free-boundary formulation, for the actual shape of the undeformed body is also unknown.

I will discuss two distinct scenarios: bulk growth and surface accretion, each posing distinctive challenges. The focus will be the development of a variational framework that enables the existence of three-dimensional quasistatic morphoelastic evolutions.

This is work in collaboration with Elisa Davoli (TU Vienna), Katerina Nik (University of Vienna), and Giuseppe Tomassetti (Roma 3).

Plenary Talk

Can math be useful for current environmental challenges? Insights from a survey of recent case studies.

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Modeling plays an important role in science. Here we focus on some relevant environmental applications.
Biological control of pests in agriculture has always represented a major problem for farmers, but nowadays becomes prominent. Repeated and continuous chemicals spraying has indeed also very negative side effects on human health, because through the food web, these poisons ultimately arrive on our tables and next into our bodies.
A new phenomenon originated by global mobility is that part of these pests are alien; they are not only insects, but also vertebrates. These invasive animal species at our latitudes outcompete the the native fauna by direct interaction and possibly also by carrying alien pathogens. They thus contribute to reducing biodiversity. This phenomenon is favored also by the ongoing climatic changes, representing a current challenge of paramount importance for humanity. A glimpse on their possible gloomy consequences will be taken, to illustrate how often our "linear" way of thinking underestimates them.
On a more positive side, employment of some other resources, such as fungi, is becoming relevant in diverse applications: modeling of their use for industrial wastewaters depuration processes as well as antagonists of plant diseases in agriculture are illustrated. To conclude with a more optimistic topic, a small success in an epidemiological farming situation is presented.

Minisymposia

MS01 - PDEs and Applications

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ABSTRACT

PDE models arise in a variety of real-world applications. Usually, they are derived through microscopic approaches or from fundamental physical laws. These models often exhibit an underlying challenging structure and provide new directions for mathematical research. The main objective of this minisymposium is to bring together experts in PDE analysis and modeling, focusing on several topics of interest, such as

- *conservation laws with a spatial-dependent flux and Hamilton-Jacobi equations with a spatial-dependent Hamiltonian;*
- *modeling of a gas flow through a one-way valve;*
- *a model describing two competing populations, given by a nonlocal conservation law for predators coupled with a parabolic equation for prey;*
- *nonlocal conservation laws, arising in traffic flow and supply chains;*
- *results on the derivation of 1D conservation laws via ODEs systems of deterministic particles interacting via follow-the-leader interactions;*
- *radiative transfer equation for cell tracking, with uncertainty in the geometry and possible sparse controls.*

The presentations will include mainly analytical but also computational advances. The speakers will report recent progress, exchange ideas, and highlight novel analytical problems.

Evolution of populations structured by dietary diversity and starvation: cross-diffusion systems

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Cross-diffusion systems are nonlinear parabolic systems, modeling the evolution of densities or concentrations of multicomponent populations in interaction. In this talk, we study the existence and regularity of weak solutions of a triangular cross-diffusion system, driven by a dietary diversity. Concerning the existence result, we rigorously prove the passage from an approximating Lotka-Volterra reaction-diffusion system with linear diffusion towards a cross-diffusion system at the fast reaction limit. The approximating system models the competition of two species, when one species has a more varied diet than the other one. The resulting limit gives a cross-diffusion system of starvation-driven type. The main tools used to rigorously pass the limit consist of a priori estimates, given by the analysis of an entropy functional, and compactness arguments. Moreover, we also investigate the regularity of the obtained solution, by improving the entropy a priori estimates with the use of a bootstrap argument. This work is based on [1, 2].

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Space Dependent Hamilton-Jacobi Equations & Conservation Laws

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The focus of this presentation is on conservation laws and Hamilton-Jacobi equations in the scalar, one dimensional, space dependent case.

First, a single framework is identified where, without any convexity assumption, the Cauchy problems for both equations are well posed and equivalent. The setting introduced in [3] is extended to the x–dependent case as considered in [4]. Instrumental, in the case of conservation laws, is the construction of a *"foliation"* consisting of $\mathbf{L}^\infty$ stationary solutions, i.e., possibly with unbounded total variation. Thus, they may well display infinitely many stationary and entropic shocks.

Then, in the convex case, we solve the *"inverse design"* problem, which consists in the characterization of the attainable sets and of those initial data that develop into a given profile. Finally, an explicit example shows the deep, somewhat counter intuitive, effects of the x dependence. Refer to [3] for the details.

References

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Modeling and management of fluid flows in pipelines with valves

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The aim of this talk consists of reviewing some recent advances in the mathematical modeling of fluid flows through pipes in presence of valves [1]–[5]. This subject falls into the more general framework of analyzing coupling conditions among different set of equations.

The flow is usually modeled by the isothermal Euler equations, even if more general systems can be considered. A fundamental step in the modeling is the study of *constrained* Riemann problems, which occur at the valve position; the constraint depends on the features of the valve under consideration.

A key feature is the appearance of *chattering*, i.e., the rapid switch on and off of the valve at some critical states. We provide both analytic and numerical evidence of this phenomenon and show how it is theoretically possible to eliminate it by redesigning the valve.

References

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Cell Tracking for the Radiative Transfer Equation

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We are interested in cell tracking using the radiative transfer equation and medical images. This problem will be formulated as an optimization problem with respect to a possibly high-dimensional partial differential equation. We will solve it using a consensus-based global optimization algorithm. In particular, we will optimize and simultaneously simulate the partial differential equation forward in time. Numerical results will be presented.

Nonlocal conservation laws with p-norm, the singular limit problem and applications in traffic flow

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We investigate nonlocal conservation laws where the nonlocal operator is not integrating the solution in L^1 but in L^p for $p \in (1, \infty)$. We show existence and uniqueness of weak solutions and a maximum principle when the initial datum is bounded away from zero. We also demonstrate that solutions exist for the more general case and turn our attention then to the singular limit problem, i.e., whether the entropy solution of the corresponding local conservation law can be recovered when the nonlocal kernel converges to a Dirac measure. And indeed, under rather general assumptions Oleinik's entropy condition holds, proving the claim. We conclude with some numerical illustrations.

Conservation laws with discontinuous flux and traffic modeling

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We provide an overview of results on the derivation of 1D conservation laws via ODEs systems of deterministic particles interacting via follow-the-leader interactions. The main motivation behind this problem arises in traffic flow and pedestrian modelling. We present results on the derivation of entropy solutions of the Cauchy problem of the LWR model [5] and later extensions of this result on problems with Dirichlet boundary data [3] and on similar models such as the ARZ model [2] for traffic flow and the Hughes model [1, 4] for pedestrians. The results are joint with B. Andreianov, M. Di Francesco, S. Fagioli, G. Russo and G. Stivaletta.

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On a class of mixed non linear and nonlocal hyperbolic–parabolic systems

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We consider two competing populations characterised by their densities, and describe their evolution and interactions through a system of PDEs. In particular, the first population, the predators, evolves according to a non linear and non local hyperbolic equation. Indeed the movement of predators is directed towards the regions where the concentration of the other population is greater. This is modelled by a non local and non linear function of the other population's density. The second population, the prey, is assumed to diffuse according to a parabolic equation. The source terms of the two equations generalised Lotka–Volterra equations, including also control functions.
This class of mixed systems is motivated by the description of predator–prey dynamics, and provides a usable structure for the search of an optimal control strategy in biological pest control problems.
We present both analytical results regarding the well posedness of this class of systems as well as numerical simulations, which give insight into the qualitative properties of the solutions.

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MS02 - Mathematical modelling and control for healthcare and biomedical systems

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ABSTRACT

Mathematical models and computer simulations are playing an increasingly important role in medicine, since they represent a useful tool to complement theoretical and experimental work. Moreover, models pave the way for investigating control problems consisting of personalized approaches for patient treatment. Smart healthcare and medical devices have become common in clinical everyday use. Popular examples include insulin pumps, inhalers and ventilators for breathing conditions, as well as implants, microcapsules and nanoparticles for drug delivery. Many of these technologies are controlled drug delivery systems, combining a platform or a carrier with a drug to be delivered efficiently to a target tissue or organ, while maintaining the dose within a therapeutic window. While many have achieved successful results clinically, there remain a number of scientific and technological challenges and an opportunity for further fine-tuning and optimization. Addressing these challenges requires multi-disciplinary approaches and competences ranging from clinical expertise and academic research to the industrial sector.

Electrical conduction and heat diffusion in composites with imperfect contact conditions

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Composite materials play an important role in the study of biological tissues and material sciences because of their wide spectrum of applications in clinical and industrial processes. In the recent years, the improvements of the industrial techniques have permitted to obtain more efficient materials constructed by assembling different constituents, whose mechanical, thermal or electrical properties are definitely superior of the ones of the single components. However, this bonding does not give rise, in general, to perfect contacts between the different components, so that discontinuities in the involved physical fields can appear.
The most common models dealing with imperfect contacts involve jumps of the solution and continuity of the flux across the interface or jumps of the flux and continuity of the solution. Also, in some of these models the Laplace-Beltrami operator appears, due, for instance, to the presence of highly conducting interfaces. More recently, models which exhibit simultaneously jumps in the solution, jumps in the flux and the Laplace-Beltrami operator, have been proposed in the engineering context and some of them involve also a new operator, i.e. the mean average of the physical fields representing the different phases. The purpose of this talk is to present some models with imperfect interfaces which origin in the description of composites made by a hosting medium containing a periodic array of inclusions of size ε, where the inclusions are coated by a thin layer consisting of two sublayers of different materials (with thickness of the order $\varepsilon\eta$ and $\varepsilon\delta$, respectively), disposed in such a way that one of them is encapsulated into the other ([1, 2, 3]). This two-phase coating material is such that one of the two components has a low diffusivity in the orthogonal direction and the other one has a high diffusivity in the tangential direction. All the parameters ε, δ and η are supposed to be very small, but with different orders. In particular, the smallness of δ and η, with respect to ε, leads us to perform, for fixed ε, a two-step concentration procedure, which produces on the resulting interface between the hosting material and the inclusions some conditions involving the jump and the mean value of the two bulk potentials and the jump of their fluxes. Moreover, also the appearance of a new surface heat potential can happen ([3]). The concentrated problems thus obtained are then homogenized, i.e. we let ε tend to zero, and we briefly discuss the different resulting models.

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[3] M. Amar, D. Andreucci, C. Timofte *Interface potential in composites with general imperfect transmission conditions*, submitted (2023).

Stochastic differential modeling of oscillatory biological mechanisms: the circadian rhythm model in *Drosophila*

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Shedding light on the oscillatory mechanisms occurring in some relevant complex biochemical processes is an intriguing challenge. Here we focus on such topic by modeling, with a stochastic approach, the biological process of the circadian clock. In almost all living organisms, countless molecules synchronize their dynamic behavior to produce periodic oscillations observable at the macroscopic level, with a period close to 24 hours. The main biochemical process from which these oscillations originate is the negative self-regulation exerted by the so-called *clock protein* on the expression of its gene [1], [6]. In this framework, in a previous work [4] we proposed a stochastic model governed by Chemical Master Equations (CMEs) [5] for the central biochemical mechanism of circadian rhythm in *Drosophila* which is based on the negative autoregulation exerted by the PER clock protein alone [2], [3]. In this work, we provide a possible extension of the stochastic approach by using stochastic differential equations (SDEs) which, on the one hand, overcome the curse of the dimensionality of the discrete-state CME approach and, on the other hand, preserve (by means of an approximate formulation) the stochastic nature of the phenomenon under study.

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Cell motion in response to mechanical stimuli: a single-cell non-local model

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Directed cell migration is fundamental in many physiological and pathological processes as organogenesis and tissue reparation, or tumor growth and invasion. It is thereby one of the phenomena that mostly attract the interest of researchers. In particular, experimental results highlighted that the migration of a cell is strongly affected by different types of cues, e.g., chemical or mechanical signals. Cell migration due to chemical signals, i.e., chemotaxis, has been widely studied in the past. Conversely, cell dynamics driven by mechanical stimuli such as the stiffness (*durotaxis*) or the stress/strain (*tensotaxis*) of the underlying substrate, are not completely clear from a biological point of view.
In this regard, inspired by the integro-differential model proposed in [1], we propose a general mathematical framework to investigate single-cell migration due to mechanical stimuli. Specifically, a cell is represented as a point particle characterized by its position and two further quantities describing cell polarization direction and motility. These quantities evolves according non-local integro-differential equations accounting for cell capacity to sense the mechanical properties of the substrate around its actual position (non-locally). An additional stochastic term implements random Brownian crawling typical of cell dynamics. The above general model can be then specified in order to reproduce cell dynamics driven by either durotaxis or tensotaxis, by properly defining the mechanical stimulus to be integrated in the equation of motion.
In this respect, we will show different numerical simulations that qualitatively reproduce different experimental scenarios, thereby validating the proposed model. Specifically, in the case of durotaxis, we consider different patterns of substrate stiffness defined according to experimental scenarios described in literature. Conversely, in the case of tensotaxis, substrate stress and strain are computed by assuming that the extracellular matrix behaves as a hyperelastic Yeoh's solid, and dealing with small deformations of inspired by the experimental literature.

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A Computational Aortic Hemodynamics model to study Transcatheter Aortic Valve Degeneration

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Transcatheter Aortic Valve Implantation (TAVI) is a minimally invasive procedure for the replacement of a stenotic aortic valve with a bio-prosthetic device. Assessing the long-term performance of TAVI valves is still an open question due to a lack of follow-up data. In particular, valve durability can be drastically reduced by an early onset of Structural Valve Deterioration (SVD) that can lead to valve failure [2].
The idea behind this project, which builds on top of [1], is to employ a Computational Fluid Dynamics (CFD) approach to study post-TAVI aortic hemodynamics in order to increase our knowledge regarding SVD. In particular, the aim is to discriminate among patients with SVD (degenerated) and patients without SVD (non-degenerated) at follow-up examination. Monzino Cardiology Centre provided us with a database of TAVI receivers with follow-up data. Patient-specific post-TAVI computational domains are generated starting from pre-TAVI CT scans by inserting a virtual bio-prosthetic valve in the segmented geometries. CFD simulations are then carried out in order to identify hemodynamics indicators allowing to discriminate between the two subsets of patients.
We solve the hemodynamic problem by means of Finite Elements using the library life^x, developed at MOX laboratory within iHeart European project (https://iheart.polimi.it/en/it/). A physiological flow rate is imposed inside the aorta, valve leaflets in open and closed configurations are managed with Resistive Immersed Implicit Surface method and turbulence is accounted for by using a Large Eddy Simulation model.
CFD results show that degenerated patients are characterized by great shear stresses on the aortic wall, a highly chaotic flow inside ascending aorta and oscillating shear stresses on the bio-prosthetic valve leaflets. Thus, by scoring each patient with respect to these indicators we are able to clearly separate the two subsets of patients
The presented CFD approach could be employed before TAVI procedure in order to assess its feasibility and could assist clinicians in planning patient-specific follow-up exams based on the risk of valve failure due to an early onset of SVD.

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The role of fractal surfaces in diffusion phenomena

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We will present some recent result on diffusion across fractal surfaces [1]. These irregular geometrical objects are good tools to model many physical phenomena which take place across irregular interfaces. The results are part of an ongoing project with M. Cefalo, S.Creo and J.Rodriguez Cuadrado.

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Alternative approaches in the modelling and control of tumour growth and treatment

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The mathematical modelling of tumour growth and treatment offers a fundamental tool for investigating the effects of antitumour drugs, as well as for designing efficient and personalized therapies. Although mechanism-based approaches are usually exploited to build up tumour models, an alternative approach grounded on the formalism of Chemical Reaction Networks (CRN) has been recently proposed by Drexler et al., (2019) [2]. In this note we generalize the proposed CRN-based approach in order to provide a double characterization, deterministic vs stochastic, of the system, which is useful for targeting different investigation issues. Indeed, the advantage of the CRN is that it can be straightforwardly translated both in a stochastic framework, by exploiting the Chemical Master Equation (CME) tool that is able to account for the inherent random fluctuations of the network chemical players, and in a deterministic framework, by means of the usual ODE models that can be viewed as linear approximations of the average dynamics coming from the CMEs [1]. The double approach is here applied to a minimally parametrized and low-dimensional model of tumour growth and treatment, showing by means of numerical simulations that the deterministic framework is definitely appropriate to characterize the system behaviour whenever the number of tumour cells is very high, so allowing to design deterministic control strategies. In particular, we analysed two alternative deterministic control approaches: the first one assumes a constant drug administration, while the second one exploits a state-feedback control scheme, with complete or partial knowledge of the state [3]. The results obtained show the advantages and the limitations of both the proposed strategies, highlighting also that the tumour size at the beginning of the therapy can play a role of paramount importance in the treatment outcome.

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Personalized computational modeling of myocardial perfusion in coronary artery disease

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Introduction - Quantitative assessment of coronary blood flow and myocardial perfusion is of critical importance in the prognostic stratification of patients with coronary artery disease. Despite the high potential of computational models to this aim, many issues remain to be addressed to use them in a predictive way, such as model personalization and capture of the interplay between ventricle contraction and coronary flow [1]. Here, we propose a multiscale framework to run simulations of hyperemic coronary blood flow up to the microvasculature, with novel elements to address these issues. *Methods* - Patients anatomy is reconstructed through 3D segmentation of CT angiographic images. The multiscale perfusion model is an evolution of what we proposed in [2] and features a 3D description of blood dynamics in the epicardial arteries, coupled with a multicompartment Darcy formulation for the microvasculature, including a treatment for microvessels compliance and ventricular contraction. Tailored hyperemic pressure boundary conditions are built using routine clinical measures. Blood flow simulations are run in 8 patients using the Finite Elements software LifeX, developed at MOX - Mathematics Dep. (PoliMi) during the iHeart project (https://iheart.polimi.it/en/it/) and their predictive power is assessed through direct comparison of quantities of clinical interest (Fractional Flow Reserve FFR and Myocardial Blood Flow MBF) with the outcomes of the respective clinical exams. *Results* - Characteristic phasic flow patterns with high arterial inflow in diastole, mainly diastolic perfusion and high venous outflow in systole are recovered. MBF maps show significantly higher values in patients with non-significant stenosis i.e. $FFR > 0.8$ (mean MBF = 2.89 ml/min/g) compared to patients with at least one lesion with $FFR < 0.8$ (mean MBF = 1.83 ml/min/g). Perfusion defects associated with such lesions were also highlighted in the obtained maps. FFR results show excellent agreement with the invasive values, with per-vessel sensitivity and specificity of 95.8% and 100% respectively. MBF results show good agreement with clinical values, although we notice a slight MBF overestimation MBF in ischemic myocardium.

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Modelling smart drug delivery with functionally graded materials

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Technological advances over the past decades have led to the development of sophisticated drug delivery devices that enable targeting and control of drug delivery [1]. A better controlled and personalized release is often desired and many new technologies and strategies are being developed to try to address this objective.
Recently, more attention has been paid to functionally graded materials (FGMs), a variety of composite materials in which the constitutive properties vary smoothly and continuously from one region to another [2].
Through a mathematical mechanistic model and a simulation approach, we explore the potential of FGMs as a new class of controlled drug delivery materials, in the attempt to establish whether varying shape material properties can provide an advantage over homogeneous or layered media. We develop a continuum model to describe drug transport within, and release from, a FGM drug-eluting stent system. A numerical solution is presented and the differences and the potential of functionalized release over a homogenous stent coating are outlined.

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MS03 - Recent Advances on the mathematical and numerical modeling of epidemics

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ABSTRACT

This minisymposium is devoted to the mathematical and numerical modeling of epidemics and aims at presenting an extensive overview of the recent advances in mathematical epidemiology, focusing, in particular, on the contributions of early career researchers. The problems addressed, that were often inspired by the recent Covid-19 pandemic, range from theoretical analysis, to the development of computational methods, including (but not limited to) spatio-temporal models, optimal control problems, parameter estimation techniques, data-driven and machine learning approaches.

Two epidemic models with cautionary response in the presence of asymptomatic individuals

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Mathematical models for the spread of infectious diseases date back almost a century. From the early classical models with no demographics, fixing in size the population at risk, the subject evolved to encompass size-varying populations. The COVID-19 epidemic has highlighted an essential feature of transmissible diseases. Namely, asymptomatics play a relevant role. In fact, in the earlier phases of this pandemic, the spread was mainly due to contact among susceptibles and asymptomatic infected.

From a theoretical point of view, we investigate the transmission of a generic disease appearing in two forms, asymptomatic and symptomatic, accounting for demographics. The main feature is the epidemic-induced fear of the population that reduces contacts, responding to increasing symptomatic numbers. Essentially, we consider a variation of the classical SI infection model, in which asymptomatic individuals are also accounted for, by splitting the infected into asymptomatics and symptomatics. The latter, however, are assumed to be isolated; therefore, it can also be interpreted as a SIR model. In such a view, the third class denotes those individuals removed from circulation who are no longer spreading the disease rather than those who recovered from the illness. We propose two versions: without and with vertical transmission.

In case of a high progression rate from asymptomatic to symptomatic, the proposed SAI models can preserve some susceptibles from the contagion. The main findings of this investigation show that in the presence of asymptomatic individuals, people voluntary means to reduce their possible contagion must be undertaken more strictly, by suitably lowering the overall transmission term, than in the case where the epidemic symptoms are immediately manifested. The results also elucidate the importance of assessing transmission rates as quickly as possible.

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Solving inverse and forward problems of multiscale epidemic spread with neural networks

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The purpose of this talk is to discuss some new achievements in the mathematical modeling of epidemic events employing kinetic equations and their numerical solution using physics-informed machine learning approaches.
To account for spatial heterogeneity, the spatial spread of an infectious disease can be described by a class of multiscale systems of partial differential equations, in which a portion of the population acting on an urban scale exhibits parabolic diffusive behavior and the remainder, acting on an extra-urban scale, exhibits a hyperbolic transport mechanism [4]. The model parameters necessary to mimic the dynamics of the virus of interest necessitate a delicate calibration phase, which is frequently made more difficult by the unavailability and uncertainty of data from official sources [2]. Furthermore, determining the problem's initial and boundary conditions is usually challenging.
In this context, Asymptotic-Preserving Neural Networks (APNNs) for hyperbolic transport models of epidemic spread are designed to solve the inverse problem (of estimating model parameters) and the forward problem (of predicting epidemic evolution) despite sparse and incomplete observed data, and without losing the ability to describe the phenomenon's multiscale dynamics, thanks to an appropriate asymptotic-preserving (AP) formulation of the neural network loss function [1, 3].
A series of numerical experiments accounting for different epidemic dynamics validates the proposed technique, emphasizing the relevance of the neural network's AP feature for the study of multiscale systems, particularly when partially observed.
This work is part of a collaboration with Lorenzo Pareschi (University of Ferrara), Chuan Lu and Xueyu Zhu (University of Iowa).

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PREDATORS AS A POSSIBLE STRATEGY FOR CONTROLLING A *XYLELLA FASTIDIOSA* EPIDEMIC

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In Southern Italy, since 2013, there has been an ongoing Olive Quick Decline Syndrome (OQDS) outbreak, due to the bacterium *Xylella fastidiosa*, which has caused a dramatic impact from both socio-economic and environmental points of view. Current agronomic practices are mainly based on uprooting the sick olive trees and their surrounding ones, with later installment of olive cultivars more resistant to the bacterium infection. Unfortunately, both of these practices are having an undesirable impact on the environment and on the economy. Here, a spatially structured mathematical model has been proposed to include a predator *Zelus renardii* as a possible biocontrol agent of the *Xylella* epidemic. The fact that *Z. renardii* has been reported to be a generalist predator implies that its introduction is not an efficient control strategy to eradicate a *Xylella* epidemic. Instead, a specialist predator, whenever identified, would lead to the eventual eradication of a *Xylella* epidemic. In either cases it has been confirmed that a significant reduction of the weed biomass can lead to the eradication of the vector population, hence of a *Xylella* epidemic, independently of the presence of predators.

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A numerical method for the stability analysis of linear age-structured models with nonlocal diffusion

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Nonlocal diffusion problems can be formulated as linear integro(-partial) differential equations in which the diffusion term is represented by a convolution operator. On the one hand, compared with Laplace diffusion, nonlocal diffusion is more suitable to describe many biological and physical phenomena [3]. On the other hand, the local stability analysis of models with nonlocal diffusion is more challenging since the associated semigroups are not eventually compact [2]. Nevertheless, for linear age-structured models with nonlocal diffusion, *i.e.*, population models depending on time, age and spatial position, it can be shown that the asymptotic behavior of the semigroup is determined by the spectral abscissa of its infinitesimal generator. The spectrum of the latter typically needs to be approximated numerically due to the infinite dimension of the state space. In this talk we present a method based first in reformulating the problem via integration of the age-state and then on discretizing the generator via spectral projection in space and pseudospectral collocation in age [1]. Numerical tests showing expected convergence properties are presented.

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Optimal control on a kinetic epidemic model with uncertain social features

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The transmission of infectious diseases is greatly influenced by variations in social interactions among individuals. However, due to limited data and the varying statistical characteristics of these interactions over space and time, it becomes challenging to develop effective control strategies that mimic the impact of non-pharmaceutical interventions. In this research, we employ a recently developed kinetic model for studying the dynamics of epidemics, which takes into account both the influence of social contacts and the uncertain nature of contact formation. By analyzing the effects of an optimal control strategy using traditional methods of kinetic theory, and integrating uncertainty quantification techniques, we evaluate the impact of social limitations. Through the use of available data, we illustrate the efficacy of our proposed targeted measures in reducing uncertainties and mitigating the spread of epidemics.

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Understanding and Controlling COVID-19 classical methods for current challenges

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The seminal work of Kermack and McKendrick (1927) has consistently influenced the mathematical modeling of epidemics since about one century and their celebrated model is still the basis of any attempt to understand the spread of infectious diseases and to also recommend control/mitigation interventions.
The specific forms of the COVID-19 pandemic, evolving into a sequence of growth vs control phases, requires attention to the interplay of the different factors that determine the course of an epidemics. Thus the basic model needs to be endowed with mechanisms able to produce the different epidemic waves and phases according e.g. to non pharmaceutical measures (social distancing, testing and tracing, etc.), vaccination, onset of virus variants.
In a series of papers ([2, 5]) we tuned the classical version of the Kermack-McKendrick model to address the description and analysis of multi-phasic epidemics. In our model, the infection dynamics is governed by an age-since infection epidemiological equation including a role of the vaccination campaigns ([2],[4]). The analysis of selected sub-cases, using specific infectiousness and recovery kernels allowing reducibility, leads to draw simple O.D.E and D.D.E sub-models to be parsimoniously fitted to data. The framework is applied to the COVID-19 epidemic in Italy since its very beginning (March 2020) up to the onset of the Omicron variant. The model provides an excellent reproduction of the overall story of the pandemic by minimal parametrization, confirming the validity of the multi-phasic epidemic concept.
Finally, classical methods of optimal control allow to investigate optimal strategies based on distancing and vaccination ([3],[5]). An ad-hoc computational tool is set up to minimize a cost function combining both direct and indirect costs of the epidemic and to compare the resulting optimal strategy with the one emerging from the Italian response data.

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Modelling the role of individuals' viral load in the spread of infectious diseases

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In classical epidemic models, a neglected aspect is the heterogeneity of disease transmission and progression linked to the viral load of each infected individual. In the present talk I will present some models allowing to investigate the interplay between the evolution of individuals' viral load and the epidemic dynamics from a theoretical point of view. We propose a stochastic particle model describing the infection transmission and the individual physiological course of the disease. Agents have a double microscopic state: a discrete label, that denotes the epidemiological compartment to which they belong and switches in consequence of a Markovian process, and a microscopic trait, measuring their viral load, that changes in consequence of binary interactions or interactions with a background. Specifically, we consider Susceptible–Infected–Removed–like dynamics. Then, we shall consider two models: in a first model infectious individuals may be isolated and the isolation rate may depend on the viral load–sensitivity and frequency of tests; in a second model the transmission rate may depend on the viral load. I will present a derivation of kinetic evolution equations for the distribution functions of the viral load of the individuals in each compartment, whence, via upscaling procedures, we obtain macroscopic equations for the densities and viral load momentum. A qualitative analysis of the ensuing macroscopic model will be peformed. Finally, I will present some numerical tests.

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After COVID-19: remarks on pandemic control

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The COVID-19 pandemic has clearly highlighted the frailty of modern public health systems with respect to pandemic events. The post-pandemic review process of the failures occurred in COVID-19 control at many different levels and scales (e.g., [3]) is just initiated. My departure point is that the COVID pandemic, though dramatic, has not been the "the worst of the worst", which would be represented by a pathogen combining short generation and doubling times, thereby making contact tracing (even digital) largely ineffective, with high mortality rates among young and young-adults. This will require a take-off of future "preparedness science", going beyond merely technical aspects and promoting equitable interventions by considering fully new dimensions such as holism and sustainability in societal protection, within and between countries solidarity. Based on previous motivations, in this talk i depart from the centrality of social distancing to make an attempt to link together and unify a number of policy keywords and modeling bits that will be key in future pandemic preparedness. Among these, i will discuss the (unavoidably) multi-phasic nature of pandemic outbreaks [2], the role of optimal control in preparedness plans, the possible ambiguities of tiers-based response policies [1], the role of behavioural responses and policy resistance at different societal scales, and the critical issue of defining a truly optimal governmental responses capable to align with the responses coming from different societal layers.

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On the control of SEIR models in epidemiology

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The study of SEIR-type models has been largely developed in literature to examine the evolution of an epidemic [3]. We use the SEIR model as the basis to develop a control approach, i.e. to develop strategies to control the spread of the disease and to define optimal strategies to be applied. We consider two main ingredients: vaccination and restrictive measures. The final goal is to have a rather flexible model to mimic different scenarios, in order to evaluate both the effects and the costs of various choices.
We will compare two numerical methods to compute the control policy, highlighting their pros and cons, not only from the computational point of view, but also from the modelling one. The first is based on Dynamic Programming [1]. In this theory, the value function plays a crucial role and it is characterised as the unique viscosity solution [2] of a first order partial differential equation of Hamilton-Jacobi type. Clearly, the solution of this equation needs the development of ad-hoc numerical methods [4] because of its non-linearity and of the non-regularity of the solution. Once the value function is calculated, one can obtain the optimal control laws in *feedback* form. The other approach is based on Pontryagin's principle [5]. Using some basic tools from calculus of variations, one can obtain a system of ordinary differential equations coupled with an optimality condition, that leads to the calculation of controls in *open-loop* form.
We will briefly sketch the two approaches and describe via several examples how and when they can be applied in the framework of epidemiological modelling. Several aspects will be discussed, including e.g. the presence of a constraint on the Intensive Care Units, vaccine availability, incoming individuals from abroad.

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Novel methods for the analysis of household-stratified infection data

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Households are well known to be amplifiers of transmission of respiratory pathogens, due to the intimate and stable nature of contacts within them. Household-stratified epidemiological data can be seen as a collection of repeated "transmission experiments" that naturally lends itself to parameter estimation. With the explosion of data collection caused by the pandemic, household studies are only likely to become more common in the future. I will discuss available methods and the novel extensions we had to develop to adapt them in real time to the household datasets collected during the pandemic [1]. Among such datasets, I will focus on the ONS COVID-19 Infection Survey [2], one of the largest studies of community SARS-CoV-2 infection in the world, because its sheer size and unique design – a household longitudinal study – pose interesting mathematical and computational challenges.

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Numerical methods for time since infection models in public health

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In a deterministic, continuous-time framework, time-since-infection models for the spread of infectious diseases are described by renewal integral equations or hyperbolic partial differential equations (PDEs). Compared to the more widespread ODE compartmental models, time-since-infection models are: more flexible in the type of parameters that can be incorporated; more complete in terms of the dynamics they can reproduce; and more powerful for mechanistic modelling. I will illustrate these points with examples in the context of contact tracing [5] and waning immunity. Today, the use of time-since-infection models in public health is severely hampered by the lack of numerical methods and software, which is nowhere nearly as developed as that for ODEs. I will review some of the work done by the author and collaborators in this direction since 2016 [2] regarding the numerical bifurcation analysis of delay equations, including recent extensions to equations with infinite delay [3]. In particular, a recent approach that maps the systems to more regular spaces via integration has proven particularly convenient in the case of renewal equations [4] and PDE models with one or two structuring variables (e.g. time since infection and demographic age) [1].

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A general kinetic model for the spread of infectious diseases in continuously structured compartments

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We propose a general kinetic compartmental model for the spread of infectious diseases, wherein each compartment is structured by a continuous variable that captures inter-individual phenotypic variability [1, 2, 5]. The model comprises a system of integro-differential equations for the dynamics of the population density functions (i.e. the phenotype distributions) of the different compartments. First, we formally derive this model from an underlying stochastic model, which describes the evolutionary dynamics of single individuals. Then, we explore the connections between this general model and specific compartmental models employed in epidemiology [3, 4, 6]. Finally, we discuss possible applications of the model in different epidemiological scenarios.

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A geometric analysis of the SIRS model with secondary infections

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We propose a compartmental model for a disease with temporary immunity and secondary infections [1]. From our assumptions on the parameters involved in the model, the system naturally evolves in three time scales. The analysis of the system is performed using tools from Geometric Singular Perturbation Theory (GSPT) [2], particularly suitable to analyze systems with this time scale separation [3, 4].
We characterize the equilibria of the system and analyze their stability. We find conditions for the existence of two endemic equilibria, for some cases in which $\mathcal{R}_0 < 1$. Then, we unravel the interplay of the three time scales, providing conditions to foresee whether the system evolves in all three scales, or only in the fast and the intermediate ones. We conclude with numerical simulations and bifurcation analysis, to complement our analytical results.

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Enhanced methods for reliable predictions and for epidemic control

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The SARS-CoV-2 pandemic has involved many members of the mathematical community in different respects in order to contribute to containing the spread of COVID19. Many works aimed at establishing robust methods for making reliable forecasts, for example by coupling different epidemic models retrieving ensemble means [2]. Instead, other works focused on prescribing concrete guidelines for policy makers to optimize Non-Pharmaceutical Interventions (NPIs) or medical treatments [3]. In this context, compartmental models have played a significant role, as they have been carefully adapted to suit this specific scenario. Nonetheless, the modeling assumptions that limit the applicability of such models can often be overly restrictive and unrealistic in many real-world cases. As a result, they may lead to unreliable forecasts and predictions. In this presentation, we will discuss our latest findings regarding methodologies aimed at generating accurate and data-driven predictions. In particular, we present the $SIRDVW$ age-stratified model [3], which is a model featured in the Italian scenario of SARS-CoV-2 spread and conceived with the introduction of medical vaccinations. Moreover, we formalize an optimal control framework based on the Pontryagin's maximum principle for ODE systems with delay: we consider (1) the aforementioned model as state problem, (2) the administrations of vaccine-doses as controls and (3) the total amount of infected, deceased and hospitalized as cost functionals. Precisely, we solve a numerically-consistent inexact adjoint system reducing significantly the computational cost and preserving the accuracy. Finally, we will address some advances for data-driven models derived from Machine Learning theory [1].

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MS04 - Space-time numerical methods and applications

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ABSTRACT

The space-time (XT) paradigm is one of the most promising trends in modern numerical schemes for evolution PDEs. XT methods have existed for more than 30 years, but only in the last decade have gained wide popularity, have been applied to realistic applications, and many mathematical tools for their treatment have been developed. By interpreting the time variable as an additional space dimension, XT methods allow for high-order accurate approximations in all dimensions, parallel-in-time solution methods, and adaptive solvers. The aim of the minisymposium is to bring together experts in the field of space-time methods to foster scientific exchange and collaboration in an innovative research area.

Time-domain Boundary Elements for elastodynamic contact problems

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The presented work deals with the numerical solution of unilateral contact problems, which consider the elastodynamic stresses that a body undergoes when in contact with a rigid obstacle. The numerical investigation of such problems finds numerous applications in mechanics, from fracture dynamics and crash tests to rolling car tires.
The contact boundary conditions correspond to a variational inequality for the linear elastodynamic equations. While there is a vast computational literature on the topic [3, 5], the theoretical and the numerical analysis are widely open and restricted to simplified model problems. Boundary Element Methods (BEMs) are perfectly suited in this context [4], given that the contact is confined to the boundary while the interior dynamics is linear. In this work we introduce an Energetic BEM for such problems (see e.g. [1]). For linear elastodynamics, this approach provides an efficient and stable numerical tool, here adapted for the solution of dynamic Signorini contact problems [2].
The numerical implementation requires the assembly of E-BEM matrices, that allow an accurate discretization of the involved Poincaré-Steklov operator. An Uzawa method is used for the solution of the variational inequality, a standard iterative solver for this nonlinearity. Both theoretical and algorithmic aspects are discussed. Numerical experiments, presented for different 2D geometries, show the optimal performance of the proposed approach.

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Efficient solution of 2D wave propagation problems by a CQ-wavelet boundary element method

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We consider wave propagation problems in 2D unbounded domains, reformulated in terms of space-time boundary integral equations. For their solution, we employ a Convolution Quadrature (CQ) for the temporal discretization and a Galerkin Boundary Element Method (BEM) for the spatial one. It is known that one of the main advantages of the CQ-BEMs is the use of the Fast Fourier Transform (FFT) algorithm to retrieve the discrete time integral operators with an optimal complexity in time. Besides, it is also known that a key ingredient for the success of such methods is the efficient and accurate evaluation of the integrals that define the matrix entries associated to the full space-time discretization. This topic has nowadays been successfully addressed when standard Lagrangian basis functions are considered for the space discretization. However, for such a choice of the basis, the BEM matrices are in general fully populated, a drawback that prevents the application of CQ-BEMs to large scale problems. In [1], as a possible remedy to reduce the global complexity of the method, we have considered approximant wavelet functions. For the particular choice of the bior2.2 wavelets, we have obtained an a priori estimate of the decaying behavior in time of the matrix entries, and we have computed only the elements which are significant with respect to a prescribed tolerance. In this talk, which focuses on the results published in [2], we present a more general numerical procedure that allows the use of wavelet basis of any type and order, combined with CQ based on any stable ordinary differential equations solver. By taking advantage of the fast wavelet transform, the proposed method allows on the one hand to compute the matrix entries associated to the choice of wavelet basis functions by maintaining the accuracy of those associated to the Lagrangian basis ones and, on the other hand, to generate sparse matrices without the need of storing a priori the fully populated ones. Several numerical results, showing the accuracy of the solution and the gain in terms of computer memory saving, are presented and discussed.

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Mapped and Unmapped Tent Pitching

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Mapped Tent Pitching [1] is one of the most successful current time parallel algorithms for the parallel in time solution of hyperbolic problems. It uses the typical property of the finite speed of propagation of information in hyperbolic problems in its design and can thus not be used for parabolic problems. The algorithm is highly scalable and among the best for solving Maxwell's equations currently in large parallel architectures, see e.g. [2].
Mapped Tent Pitching needs a geometric mapping of the tents to cylindrical domains to solve the problems in the tents in parallel, and then a mapping back to physical space. These mappings can lead to order reduction in the time stepping method used.
We present a new, Unmapped Tent Pitching algorithm which replaces these mappings by redundancy in the computations. The algorithm is based on waveform relaxation techniques, and can even be implemented in a completely algebraic way on the all-at-once space-time system using Restricted Additive Schwarz. It computes equivalent approximations at lower computational cost, since the volume of computation is equivalent to the volume in the mapped tent pitching algorithm, but the computation of the mappings is avoided. It can therefore also not suffer from order reduction. We illustrate the new algorithm with numerical experiments. This is joint work with Gabriele Ciaramella and Ilario Mazzieri [3].

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A Space-Time tensor-product B-spline discretization for Schrödinger equation

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We introduce a Petrov-Galerkin discretization for a well posed space-time variational formulation of time-dependent Schrödinger equation as formulated in [1]. We consider the trial space of maximum smoothness tensor product B-splines, while the test space is the image of the trials using the Schröedinger operator $A = i\frac{\partial}{\partial t} - \Delta$. The proposed discretization is infsup stable, and the matrix associated with the problem has a tensor structure in space and time as the ultraweak discretization in [2]. Exploiting this structure, we propose a preconditioner for the resulting linear system, easily assembled and invertible with Fast Diagonalization techniques. We provide numerical tests showing high order approximation rates of the proposed method, and we highlight the competitive behavior concerning wall-clock time compared to classical algebraic preconditioners.

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A space-time least squares approach for the wave equation with right-hand side in $L^2(Q)$

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For the discretization of time-dependent partial differential equations, classical approaches are explicit or implicit time-stepping schemes together with finite element methods in space. An alternative approach is the usage of space-time methods, i.e., the temporal variable t is just another spatial variable. Thus, the space-time domain Q is discretized, and the resulting global linear system has to be solved at once.
In this talk, the model problem is the wave equation in second-order formulation. First, we recall a space-time variational formulation of the wave equation in a strong sense, which is inf-sup stable in an appropriate trial space $X \subset L^2(Q)$ and the test space $L^2(Q)$, see [1, Section 4.3]. Based on this variational setting, we introduce a least squares formulation, leading to a continuous and elliptic bilinear form in X. Next, we discuss possible conforming space-time discretization schemes for this approach. In the last part of the talk, numerical examples are presented.

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MS05 - New trends in data processing

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ABSTRACT

The main goal of this minisymposium is to bring together researchers working in different fields of data approximation and to present recent advances from both a theoretical and a numerical perspective. The topics address typical problems in data processing, including compression, reconstruction, denoising and classification, and involve data of different nature: volumetric, biomedical, image and scattered data. Various approaches will be proposed by the speakers, to process, analyze and classify different types of data. Such methodologies involve, for example, cutting-edge advancements in classical spline, wavelet, RBF techniques, as well as innovative machine learning and deep learning-based models and algorithms.

(This minisymposium is dedicated to Prof. Luigia Puccio, on the occasion of her recent retirement, in recognition of her contributions in the fields of data processing and the activity carried out as a member of the Board of Directors of SIMAI from 2001 to 2012)

Problems related to data analysis in non-Euclidean spaces: iterative filtering for signals defined on the sphere

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Since real-life data are non-stationary, it would be better to study them through non-stationary techniques, and 'Fast Iterative Filtering' has proven to be an interesting and useful method to achieve this goal, especially in classic 1D or 2D cases [3]. But some problems arise in non-Euclidean settings since the filtering relies on convolution.
After developing a continuous operator we analysed its discretisation through the Generalised Locally Toeplitz (GLT) sequences of matrices [2]. Using some property from the GLT theory we studied the convergence of this procedure [1].
In this talk, after a brief review on the topic, we will describe some problems related to this setting and what we have obtained so far to overcome them. We conclude our talk with a few examples of applictions of this method to real life signals.

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Global interpolation on the sphere through multinode Shepard method

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In 1985 Little announced the possibility of improving the approximation qualities of the classic Shepard interpolant using a convex combination of Shepard-like basis functions based on triangles with local linear polynomial interpolants based on the vertices of those triangles. Similarly to the Shepard basis functions, the triangular Shepard basis functions are the normalization of the product of the inverse distances from the vertices of the triangles. Starting from the 2016 paper [1], a new light is given to the triangular Shepard method by proving its quadratic approximation order theoretically and computationally and by enlarging its applicability to compact triangulations. After this insight, the ideas in Little's paper are realized, and they lead to the introduction of the multinode Shepard method [2, 3], a powerful method for interpolation of scattered data based on inverse distance weighting and local polynomial interpolants on sets of unisolvent nearby nodes. In this talk, we discuss the suitability of the multinode Shepard method in interpolating scattered data on the sphere.

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Cell contour dynamics and the kymograph picture

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The analysis of cell motility is essential for a wide range of biological processes including wound healing, embryonic morphogenesis, and cancer metastasis. In general only a sequence of time frames of the contour of the cells are available. We show how to describe the cell contour dynamics by means of the kymograph mapping. The latter is based on a family of regularized flows based on virtual markers. Their dispersion rate allows us to define local membrane expansion which in turn can be linked to the protrusion activity of the cell. The analysis is available as a python package on https://zenodo.org/record/7539065

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Quaternary Image Decomposition with Cross-correlation-based Multi-parameter Selection

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An important problem in image analysis is to separate different components/features in images, such as, e.g., cartoon, smooth and texture components. However, when the image is corrupted by noise, the decomposition process becomes challenging, especially in the separation of the textural part.

The talk will illustrate a novel two-stage variational approach - see [1], [2] - for the additive decomposition of images into piecewise constant (cartoon), smooth, textural and white noise components. The challenging separation of white noise from texture is successfully achieved by including a normalized whiteness constraint in the model, and the selection of the regularization parameters is performed based on a novel multi-parameter cross-correlation principle. The two resulting minimization problems are efficiently solved by means of the alternating directions method of multipliers (ADMM). Numerical results show the potentiality of the proposed model for the decomposition of textured images corrupted by several kinds of additive white noises.

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Identification of Different Brain States from Brain Activity Maps

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In neuroscientific studies, it is of paramount importance to be able to identify features that allow to recognize different functional states of the brain. In particular, it is important to be able to recognize at an early stage any abnormalities in brain function due to pathological situations. In [1], a methodology was proposed to identify the regions of the brain involved in different meditation states. In this talk I will show how this technique can be refined to obtain additional information about the behavior of these regions. A further development will be to apply the same methodology to identify the brain areas most affected by mental disorders.

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Non-local and non-linear versions of the osmosis PDE model: properties and applications on images and graphs

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Osmosis is a parabolic linear isotropic diffusion-transport PDE model, which respects conservation properties about the average value and non-negativity of the initial data [2]. We consider both the model itself and a non-local approximation, analysing existence, uniqueness and regularity of the solution in time and space, depending on the properties of the drift vector field. Moreover, we study continuum limits of the problem when defined on weighted graphs with n vertices, as n grows. The model is then discretised as a time-evolutive process using both explicit and implicit iterative schemes, for which conditional and unconditional stability is proved, respectively [1]. The model is able to address the tasks of shadow/spot-light removal and compact data representation, for data defined both on 2D images and 3D graphs. For these applications, a non-linear variant is considered [3], with the introduction of a scalar diffusivity term that balances the diffusion intensity on the different regions of the domain, preventing smoothing effects. This new variant qualitatively improves the results obtained by the linear model, while keeping the computation efficient.

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Curve network interpolation by quadratic B-spline surfaces with multiple knots and free parameters

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In this talk, we propose a method for the construction of B-spline surfaces interpolating a B-spline curve network. Starting form the results obtained in [1, 2], in order to model the interpolating surface, we allow the presence of free parameters and of multiple knots in the spline space. We provide a constructive algorithm for surface generation in the case of both biquadratic tensor product B-spline surfaces and bivariate B-spline surfaces on criss-cross triangulations. Finally, we present graphical results showing the performances of the proposed methods.

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On Polyharmonic B-splines

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The aim of this talk, is to provide a review on the present possible application of various kinds of polyharmonic B-splines, discuss different constructions and present a simple procedure for to provide quasi-interpolation operators in spaces of cardinal $m-$harmonic splines in dimension d which reproduce polynomials of high degree.

Wavelets for Compression and Analysis of Large 3d Volumes

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Modern industrial computed tomography is capable of generating huge datasets. A size of 1TB per scan is no more special and in the context of sychrotron tomography we can expect files larger than even 10TB soon.
To be able to handle and even visualize such amount of data on normal or consumer hardware, it is necessary to apply compression, where compression by 3d tensor product wavelets offers quite a few advantages. These advantages, including an efficient computation of TV regularization, are listed and explained in the talk.

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Big Data and AI in Natural Disaster Management: The TEMA EU-Project Experience

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Natural Disaster Management (NDM, e.g., for forest fires, floods, etc.) can be greatly improved by developing automated means for precise semantic mapping and phenomenon evolution predictions in real-time. Several extreme data sources can significantly help towards achieving this goal: a) autonomous devices and smart sensors at the edge, equipped with AI capabilities, b) satellite images, c) topographical data, d) official meteorological data, predictions or warnings published in the Web, and e) geosocial media data (including text, image and videos). Such heterogeneous data sources provide a prime extreme data example: a) they are diverse (images, videos, text, scientific measurements) b) voluminous (images and videos), c) fast (most of them come in real-time) and frequently updated, d) complex (many of them are unstructured), e) multilingual (text), f) have very disperse sources (satellite, drone, sensors, social media, maps), g) are sparse/missing (as forest fires and floods can only be sparsely observed in space and time) and h) have extreme values (by definition, as forest fires and floods are exceptional events).
TEMA ([1]) is going to develop state-of-the-art (SoA) technologies facilitating this vision, focusing on real-time semantic extraction from multiple heterogeneous data modalities and sources, on-the-fly construction of a meaningful semantically annotated area map, near-real-time prediction of phenomenon/emergency evolution and automated response recommendations. Semantic analysis computations will be distributed across the edge-to-cloud continuum according to emergency response needs, in a federated manner, so as to keep latency to a minimum. Heterogeneous data analytics will be performed, mostly based on artificial intelligence (AI) and Deep Neural Networks (DNNs) in a trustworthy, transparent and flexible way, deployed as fit to the emergency and catering to various user needs. The constantly updated 3D map, the predictions and the recommendations will be used as the basis for an advanced, interactive, Extended Reality (XR)-based interface, where the current situation will be visualized and different alternatives for device/sensor deployment and response strategies can be dynamically evaluated by human operators. TEMA will provide a highly advanced and versatile Augmented Reality (AR) interface will be developed for integrating and visualizing live all TEMA results (semantically annotated 3D map, predicted outcomes, AI prediction explanations and proposed recommendations), as support for the human user in an operational "control room", while also allowing them to interactively assess contingent response alternatives via simulation. TEMA will deliver a technical solution to make modern AR systems exploitable in disaster response and management, bringing situational data to relevant end-users, thus providing the relevant information that can help make the best possible operative decisions.
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GNN-based construction of Laplace-Beltrami Operator basis for intrinsic 3D shape representation

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In recent years, neural fields have been proposed as a new 3D shape representation paradigm. The recent success of Euclidean-based neural fields has been enabled by the random Fourier features [3] embedding technique. Similarly the intrinsic neural fields rely on an analog embedding based on the Laplace-Beltrami Operator (LBO) spectrum on closed compact manifold. In the proposed work, we compute the LBO basis by a Graph Neural Network [2], whose kernel has been derived in a variational framework.

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MS06 - Advances in Shock-Fitting/Front-Tracking methods

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ABSTRACT

High speed flows are governed by hyperbolic conservation laws, which often exhibit discontinuous solutions. Shock-waves, one of the possible gas-dynamic discontinuities, exert severe thermal and aerodynamic loads on vehicles flying at high speed, such as spacecrafts re-entering the atmosphere. Accurate numerical modeling of gas-dynamic discontinuities is therefore of paramount importance when building Computational Fluid Dynamics (CFD) simulation codes to be used in the design of supersonic and hypersonic vehicles.

Over the years, the quest for general-purpose CFD codes contributed to the widespread popularity of the so-called Shock-Capturing algorithms [3], which lay their foundations in the conservation-law-form of the governing equations and consist in adding artificial viscosity in the vicinity of the discontinuity, thus widening its width well beyond the physical value. Coding simplicity comes not for free, however, and Shock-Capturing algorithms are plagued by a number of defects that often hinder the predictive reliability of the simulation.

In contrast, Shock-Fitting and Front-Tracking algorithms, which were respectively pioneered by Gino Moretti [2] and James Glimm [1], consist in modeling discontinuities in the "true" mathematical sense, i.e. surfaces of negligible thickness that bound regions of the flow-field where a smooth solution to the governing PDEs exists. Despite their capability to deliver accurate solutions using coarse-mesh discretizations, Shock-Fitting/Front-Tracking algorithms require a fairly complex computational logic which probably contributed towards making CFD practitioners shy away from this class of techniques. Over the last decade, however, the increasing use within the CFD community of high-order-accurate discretization, which in turn require accurate shock-modeling, led to a renewed interest in Shock-Fitting/Front-Tracking algorithms. In the proposed Mini Symposium we plan to address the most recent developments in Shock-Fitting/Front-Tracking algorithms including application areas not limited to compressible fluid dynamics and including other physical systems where sharp interfaces are encountered.

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Shock-fitting simulations of transonic flows in a channel with a half lenticular profile

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The transonic flow past a NACA0012 profile [1] in the Mach number range $0.91 < M_\infty < 0.95$ exhibits the so-called "fishtail" shock-pattern, which is characterized by the interaction between the oblique shock that originates at the trailing edge (TE) of the airfoil and a nearly normal shock standing at some distance downstream of the TE. Shock-Fitting numerical simulations of the aforementioned transonic flow, coupled with standard shock-polar analysis, reveal [1] that this particular shock-shock interaction cannot be explained using von Neumann's three-shocks-theory (3ST), but the less known four-waves model (4WT), proposed by Guderley, should be used instead.
In order to gain further insight into this kind of interaction, we numerically studied a similar geometry which consists in a planar channel whose bottom wall takes the shape of a 10^0half lenticular profile close to the inlet section and then continues as a straight wall. A weakly supersonic, uniform flow at Mach number M_{in} is prescribed along the inlet section, whereas a subsonic outflow at a fixed pressure ratio P_{exit}/P_{in} is set at the exit section. The transonic flow that develops inside this channel is very similar to the one around airfoils exhibiting the fishtail, but the possibility of varying both M_{in} and P_{exit}/P_{in} allows to obtain a wider range of possible interactions. Numerical simulations have been carried out using an hybrid Shock-Fitting/Shock-Capturing approach: the shock originating at the TE is fitted, but the detached shock is captured. By looking at the upstream Mach number and slope of the oblique shock close to the interaction point, both of which depend upon the P_{exit}/P_{in} ratio, it is possible to establish whether a three-shocks or four-waves interaction takes place. In the conference presentation other numerical solutions obtained with different values M_{in} and P_{exit}/P_{in} will be shown and analyzed.

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An overview of second-order-accurate Shock-Fitting algorithms on structured and un-structured grids

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Over the last decade or so, Shock-Fitting/Front-Tracking methods have met a renewed interest among CFD developers: research groups from all over the globe developed different flavours of Shock-Fitting/Front-Tracking algorithms to be used in conjunction with either Finite Volume, Finite Element or Fluctuation Splitting discretizations.
The talk will summarize a fifteen-years-long joint activity involving four research teams that led to the development of second-order-accurate, Shock-Fitting algorithms, suitable to be used both on structured and un-structured grids. In our approach [3, 2], the discontinuities are described (in 3D) using double-sided, triangulated surfaces that are free to move throughout a background tessellation of the computational domain, which can be filled with either a structured or an unstructured mesh. The flow variables on the two sides of the discontinuities obey the Rankine-Hugoniot jump relations, which also provide the local speed with which the discontinuity surface moves. The moving discontinuity surfaces are handled as internal boundaries of zero thickness by shock-capturing CFD codes (either structured or un-structured) which are used to discretize the governing PDEs in the smooth regions of the flow-field and, eventually, also used to "capture" those discontinuities that are not explicitly fitted.
In order to accommodate the moving surface of discontinuity inside the background tessellation, two different approaches have been used: local re-meshing [3, 2] or immersed interpolation/extrapolation [4], both limited to the neighbourhood of the discontinuities.
Thanks to a modular algorithmic structure, different mesh generators and CFD codes can be used, while keeping the coding effort to a minimum to include fitting/tracking capabilities to an existing solver.

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Front Tracking and Application to Parachute Simulation

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We introduce an integrated computational platform for the simulation of the parachute system using the front tracking methodology. A dual-stress spring-mass model based on the front tracking method is used to study the dynamics of fabric surfaces in air. The numerical algorithms for this complex physics system includes fabric model and its coupling with the fluid solvers, both incompressible and compressible. The fabric porosity is modeled by the ghost cell method. The collisions, including fabric-fabric, fabric-rigid, rigid-rigid and string colissions with fabric and rigid are inplemented. This presentation will introduce on the algorithms and simulation of the supersonic parachute simulation. We will also present other applications, including fluid interface instabilities, phase transition and particle tracking with the front tracking software library.

On Moving Discontinuous Galerkin Method with Interface Condition Enforcement for Discontinuous Flows

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The necessity of enforcing conservation in computational elements or cells (element conservation) for discontinuous solutions is well understood and respected for solving conservation laws in computational fluid dynamics (CFD). In contrast, interface conservation, where the conservation across cell interfaces is enforced, is long ignored, and yet is also ruled and required by the underlying physics just like element conservation. Violation of the interface conservation across discontinuities is the root cause why an exact discontinuous solution can never be achieved in shock capturing methods. The interface conservation is examined and explored in this talk. Moving discontinuous Galerkin (MDG) finite element method with interface conservation enforcement (MDG-ICE) [1],[2] are then presented for solving compressible flow problems with discontinuities based on the observation that the interface conservation can only be satisfied, only when mesh interfaces are aligned with discontinuities. In the MDG-ICE formulation, both conservative quantities and grid geometry are considered as independent variables. A space-time DG formulation is used to solve the multi-material compressible Euler equations in the standard discontinuous solution space and the discrete grid geometry is solved using a variational formulation in a continuous space. A self-adaptive Levenberg-Marquardt method is utilized to solve the resulting over-determined system of nonlinear equations arising from the MDG-ICE formulation. A number of numerical experiments for a variety of flow problems are conducted to assess the accuracy and performance of the MDG-ICE method. Numerical results obtained indicate that the MDG-ICE method is able to deliver the designed order of both h- and p-convergence even for discontinuous solutions, and detect all types of interfaces, via interface condition enforcement and satisfy, via grid movement, the compressible Euler equations and the associated interface condition.

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Numerical modelling of hypersonic flows past inflatable shields through a shock/wall - tracking technique

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The shield is an essential component of a re-entry vehicle or an interplanetary probe in an aerocapture maneuver, as it decelerates the capsule and protects it from the aerothermal loads. An inflatable shield increases significantly the surface exposed to the flow without adding mass, thus reducing the ballistic coefficient and ensuring paths in the atmosphere that are less critical in terms of aerothermal loads. In the proposed study we present a new numerical technique able to model the behaviour of inflatable walls in hypersonic flows. To do so, we couple a commercial structural solver with the in-house gas-dynamic solver `UnDiFi`, which is based on the shock-fitting approach [1]. Shock-fitting methods consist in identifying and tracking the motion of shock waves within the flow-field and in computing their space-time evolution by enforcing the Rankine-Hugoniot jump relations. The fitted discontinuities bound smooth regions of the flow-field where a shock-capturing solver is used to discretize the governing PDEs. In a similar manner, the thin wall of the inflatable shield is treated as a new type of discontinuity, which is deformed due to the combined effect of the external aerodynamic pressure and internal inflation pressure. The wall of the inflatable shield, featuring negligible bending stiffness, is modelled as a shell, and its displacement and deformation are calculated using the non-linear structural solver SOL400 of MSC Nastran. More details about this new computing technique and some 3D test-cases will be discussed and analyzed in the conference presentation.

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Optimized quantum drift diffusion model applied to a resonant tunneling diode

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The purpose of the study is to optimize a Quantum Drift Diffusion model (QDD) by comparing the solutions with those obtained by the Wigner Transport Equation (WTE) [1], in the case of a Resonant Tunneling Diode (RTD) made of GaAs with two barriers potential made of GaAlAs. The QDD model has been numerically solved by using finite difference scheme for Poisson equation and Scharfetter-Gummel scheme for continuity equation, in the stationary case. To solve the WTE we have adopted a signed Monte Carlo method [2]. To optimize the QDD model we have used a constrained optimization procedure.
A good agreement between the two models is found when the applied bias voltage is low. Furthermore, we have compared the QDD model with a Quantum Hydrodynamical model [3], solved by using a Runge-Kutta Discontinuos Galerkin method.

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MS07 - Models and Methods for Biomedical Applications

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ABSTRACT

In the last decades, mathematics has played an increasingly prominent role in the fields of biology and healthcare. The main aims range from developing models to perform in silico simulations to applying data-informed models to make patient-based predictions and getting deeper insights into specific biological mechanisms with formal and numerical analysis of the related models. Not secondly, mathematical challenges arising from these problems allow the improvement of mathematical methods. In this Mini-Symposium, we want to illustrate some recent research opportunities arising in the mathematical biology field, highlighting the interactions between mathematical and biomedical sciences. Different modeling approaches and methods will be presented for describing biological phenomena that characterize both pathological and physiological conditions.

Based on the expertise of the invited speakers, the use of a multiscale constitutive framework to computationally model blood flow in physiological conditions will be discussed, showing how it is possible to reconstruct different types of blood propagation phenomena through the implementation of the viscoelastic contribution at the boundaries. Moreover, the problem of cell migration through thin membranes will be presented along with the derivation, by the means of a formal asymptotic procedure, of effective interface conditions for a mechanical model. In particular, this study will show several applications to developmental biology and cancer invasion, which will be discussed. As another key problem, pathological scenarios related to inflammatory diseases and tumor progression will be presented. For the former, macroscopic and kinetic models will be presented to understand the main mechanisms driving an inflammatory response in patients with Multiple Sclerosis, through a linear and nonlinear analysis and, eventually, the study of the emerging patterns. For the latter, we will focus on both single-cell dynamics to examine cells' response to hypoxia and collective dynamics to discuss nutrient-deprived scenarios, also by the means of asymptotic analysis for the long-time behavior of the system.

Overall, with this Mini-Symposium, we aim to demonstrate the power of mathematical modeling, formal analysis, and simulations in advancing our understanding of complex biological systems and to highlight the opportunities for collaboration between mathematicians and biomedical researchers.

A multiscale constitutive framework of computational blood flow modeling

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One of the many challenges of modeling the human cardiovascular system is related to the high morphological and mechanical variability of vessels, which gives rise to complex fluid-structure interaction (FSI) mechanisms between vessel walls and blood flow [1, 4]. In unhealthy cases, this variability is further emphasized by the possible presence of calcifications, stenoses, aneurysms, or even prostheses, such as grafts or stents. In order to model the FSI that occurs between blood and vessel walls, it is necessary to consider an appropriate constitutive model that relates pressure variations to area deformations as realistically as possible [2, 3]. Thus, in this complex context, to have an easily extensible model together with an efficient, accurate, and robust method is one of the main relevant purposes.
In this talk, a very flexible multiscale constitutive framework for one-dimensional blood flow modeling is introduced and discussed. It is demonstrated that different types of blood propagation phenomena can be described using an appropriate choice of the scaling parameters of the proposed model, which are related to distinct characterizations of the FSI mechanism (whether elastic or viscoelastic) [3]. In these asymptotic limits, well-known blood flow models from the literature are recovered. Furthermore, a novel viscoelastic blood flow model is derived by examining the perturbation of the system's local elastic equilibrium.
The resulting multiscale hyperbolic model is solved using a third-order accurate asymptotic-preserving Implicit-Explicit Runge-Kutta Finite Volume method, which ensures the numerical scheme's consistency with the different asymptotic limits of the model without affecting the choice of the time step due to scaling parameter smallness constraints [3]. Several numerical experiments, including a case study of the hemodynamics of a thoracic aorta in the presence of a stent, support the validity of the suggested methodology.

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Modelling HIF-PHD dynamics and related downstream pathways in tumours

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Hypoxia can represent a challenging condition for cell survival and is a typical feature of solid tumours as result of increased proliferative rate and dysfunctional vasculature. The efficiency of the response to decreased oxygen availability is strictly related to the Hypoxia-Inducible Factors (HIFs) that are enzymatically regulated in an oxygen-dependent way by a class of Prolyl Hydroxylase (PHDs). HIFs regulate the transcription of hundreds of genes whose proteins favour changes in metabolism, promotion of angiogenic processes and elicitation of pro-inflammatory responses. These downstream effects represent driving forces of malignant progression in cancer cells. We will firstly focus on the hypoxia-induced dynamics of HIF1α and HIF2α, which are the most studied HIFα isoforms, comparing available experimental data on their evolution in tumor cells with the results obtained integrating the deduced mathematical model [1]. Secondly, we will focus on the tumor-associated inflammatory signaling that is strictly related to the interplay between HIFs and the Nuclear Factor k-light-chain-enhancer of activated B cells (NFkB), which is considered the master regulator of inflammatory responses. Then, we will examine the possible scenarios that characterize the link between hypoxia and inflammation when the dimensionless groups of parameters of the mathematical model change. In this way we will be able to discuss why and when hypoxic conditions lead to acute or chronic inflammatory states.

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Pattern formation in a chemotaxis model of acute inflammation

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Inflammation is the process by which the immune system recognises and eliminates harmful and foreign stimuli and initiates the healing process. Although it is a protective mechanism, dysregulation of this biological process can impair physiological function and lead to a significant number of serious and debilitating diseases, such as multiple sclerosis. The complex dynamics of the inflammatory process are not yet fully understood, and a thorough knowledge of these mechanisms would be key to controlling the onset and progression of inflammatory diseases.
In this talk, I will present a study on a recently proposed reaction-diffusion-chemotaxis model ([1]) that describes the activity of immune system during an inflammatory attack, from early stages to the acute phase. I will focus on the appearance of pattern solutions and their stability. These solutions represent aggregations of immune cells, which are the hallmark of an inflammatory activity. I will show that the system may undergo both stationary and wave instabilities, generating non-homogeneous steady states and time oscillating aggregation patterns, respectively. I will also analyse stationary radially symmetric solutions and show that they reproduce various inflammatory aggregates observed in the clinical practice.
The analysis is carried out using realistic parameter values and is supported by a detailed numerical investigation.
Our study shows that the model captures the main mechanisms involved in an inflammatory process and thus its analysis can provide valuable insights into the functioning of the immune system.

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Influence of mechanical properties on cell migration through thin barriers of extracellular matrix

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As cells migrate within a three-dimensional environment, they encounter a variety of barriers including other cells, cell-cell junctions and extracellular matrices (ECMs) of varying density and composition. The migration process is associated with significant cell deformation, especially when the production of proteolytic enzymes is inhibited, and experimental studies have revealed the existence of a critical ECM pore size below which cell migration is entirely hampered. Therefore, the introduction of microscopic mechanical properties of the cell, and in particular of the nucleus as the stiffest organelle, into continuum macroscopic models of cell migration is of fundamental importance in order to make a step towards a more comprehensive representation of cell invasion.
First, treating the nucleus as an elastic body covered by an elastic membrane, we derive a necessary criterion for cells to pass through a regular network of fibres, depending on the forces acting on the cell, the stretchability of the nuclear membrane, the stiffness of the nucleus, and the size of openings inside the ECM with respect to the nucleus diameter [1]. The obtained critical value is then incorporated into a continuum macroscopic model able to describe both the invasion of cell aggregates and their segregation within thick regions of extracellular matrix [1]. Finally, we consider the limit case in which such barriers become so thin that each of them can be replaced by an effective interface equipped with a set of biophysically consistent conditions for the equivalent transmission problem. Specifically, we find that the mass flux across the thin interfaces must be continuous and proportional to the jump of a term related to the tissue pressure, through a coefficient that can be related to the size of the pores of the thin membrane [2, 3].
From a mathematical point of view, these results can help to describe the invasion and segregation of an ensemble of cells within a heterogeneous environment characterised by the presence of barriers and constrictions. From a biomechanical point of view, the proposed approach could be applied to the design of synthetic scaffolds with optimal values of pore size and fibre density, which could accelerate cell transport and ingrowth, critical for regenerative treatments.

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Demyelination-remyelination patterns in Multiple Sclerosis derived from kinetic models

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We present a study for anomalous immune response that extends the one proposed in [1], where a kinetic model is proposed to describe, at mesoscopic level, the dynamics in time of a high number of interacting cells in an autoimmune framework. We propose a more realistic spatio-temporal model, considering both interactions among different populations of human cells and motion of immune cells, stimulated by cytokines, as performed in [2]. Moreover, we apply it to a particular case of autoimmune disease represented by Multiple Sclerosis, reproducing the consumption of myelin sheath due to anomalously activated lymphocytes and its restoration by oligodendrocytes. Successively, we fix a small time parameter and assume that processes considered occur at different scales. This allows to perform a formal hydrodynamic limit, obtaining macroscopic reaction-diffusion equations for the number densities of the constituents with a chemotaxis term. A natural step is then to study the system, inquiring about the formation of spatial patterns through a Turing instability analysis of the problem and basing the discussion on microscopic parameters of the model. In particular, we get spatial patterns oscillating in time that may reproduce brain lesions characteristic of the pathology.

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Modelling the evolutionary dynamics of nutrient-deprived cancer cells using structured PDEs: analysis, numerics and validation

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Glucose and oxygen are primary energy sources for cancer cells. Several lines of evidence support the idea that changes in gene expression levels (e.g. MCT1, HIF1) elicit metabolic reprogramming of cancer cells in nutrient-poor environments, promoting cancer cell survival and disease progression. A more in-depth theoretical understanding of the evolutionary processes at the root of cancer cell adaptation to nutrient deprivation can be achieved through analysis and numerical simulation of structured-population models. The focus of this talk is on non-local partial differential equations modelling the adaptive dynamics of a population of cancer cells structured by the level of gene expression. I will present an experimentally-informed mathematical model of a well-mixed population, which was calibrated with data from in vitro experiments on glucose-deprived aggressive cancer cells [1], and discuss the challenges introduced by the extension to a spatially-explicit framework [2].

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MS08 - Particle-Based Methods In Applied And Industrial Sciences

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ABSTRACT

Computer simulations of physical phenomena have nowadays become an essential tool in many areas of applied and industrial sciences (like, e.g., computational fluid dynamics, geomechanics, biomathematics, continuum mechanics, life sciences, etc.), as they are increasingly replacing expensive and time-consuming real experiments. Grid-based numerical methods, like Finite Element Method, are well established and widely used in both academia and industry. However, these approaches struggle to deal with the extreme changes of geometry associated to problems like, e.g., hypervelocity impact, crack propagation, multi-phase interactions and free surface simulations.

In recent years, numerical methods that rely on a discretization of the system based on particles turned out to be more suited to address the challenging problems described before. Moreover, some of these methods are particularly fitting the need of fine granularity parallelism required to run efficiently on massively parallel architectures, such as modern GPUs-based HPC clusters. For these reasons, researchers have devoted increasing attention to this approach and many different particle-based methods have been developed, among which we mention the Smoothed Particle Hydrodynamics (SPH), the Lattice Boltzmann Method (LBM) and the Material Point Method (MPM).

This Minisymposium focuses on the mathematical modelling, computational and implementation aspects of particle based numerical methods and their applications to industrial and applied science problems. The objective is to share state-of-the-art results on such fields, to stimulate interdisciplinary research in applied mathematics and to foster interactions of the scientific community with industry.

Material Point Method for Compressible CFD on GPUs

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Parallel computing is a key capability for effective advancement of industrial grade large scale computations. In the decade Graphics Processing Units (GPUs) based architectures are continuously evolving and delivering increasing throughput in terms of computing power, but to optimize algorithms and design GPUs based software is an actual current challenge [3]. Particle-In-Cell (PIC) like methods as Material Point Method (MPM) are particularly fitting the need of fine granularity parallelism required by GPUs based architectures.
Recently, PIC and MPM codes are being developed or ported to GPUs in various field of application [2, 5, 4]; however, few works have been published in the compressible computational fluid dynamics (CFD) realm since early 2000s [6, 1], in particular, paying attention to the High Performance Computing (HPC) capabilities of the algorithm.
This contribution will show the results obtained in developing a GPUs based MPM code with applications to compressible CFD. The focus will be on the algorithm adaptations made to suit GPUs features, and so, to obtain a high level of parallel scalability on industrial-grade clusters, the individuation of the kernel to be optimized and scaling studies. Such results will be presented with respect to some standard gas dynamics test cases which are of interest for a proof-of-concept code for industrial applications.

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Pyroresistivity of Conductive Polymer Composites: Algorithms for Aggregation, Percolation, and Thermoelasticity

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Flexible and lightweight Conductive Polymer Composites (CPCs) are a popular choice for several technological applications that require electrical materials to be responsive to external stimuli or flexible. CPCs combine the conductivity of fillers with the flexibility and lightweight of polymers. When in contact with each other, the fillers form a conductive network within the insulating polymers. However, the critical volume fractions at which CPCs with different filler sizes become conductive are poorly understood. Experimental evidence [1] suggests that the critical volume fractions range from 5.5% for small spheres (radius of 1 μm) to 28% for large spheres (radius of the order of 100 μm). In this talk, we propose a new off-lattice continuum percolation model that explains the variation in percolation threshold for different polymers and fillers. Our model consists of a contact algorithm and an aggregation algorithm. The contact algorithm takes an initial random arrangement and generates non-overlapping spheres that are at most in contact. The aggregation algorithm produces giant connected components critical for the system's percolative paths. Our method produces low-volume fraction clusters closer to the experimental ones and shows similar statistical properties.

CPCs also have a significant positive temperature coefficient (PTC), which is helpful for current-limiting devices, such as fire safety systems. As the temperature increases, the thermal expansion of the polymer creates an increasing separation between the fillers, which weakens or breaks the macroscopic conducting paths through the composite. This results in a sharp transition from an electrical conductor to an insulator. The causes of such a switch are still not well understood. We hypothesize that it depends on the actual polymer strain distribution and the bonding stiffness between filler and polymer.

For this purpose, we solve numerically the 3D thermoelastic equations. However, mesh-based numerical schemes are impractical, as meshing around many spheres in contact is arguably impossible. For this reason, so we employ a mesh-free numerical method. Additionally, we determine the resulting electrical conductivity by extracting the connected components of the graph and solving the corresponding electrical circuits. This enables us to calculate the resistivity curve for varying thermal strains, closely resembling the experimental ones. Notably, we can identify the thermal strain at which resistivity approaches the singularity, indicating a broken-down conductive network.

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From geophysics to industrial applications: high-performance Smoothed Particle Hydrodynamics with GPUSPH

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The Smoothed Particle Hydrodyamics (SPH) method [1] was initially developed for astrophysics, has grown to find application in many applications computational fluid dynamics, and particularly in modeling and simulation of complex fluids [2]. Weakly-compressible (WCSPH) formulations are commonly used to close the system of equations, which allows the evolution of the particles to be computed directly: at the cost of more stringent conditions on the time-step, this has the benefit of an embarrassingly parallel algorithm that is a natural fit for the emergent use of low-cost high-performance parallel computing hardware such as modern video cards (GPUs) to accelerate computations.
GPUSPH [3] was the first implementation of WCSPH to fully run on GPU. Featuring a wide range of formulations and rheological models, GPUSPH has found application in applied and industrial sciences, ranging from geophysics [4] and volcanology [5] to structural engineering [6] and the energy industry [7].
Here we present some of the more recent applications of GPUSPH, highlighting the benefits offered by the SPH method and its GPU implementation, and covering some of the common pitfalls to be avoided to ensure numerical robustness and maximize accuracy.

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A dynamic-Immersed Boundary approach for Fluid/Structure Interaction in Biology

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Margination is a process that occurs in bloodstream, in which particles, such as white blood cells and platelets, accumulate along the walls of blood vessels, thus resulting easily accessible to tissue that may be damaged or infected. Here a numerical framework for computing the vascular journey of blood borne particles and cells is presented. The incompressible Navier–Stokes equation is modeled through a BGK-Lattice Boltzmann scheme endowed with a forcing term accounting for the presence of immersed geometries. Dirichlet boundary conditions are imposed on moving deformable or rigid geometries through a dynamic-Immersed Boundary method, while, on fixed immersed geometries a second-order mass-conserving bounce-back technique is adopted. The proposed computational framework is thoroughly analyzed in term of its stability and accuracy. This approach is employed to detail transport, dynamic, and deformation of micrometric capsules into microfluidics chip and capillaries [1, 2]. Moreover, preliminary findings on the problem of coupling the incompressible Navier-Stokes with nonlinear peridynamics [3] will be discussed.

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Simulation of hydrological hazards and their interaction with protection systems using the Material Point Method

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In the last decades we have observed a significant growth in the intensity and frequency of extreme hydrological events involving large mass movements such as landslides, debris flows, and mud flows that may cause serious damage to civil structures. Since, as a consequence of climate change, this tendency will keep worsening in the near future, it is important to develop numerical tools that are capable of playing an important role in the minimization of the damage induced by these natural hazards by simulating the interaction between the rock/fluid or debris flow and the surrounding terrain and structures. However, the numerical simulation of these multiphysics events still represents a challenge. One of the main reasons is that these kind of problems naturally involve large deformations that affect the accuracy of the solution obtained using a well-known method like the standard Finite Element Method (FEM). In the last decades many different methods have been proposed and developed with the purpose to deal with the big changes of geometry associated to these extreme events. Among these methods there is the Material Point Method (MPM). The talk will give an overview of some recent advances in MPM formulations, presenting both an irreducible and a mixed UP formulation [1] stabilized using Variational Multiscale (VMS) techniques. Moreover, some partitioned strategies to couple MPM with other techniques such as FEM or DEM are also presented [2, 3]. All the algorithms discussed are implemented within the Kratos-Multiphysics open-source framework and available under the BSD license.

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Run-out simulations of fast flow-like landslides with a semi-conservative Depth Averaged Material Point Method

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Landslides are one of the most troublesome natural occurrences for human safety, not only because of their intrinsic unpredictability but also because they might be disastrous in terms of human and financial losses [1, 2]. For these reasons it is crucial to constantly monitor landslide-prone locations. Satellite surveys can offer extensive topography and elevation information of the study area, while in-situ detection equipment like piezometers and strain gauges allow accurate monitoring of internal pressures and movements of the region of interest created by cracks [3, 4]. However, empirical monitoring alone is not sufficient to ensure effective management of a hazardous situation, especially in a preventive capacity. The great economic cost, as well as very limited practicality in carrying out real experiments, have made the development of numerical techniques capable of simulating landslide phenomena increasingly necessary. In this work we present a two dimensional time-adapted particle numerical method to modeling flow-like landslides, developing a semi-conservative variant of the Depth-Averaged Material Point Method (DAMPM) [5]. The mathematical model is given by the Shallow Waters equations, derived from depth-integrating the Navier-Stokes equations. Both bed friction and the rheology are considered in the presented framework, following the Voellmy model and the depth integrated Bingham visco-plastic stress model respectively [6]. After verifying the performances of the numerical method through different benchmarks and idealized settings, it has been tested on a realistic scenario.

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MS09 - A journey into brain imaging: from the MEG/EEG inverse problem to brain fingerprint

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ABSTRACT

Understanding brain function from magneto-electroencephalographic (M/EEG) measurements requires advanced mathematical and signal processing tools. Although the analysis of M/EEG data at sensors level sheds light on important brain mechanisms, full exploitation of the information contained in such brain data could be achieved by reconstructing the active neural sources from M/EEG measurements. This involves solving an ill-posed and ill-conditioned inverse problem in which not only the identification of the most suitable inversion method [1, 2] but also the calibration of the regularization parameters is of paramount importance. Once time series representing brain activity are available, a next step is to develop tools to extract meaningful information that characterizes brain activity [3, 4], for example, when the subject under study is affected by diseases that impair brain function.

The mini-symposium brings together researchers from various disciplines who have developed methodologies that are being successfully used for the analysis of the M/EEG data, the solution of the underlying inverse problem and in the definition of brain fingerprint. The purpose is not only to present the latest research results in this area but also to create a fruitful environment for the development of new ideas.

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Fractality measure and deep learning techniques for studying the cortical neurodynamics

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The neuronal ongoing electrical activity of the brain network, the neurodynamics, reflects the structure and functionality of the generating neuronal pools. Their activity, investigated via encephalographic brain recordings, often exhibits a non-periodic, fractal-like behaviour. Thus, here, using the intra-cranial stereo-electroencephalographic (sEEG) recordings from Montreal Neurological Institute (MNI), we investigated the neurodynamics of precentral (144 channels), postcentral (64 channels) and superior temporal (79 channels) gyri across wakefulness and three sleep stages: REM, N2 and N3. The aim of the study is to assess the spectral and fractal features of the neurodynamics, in time and frequency domains, across the three cortical regions, and to verify if they can constitute a signature for distinguishing cortical areas, possibly despite the state. For this study we calculated several signature candidates such as the mean power spectrum and the power-law β exponent ($\frac{1}{f^\beta}$) of the power spectrum, and we compared theses signatures between areas and wake/sleep stages. We also deployed a convolutional neural network (CNN) for automatic pattern recognition of the temporal sEEG series of the three areas. The achieved results suggest that both with deterministic estimates and with less "controllable" techniques, such as deep learning neural networks, we are able to extract different characteristics of neurodynamics and the classify the three cortical areas from the intracerebral intracranial recordings. The potential impact of this study stands in automatic mapping of the brain parcels according to the ongoing neuronal activity in resting states.

Investigating the Impact of Signal-to-Noise Ratio on EEG Resting-State source reconstruction

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The impact of Signal-To-Noise Ratio (SNR) on source localization accuracy is commonly assessed in relation to task-evoked cortical activity. The evaluation of the SNR effect is more challenging in the resting-state condition, i.e., in the absence of stimulus or task, because of the signal's low amplitude and the lack of external stimuli. In this study, we explore the impact of varying SNR values on source estimation performance (SNR LOC) of EEG resting-state activities, using Minimum Norm Estimation (MNE) and a realistic head model. We simulated synthetic resting-state EEG signals with different known SNRs for three neural networks: the Motor Network (MN), the Visual Network (VN), and the Dorsal Attention Network (DAN). The synthetic source-based signal was 1 min long and sampled at 256 Hz. We considered eight non-linear sources for the MN, six for the VN, and fourteen for the DAN. For each network, the sources presented a time delay of 15 ms [1]. In addition, fifty uncorrelated noise sources were randomly distributed over the whole cortex. Using a boundary element method (BEM) volume conduction model based on the New York head model, we obtained the inverse solution through MNE on brain Independent Components (ICs), with different regularization parameters (defined as λ proportional to $1/SNR^2$). The SNR of the simulated EEG signal was set equal to [1, 5, 10, 15, 20, 30, 40, 50, 75, 100]. Differently, the SNR LOC values varied across [0.1, 3, 10, 100]. The performance was assessed using three metrics: localization error, source extension, and source fragmentation. The results of all three networks indicated that the localization error decreases as the SNR LOC increases, following a 1/SNR trend. Regarding source extension, higher SNR LOC values resulted in more focal sources. Additionally, when evaluating source fragmentation using the *dbscan* algorithm, the number of clusters was significantly higher for an SNR LOC of 100 compared to SNR LOC values of 0.1, 3, and 10. The statistical analysis based on the repeated-measures ANOVA (α=0.05), with Bonferroni correction for post-hoc multiple comparisons, revealed that 10 for SNR loc represents a good trade-off between the three metrics, as it provides a focal source reconstruction and ensures a low localization error. In conclusion, the SNR LOC significantly impacts the spatial resolution of the source-level analysis.

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Hierarchical Bayesian models for EEG, MEG and beyond

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In this talk, a review of hierarchical Bayesian methods for solving inverse problems with sparsity or group sparsity constraints as a prior. Hierarchical Bayesian models are based on the idea that simple and computationally efficient prior probability densities such as Gaussian densities can be enriched significantly by using them as building blocks in layered models. On overview of algorithms combining hierarchical models, iterative solvers and sampling techniques to solve the inverse problem in brain activity imaging [2]-[9] is given, along with some extensions to dictionary learning problems inspired by these algorithms [1, 10].

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THE TOPOCHRONIC MAP OF THE LARGE-SCALE BRAIN DYNAMICS

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Large-scale brain activity evolves dynamically over time, across multiple time-scales. The structural connectome imposes a spatial network constraint since two structurally connected brain regions are more likely to coordinate their activity [1, 2]. It also imposes a temporal network constraint by virtue of time delays via signal transmission, which has modulatory effects for oscillatory signals CC. Specifically, the lengths of the structural bundles, their widths, myelination, as well as the overall organization of the structural scaffold, influence the timing of the interactions across the brain network. Here, we directly estimate the functional delays across the whole brain - in vivo, from magneto/electroencephalography - and integrate them with the structural connectome - derived from magnetic resonance imaging. Hence, we provide a map of the functional delays characterizing the connections across the human brain DD. Furthermore, we show in multiple sclerosis patients that demyelinating lesions correspond to higher transmission delays as compared to controls. Methods and results We estimate in vivo, non-invasively, the functional delays of transmission across the network of white matter bundles, combining source-reconstructed magnetoencephalography and tractography. Previous work showed that fast bursts of coordinated activations ("avalanches") spread in the human brain along the white-matter bundles. To track avalanches, we z-scored (in time) the source-reconstructed MEG signals, and defined the start of an avalanche as the moment when at least one region is "active" - i.e. when it is above threshold – and the end of an avalanche as the moment when no region is active anymore. Once a region becomes active, the other regions were considered recruited in the avalanche if they went above threshold at subsequent timesteps. The time it took region j to be recruited by a perturbation started in region i was measured, building a matrix of delays, where rows and columns represent brain regions, and each entry represents the delay between those two regions. Using tractography, we also built a structural matrix, containing the length of the structural bundles. Finally, we obtained a velocity matrix, dividing the trait length by the corresponding delays. The range of the delays is much narrower than what would be expected given constant velocities of propagation. When estimating the velocities, we show that a well behaved, fat tailed distribution emerges. As expected, due to the heterogeneity of the tracts, the velocities appear to be far from homogeneous, and range from 2 to 60 m/sec. We found that the delays grow as a function of the length of the traits, as shown by the Spearman correlation between edge length and delays (r=0.45, p=3.85e-205). Such relationship holds at the individual level (figure 1, top-right). However, while the delays are related to the trait lengths, they are not only determined by the lengths. In fact, the trait lengths range across an order of magnitude, while the corresponding growth of the delays is only moderate. For comparison, in figure 1, bottom-left, we showed the expected delays given constant velocities, and the observed delays are remarkably steady, despite the difference of the lengths of the structural traits. Next, we sought to establish if our results are likely to be obtained by chance alone. To this end, we build surrogate data based on randomized avalanches, whereby we shuffle the time sequence, while preserving the spatial structure. In other words, for each avalanche, the time points where randomly shuffled, but the regions

recruited at any given time points were fixed. This way, the time-structure of the recruitment of regions was disrupted, while the purely spatial component retained. After the permutations, the average delays were again computed per each edge. The procedure was repeated 100 times, yielding a hundred surrogate delays per each edge. Firstly, we compared the delays retrieved from the random timeseries to the trait lengths, obtaining 100 Spearman's R's, to which we compared the observed correlation, p<0,001. We then used the random surrogates to compute random velocities, i.e. dividing each edge length by the corresponding delay derived from the random surrogates. Similarly, as before, this procedure was carried out 100 times (once per each of the 100 random surrogates), retrieving a distribution of the correlations obtained between trait lengths and random velocities (i.e. the velocities computed using random delays). As expected, the random velocities appear to be related more strongly to the trait lengths, as compared to the observed velocities (p<0.001). In other words, when one divides the lengths by the randomized delays, the resulting velocities become a function of the trait length alone. On the other hand, when one divides the trait lengths by the observed delays, these show that the longer traits appear to be faster than if the delays were only a function of distance. The mean (red line) and upper and lower bounds (shaded area) of the surrogate velocities derived from surrogate delays (grouped by the percentile of the corresponding trait length) are shown in figure 1, bottom - middle, confirming in real data that the velocities of transmission grow as a function of the length of the traits, such that the longer traits are also the faster ones. Next, we sought to test our framework in patients affected by multiple sclerosis, which is a prototypical disease where myelin in the central nervous system is selectively attacked by the immune system. We expect to observe higher delays in patients (KS test, p<0,001). Then, for each patient, the average delay of each edge was compared to the average delay of each corresponding edge in the controls. Hence, we obtained, per each patient, the difference between the edge-specific delay and the corresponding average delay in the controls. We found higher delays in patients as compared to controls. Finally, while it is reasonable to expect globally higher delays in patients as compared to controls, the edges that are directly lesioned might be more prominently affected as compared to unaffected ones. We identified, per each patient, based on the structural damage, healthy and lesioned edges. The delays in the lesioned edges are more slowed down (with respect to the corresponding delays in the healthy population) as compared to healthy edges (p<0.0001). Conclusions Our technique provides a practical approach for estimating functional transmission delays in vivo at the single-subject and single-fiber level and, thus, opens the possibility for novel diagnostic and curative interventions as well as providing empirical, subject-specific constraints to tailor brain models. Furthermore, our technique captures the longer delays that are likely to be induced by myelin lesions in multiple sclerosis.

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SESAME: a powerful Bayeisan method for Magneto/Electro-EnchephaloGraphy inverse problem

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Magneto/Electro-EnchephaloGraphy (M/EEG) is a non-invasive medical imaging technique whose aim is the reconstruction of underlying neural current given the magnetic or electric field measured outside the scalp.
The localization of the brain activity is of particular interest in several fields, such as: the pre-surgical evaluation of epileptic patients and the study of degenerative diseases such as Alzheimer and schizophrenia.
For the resolution of the M/EEG inverse problem many sophisticated methods have been developed considering different techniques: regularization, machine learning and probabilistic approaches.
SESAME (Sequential Semi-Analytic Monte Carlo Estimation) [1, 2] is a probabilistic algorithm based on a specific class of Monte Carlo methods, the Sequential Monte Carlo (SMC) samplers, whose output is the estimated probability distribution for the number of sources and the source localization, and an analytical estimate for the source intensity.
The main advantage of using a Bayesian approach is the possibility of obtaining not only estimates from the approximated posterior distribution, such as the mean or the maximum of the distribution, but also to evaluate uncertainty quantification. This is a useful advantage for SESAME; indeed having knowledge on how much one can trust the obtained solution is crucial in an inverse problem where there are multiple configurations of active brain regions that generate the same magnetic/electric field. But what makes SESAME unique in the M/EEG world, is its capability of exploring different configurations for the number of active regions, giving an approximation of the probability distribution for the number of sources in addition to the distribution for their locations.
Nowadays SESAME is available both open source and in a commercial version and it is possible to find it in the most common softwares for brain imaging such as MNE python and Brainstorm.
The talk presents SESAME from a mathematical point of view and shows some comparison with widely used inversion methods in the M/EEG world showing its performances and advantages.

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MS10 - Recent advances in polytopal methods for coupled problems

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ABSTRACT

The numerical solution of coupled problems is of utmost relevance, as the interaction of several physical laws, objects with different materials and properties, and phenomena that occur on different spatial or temporal scales are consistently found in nature. In this context, polytopal discretization methods offer several key advantages. One of the most attractive aspects consists in their flexibility to handle complex geometrical situations such as those arising from multiphysics, multiscale, mixed-dimensional, and interface problems. Indeed, these models often involve coupling terms and transmission conditions localized on sub-regions of the computational domain that need to be accurately represented without compromising the efficiency. Another appealing feature of advanced numerical schemes supporting general meshes in the context of coupled problems is their arbitrary-order accuracy which usually favors stable and robust designs.

This minisymposium is devoted to new and advanced strategies based on the use of polytopal methods (such as, e.g., discontinuous Galerkin, Virtual Element, and Hybrid High-Order) and their combination with standard discretization schemes to address important challenges in the numerical solution of coupled problems. The topics of interest include (but are not limited to): i) coupled poromechanics modeling geological materials and biological tissues, ii) non-isothermal flow and deformation processes, iii) multiphysics simulation in heterogeneous media, iv) bulk-surface couplings, v) fracture and contact mechanics, and vi) fluid-structure interaction problems.

Intrinsic Surface VEM for Vector Laplacian

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We present an extension of the geometrically intrinsic formulation of the arbitrary-order Virtual Element Method (VEM) to vector-valued surface Laplacian on polygonal cells. The equation, written in covariant form using an appropriate local reference system, is discretized by the VEM approach. The knowledge of the local parametrization allows us to derive a two-dimensional VEM scheme for the contravariant components of the solution vector. The main advantage of the proposed formulation is that there is no need of additional projections or penalizations as the unknowns of the equation are objects that live intrinsically in the tangent space. We evaluate the method on several surfaces to show experimental convergence rates.

Numerical modelling of wave propagation phenomena in thermo-poroelastic media via discontinuous Galerkin methods

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Poroelasticity inspects the interaction among fluid flow and elastic deformations within a porous medium. In several applications in the context of environmental sustainability, such as geothermal energy production and CO2 sequestration, temperature plays a key role in the description of the physical phenomena. Moreover, the thermo-poroelastic model finds application in the context of seismicity and induced seismicity.
In order to correctly describe these processes, the differential problem should also take into account the influence of the temperature, leading to a fully-coupled thermo-poroelastic (TPE) system of equations [3]. To correctly describe the seismic case, the study of the fully-dynamic TPE problem is necessary. We present and analyze a a high-order discontinuous Galerkin method on polygonal and polyhedral grids (PolyDG) for the wave propagation model in TPE media [2]. For the semi-discrete problem, we derive stability and *hp*-version error estimates in suitable energy norms. The fully-discrete scheme is then obtained by coupling the space discretization with an implicit Newmark-β time integration scheme.
Finally, we report a wide set of numerical simulations, both for verification of the theoretical estimates and for examples of physical interest, such as the case where the medium is heterogeneous. A comparison with the results of the poroelastic model [1] is provided too, highlighting the differences between the predictive capabilities of the two models.

Key-words: discontinuous Galerkin method, thermo-poroelasticity, wave propagation, polygonal and polyhedral meshes.

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A coupled VEM-MFD formulation for poromechanics

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The simulation of underground deformations induced by flow in real scenarios can, in many cases, be limited or slowed down by meshing issues, especially when the numerical discretization methods are limited to polyhedra of standard shape, such as tetrahedra or hexahedra. New generation numerical methods such as Mimetic Finite Differences (MFD) [K. Lipnikov et al., *Mimetic finite difference method*, 2014] and Virtual Element Methods (VEM) [L. Beirão da Veiga et al., *A Virtual Element Method for elastic and inelastic problems on polytope meshes*, 2015], can help circumventing such issues, since they allow for more general star-shaped polygons or polyhedra and treat aligned edges and aligned faces naturally.

We describe a fully coupled scheme of multiphase flow and poromechanics, where MFD are used to discretize the flow equations and VEM are used for mechanics (the 2D version of the method was proposed in [A. Borio et al., *Hybrid mimetic finite-difference and virtual element formulation for coupled poromechanics*, 2021]). The method has the interesting feature of allowing the use of polyhedral meshes. We present some standard tests validating the method and some results on realistic domains obtained by an optimized implementation of the scheme carried out within a massively parallel open source multiphysics simulator (`https://www.geosx.org`).

A Deep Learning algorithm to accelerate Algebraic Multigrid methods in Finite Element solvers

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Algebraic multigrid (AMG) methods [3] are among the most efficient solvers for linear systems of equations and they are widely used for the solution of problems stemming from the discretization of Partial Differential Equations (PDEs). The most severe limitation of AMG methods is the dependence on parameters that require to be fine-tuned. In particular, the strong threshold parameter is the most relevant since it stands at the basis of the construction of successively coarser grids needed by the AMG methods. We present a novel deep learning algorithm to accelerate the convergence of AMG methods [1, 2]. An Artificial Neural Network (ANN), comprised of a dense and convolutional part, tunes the value of the strong threshold parameter by interpreting the sparse matrix of the linear system as a black-and-white image and exploiting a pooling operator to transform it into a small multi-channel image. To demonstrate the practical capabilities of the proposed algorithm, we apply it to the iterative solution of the linear systems of equations stemming from Finite Element discretizations of two and three-dimensional model problems with structured, unstructured, and polytopal grids. Namely, we consider diffusion equations with a highly heterogeneous coefficient, stationary Stokes problems, and linear elasticity problems with a highly heterogeneous Young's modulus. When tested on problems with coefficients or geometries not present in the training dataset, our approach reduces the computational time by up to 30% with respect to using the value commonly found in the literature.

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A novel family of hybrid Finite Volume / Virtual Element methods for incompressible flows on unstructured meshes

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We present a new family of high order accurate semi-implicit schemes for the solution of non-linear hyperbolic partial differential equations (PDE) on unstructured polygonal meshes [2]. The time discretization is based on a splitting between explicit and implicit terms that may arise either from the multi-scale nature of the governing equations, which involve both slow and fast scales, or in the context of projection methods, where the numerical solution is projected onto the physically meaningful solution manifold. We propose using a high order finite volume (FV) scheme for the explicit terms in order to ensure conservation property and robustness across shock waves while the discretization of the implicit terms, which typically calls for the solution of an elliptic problem, is handled by the virtual element method (VEM) [1]. The numerical solution is then converted from the FV to the VEM solution space and vice versa using appropriate L_2 projection operators. High order time accuracy is then achieved using the semi-implicit IMEX Runge-Kutta schemes, which are proven to be asymptotic preserving (AP) and well-balanced (WB). We investigate two representitive models, i.e. the incompressible Navier-Stokes equations (INS) [3], which are solved with the aid of a projection method to satisfy the solenoidal constraint of the velocity field, and the shallow water equations (SWE) [4], which entails multiple time scales each characterized by a different Froude number. Several numerical experiments demonstrate the accuracy and the capabilities of the new family of schemes to solve relevant benchmarks in the field of incompressible fluids.

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A virtual element method for the solution of time-harmonic elastic wave equations via scalar potentials

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Soft tissues and other nearly incompressible media present a challenge when simulating the propagation of elastic waves. This challenge arises from the disparity in the speed of shear waves compared to pressure waves. To address this issue, a classical Helmholtz-Hodge decomposition is employed to separate the displacement field into scalar pressure (P-) and shear (S-) waves. This enables the independent treatment of these two types of dynamics and facilitates the construction of discretization spaces suitable for each wave type.

This presentation focuses on the simulation of two-dimensional time-harmonic elastic wave soft scattering in isotropic homogeneous media, using the scalar potential decomposition. For problems defined within bounded domains, we propose a Virtual Element Method (VEM) that utilizes varying mesh sizes and degrees of accuracy to approximate the two scalar potentials. In the case of unbounded domains, a boundary element method is coupled with the VEM. This combined approach enables the tracking of different wave numbers associated with the propagation speeds of P-waves and S-waves. Notably, higher-order methods can be employed to approximate waves with higher wave numbers.

We establish the stability of our method and present a convergence error estimate in the L^2-norm for the displacement field. Importantly, our error estimate distinguishes the contributions to the error associated with P-waves and S-waves. To demonstrate the effectiveness of the proposed approach, we provide numerical results. This presentation is the result of collaborative work with S. Falletta and L. Scuderi from the Polytechnic University of Turin.

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Mixed Virtual Element approximation of linear acoustic wave equation

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The numerical simulation of acoustic, elastic, or electromagnetic wave propagation finds application in many scientific disciplines, including aerospace, geophysics, civil engineering, telecommunications, and medicine for instance. The present work considers a Mixed Virtual Element method on general polytopal grids for the discretization of the acoustic wave equation written as a first-order system of hyperbolic partial differential equations. In the absence of external loads, the semi-discrete method exactly conserves the system energy. To integrate in time the semi-discrete problem we consider a classical θ-method scheme. We carry out the stability and convergence analysis in the energy norm for the semi-discrete problem showing an optimal rate of convergence with respect to the mesh size. We further study the property of energy conservation for the fully-discrete system. Finally, we present some verification tests as well as engineering applications of the method.

Discrete Weber inequalities and related Maxwell compactness for hybrid spaces over polyhedral partitions

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We prove discrete versions of the first and second *Weber inequalities* on $\mathbf{H}(\mathbf{curl}) \cap \mathbf{H}(\mathrm{div})$-like hybrid spaces spanned by polynomials attached to the faces and to the cells of a polyhedral mesh [1]. Moreover, we also establish the related discrete Maxwell compactness properties within a general topological setting. The proven hybrid Weber inequalities are optimal in the sense that:

1. they are formulated in terms of $\mathbf{H}(\mathbf{curl})$- and $\mathbf{H}(\mathrm{div})$-like hybrid semi-norms designed so as to embed optimally (polynomially) consistent face penalty terms;
2. they are valid for face polynomials in the smallest possible stability-compatible spaces.

Crucially, our results make possible the analysis of hybrid polyhedral approximations of general div-curl systems on domains with arbitrary topology. As an instance, our work paves the way to the polyhedral approximation of non-linear (Hilbertian) div-curl problems, as they may arise in the modeling of ferromagnetic materials. The targeted numerical methods include the HDG (Hybridizable Discontinous Galerkin), HHO (Hybrid High-Order), or weak Galerkin methods.

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CIP-stabilized Virtual Element Method for advection-dominated problems

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In convection-dominated problems, standard numerical schemes produce unsatisfactory solutions with spurious oscillations near the element boundaries. To overcome these difficulties, one possibility is to use the method proposed by the pioneering work of Douglas and Dupont [5] which consists in adding a term that penalizes the gradient jump at mesh interfaces. This technique is known as Continuous Interior Penalty (CIP). Many Finite Element Methods (FEMs) with CIP were implemented to solve a large number of equations like the advection-diffusion-reaction equation [2], Stokes equation [3], Oseen equation [1], and Helmholtz equation [4]. We would like to extend these results to Virtual Element Methods (VEMs) and we want to devise a VEM that benefits from this technique. We will consider some well-known equations like the advection-diffusion-reaction equation. Under standard regularity assumptions, we will prove that the numerical solutions converge to the analytic solutions with the expected ratio in the L^2 and H^1 norms and we will show some convergence graphs.

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Virtual element method for the Navier-Stokes equation coupled with the heat equation

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The present talk deals with the stationary flow of a viscous incompressible fluid, in the case where the viscosity of the fluid depends on the temperature.
We present the virtual element discretization of the coupled problem, show its well-posedness and prove optimal error estimates and exploit the divergence-free property of the discrete velocity solution. Finally, numerical experiments confirming the theoretical error bounds are also presented.

Virtual Element approximation for poroelasticity problems

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In these years, the applications of the Virtual Element Method (VEM) to computational mechanics have met many successes, both for its robustness in treating general polygonal and polyhedral meshes, including hanging nodes and non-convex elements, and for its great flexibility in handling some features of the problems. In particular, for elasticity problems, whose variational formulation is based on the Hellinger-Reissner principle, the Virtual Element approach turned out to be a valid alternative to the classical Galerkin methods, for instance, Finite Elements, providing stable 2D/3D schemes which preserve the symmetry of the stress tensor, the continuity of the tractions and they are reasonable cheap with respect to the delivered accuracy [1, 2, 3]. Recently, exploiting these features of VEM, we focus our attention on the application of this technology to the quasi-static Biot's consolidation problem describing Darcian flow in a deformable saturated porous medium [4]. The idea is to design a low-order VE method for the four-field formulation, where the symmetry of the stress field is strongly imposed in the discrete space.
In this talk, we briefly introduce the Virtual Elements for the elasticity problems and then present the recent developments for the poroelasticity problems. Some numerical tests are provided to show the validity and the potential of the proposed methods.
This work is in collaboration with M. Botti, F. Dassi, A. Fumagalli, D. Prada, S. Scialò, A. Scotti and G. Vacca.

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Inf-sup theory for the Biot's equations in poroelasticity

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The quasi-static Biot equations in poroelasticity describe the flow of a Newtonian fluid inside an elastic porous medium. The main unknowns are the displacement of elastic medium and the pressure of the fluid. The analysis and the discretization of the equations are typically driven either by the Faedo-Galerkin scheme or by the theory of implicit evolution equations.

We propose a new approach, based on the inf-sup theory, i.e. on the Banach-Nečas theorem for linear variational problems. This yields a new result on the well-posedness of the equations, including a sharp stability estimate, which controls the two main variables in suitable norms as well as two auxiliary variables, namely the total pressure and the total fluid content.

We introduce a class of discretizations inspired by the above analytical results. We establish quasi-optimal and robust a priori error estimates and comment on the regularity of the solution that is necessary in order to ensure a rate of convergence of the error to zero. Finally, we discuss a possible linear solver.

MS11 - Mathematical methods and tools for Imaging Problems in real-life applications

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ABSTRACT

Imaging problems (denoising, deblurring, segmentation, classification, decomposition, etc.) arise in various real-world application fields, such as medicine, biology, security, and industrial control. Under each of these fields, technological developments of recent years have highlighted not only the need to store and analyze huge amounts of image data but also to deal with noise and artifacts due to acquisition imaging tools, for example, bias field produced by magnetic resonance scanners, speckle noise detected in medical or in Synthetic Aperture Radar images, photobleaching, and low contrast caused by fluorescence microscopy, and so on. All of these problems require ad-hoc numerical methods able to tackle several issues such as high dimensionality, uncertainty, ill-posedness, and ill-conditioning. The mini-symposium aims to foster discussion and collaboration among researchers in different application fields and promote interest in mathematical methods, algorithms, and tools to face imaging problems.

Characterization and reduction of mixed and structured noise in PRISMA hyperspectral images

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The PRISMA hyperspectral satellite mission, launched in 2019 by the Italian Space Agency, includes a hyperspectral imager that collects the reflected Earth signal in the 400-2500 nm spectral range (VNIR and SWIR), covering up to 256 spectral bands. PRISMA images are corrupted by both random noise and fixed pattern noise[3]. Striping, as well as other fixed effects, is normally related to calibration error and should be mitigated in a preliminary data processing. In new-generation hyperspectral sensors, where electronic noise is not dominant, random noise can be further decomposed in photon noise (depending on the signal intensity) and thermal noise[1]. Algorithms for preliminary destriping, for noise characterization[2] and noise reduction are presented and their performance on several PRISMA L1 (Top-of-Atmosphere radiance) images acquired on different sites is discussed.

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Variational additive image decomposition into cartoon, harmonic and oscillatory components

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Additive image decomposition into piece-wise constant (cartoon) and oscillatory (texture) components is the point of interest since early 2000s [1]. In this talk, we will discuss newer advances of additive decomposition, in particular into piece-wise constant, smooth, and oscillatory components [2, 3], which is motivated not only by image denoising and structure separation, but also by shadow and spot light removal. To that aim, we propose a nonconvex variational decomposition model which, for a given image, separates the piece-wise constant part via TV-like nonconvex regularization, harmonic term via second-order regularization, and oscillatory (noise and texture) term via a H^{-1}-norm penalty. There are interesting interactions between these three regularization terms; the proposed model clearly separates the piece-wise constant structure and smoothly varying harmonic part, thanks to having a separated oscillatory component. Various examples show the robustness against a high level of noise and applications to soft spotlight and shadow removal. Moreover, a simple adaptation of the proposed model to 1D signal decomposition [4, 5] represents a powerful pre-processing tool to frequency analysis that confirms the range of applicability of the proposed model in real-life applications.

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Cultural Heritage Preservation through Multispectral Imaging: Preliminary Results from the IMAGO Project

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The IMAGO project aims to develop an innovative system that utilizes Multispectral Imaging and Augmented Reality (AR) techniques for studying and preserving cultural heritage. By employing machine learning algorithms on multispectral images, the system can detect lost original elements and hidden features in cultural artifacts, offering a unique perspective beyond human vision.

Here we show some preliminary results related to the multi spectral analysis conducted on three paintings attributed to Cavalier d'Arpino (Giuseppe Cesari) located at the Galleria dell'Accademia Nazionale di San Luca in Rome. Non-invasive and portable techniques such as Energy Dispersive X-ray Fluorescence (ED-XRF) spectrometry, Fiber Optics Reflectance Spectroscopy (FORS), UV fluorescence imaging, and Multispectral (MS) imaging were employed. Preliminary characterization of the pictorial materials was achieved through FORS and ED-XRF analyses, allowing the identification of pigments used for the creation of the three paintings and highlighting similarities and differences in the palette.

MS images, acquired between the ultraviolet and near-infrared regions (NIR), revealed significant differences between visible and NIR images with some details of the paintings transparent in the infrared region. Furthermore, data clustering algorithms were applied to the MS images, enabling semantic segmentation and providing extrapolation of salient parts of the artwork and better perception of details.

The combined results of this work contribute to the preservation and interpretation of cultural heritage and are of paramount importance for the developing of the IMAGO system.

Acknowledgments This work is part of a project founded by Regione Lazio and MUR ("IMAGO - Multispectral Imaging for Art, Gamification and hOlografic reality" project)

Speckle noise removal via learned variational models

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In this talk, we address the image denoising problem in presence of speckle degradation typically arising in ultra-sound images. Variational methods and Convolutional Neural Networks (CNNs) are considered well-established methods for specific noise types, such as Gaussian and Poisson noise. Nonetheless, the advances achieved by these two classes of strategies are limited when tackling the de-speckle problem. In fact, variational methods for speckle removal typically amounts to solve a non-convex functional with the related issues from the convergence viewpoint; on the other hand, the lack of large datasets of noise-free ultra-sound images has not allowed the extension of the state-of-the-art CNN denoiser methods to the case of speckle degradation. Here, we aim at combining the classical variational methods with the predictive properties of CNNs by considering a weighted total variation regularized model; the local weights are obtained as the output of a statistically inspired neural network that is trained on a small and composite dataset of natural and synthetic images. The resulting non-convex variational model, which is minimized by means of the Alternating Direction Method of Multipliers (ADMM) is proven to converge to a stationary point. Numerical tests show the effectiveness of our approach for the denoising of natural and satellite images.

Deep learning methods for the automatic classification of autoimmune bullous skin diseases

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The term AutoImmune Bullous Diseases (AIBDs) is an umbrella term for a collection of rare skin disorders, in which autoantibodies attack the proteins of the epidermis and the basal membrane. The disease has a high morbidity rate, which can become fatal if not properly treated [1]. The correct diagnosis and classification of AIBDs require the analysis of ImmunoFluorescence (IF) skin images. The two main IF patterns are the Linear Pattern (LP) and the Intercellular Pattern (IP) [2]. Up to now, the diagnosis can only be performed in highly specialized centers with highly trained operators [3]. Thus, it is worth exploring the possibility of an automatic diagnosis of AIBDs.
In this study, we follow a data-driven approach and exploit deep convolutional neural networks within a transfer-learning framework to design an automatic classification of the acquired immunofluorescence (IF) skin images.
For the design of our classification model, we incorporate the visual analysis of the basal membrane, which is the diagnosis prior given by the experts in the field. To this purpose, we first adopt a segmentation framework to automatically predict the region in the IF images that our experts mostly evaluate for the diagnosis of AIBDs. Then comes the incorporation of this prior information in the two-branches Convolutional Neural Network (CNN), whose input is represented by both the IF image and the predicted segmentation mask of the basal membrane.
The results demonstrate that our classification pipeline, with the incorporation of medical diagnosis prior, increases the test accuracy with respect to baseline classifiers. This could reinforce the medical trust in deep learning algorithms for the automatic classification of AIBDs skin disorders.

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Multiple Instance Learning for Medical Image Classification

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A Multiple Instance Learning (MIL) problem [1] consists of classifying sets of points, called bags. The points inside the bags are called instances. Different from the classical supervised classification, in an MIL problem, during the learning phase, only the labels of the bags are known, whereas the labels of the instances inside the bags are unknown. Various MIL applications are found in different fields, such as text categorization, image classification, bankruptcy prediction, speaker identification, and video analysis. For example, in text categorization, the aim is to associate a text (bag) to a particular topic of interest on the basis of some keywords (instances), while, in image classification, the objective is to categorize an image (bag) on the basis of some its subregions (instances).
An interesting application of the MIL is also in diagnostics by means of medical images. In this case, the objective is to discriminate between nonhealthy and healthy patients on the basis of their medical scan (bag): a patient is "positive" if he/she presents at least an abnormal subregion (instance) in his/her medical scan; vice versa, a patient is "negative" if all the subregions (instances) in his/her medical scan are healthy. This example fits very well with the so-called standard MIL assumption, which is often adopted in the presence of two classes of bags and two classes of instances: based on this assumption, a bag is positive if it contains at least a positive instance (nonhealthy subregion), and it is negative if all its instances are negative (the healthy subregions).
We present some MIL applications aimed at discriminating, by means of medical images, between nonhealthy and healthy patients in three different medical fields: melanoma detection, pneumonia detection and diabetic retinopathy detection. Extensive numerical results are also discussed.

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MS12 - Data driven methods for inverse problems in imaging

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ABSTRACT

Inverse problems in imaging science represent a highly relevant research topic for over a decade now. The attractiveness of image processing ignited an outburst in its range of applicability and usage in many scientific and industrial areas, including medical, astronomical, seismic and automation applications.

Although each imaging application may elaborate on different data, mathematically the observed input image can be defined as product of a so called forward operator, which incorporates the specific corruption of reality during the acquisition process. A widely used strategy to recover the original image is to define and resolve the inverse problem to the forward process, which is typically ill-posed. The ill-posedness makes the choice of a prior a crucial point in getting accurate reconstructions. The main prior attribute is its capability of modelling the target solution properties in a realistic way. Classical hand-crafted priors are designed so as to exploit various global properties related to the sparsity or the regularity of the unknown original image. However, recent advances in terms of storage capability, for a wide class of applications, facilitated the availability of large amounts of training examples. These can be successfully employed in the design of more sophisticated and flexible priors, which have the ability to model complex structures in the images of interest. The aim of this session is to provide a discussion on new results and applications on data-driven approaches, with distinct focus on the variability and challenges the input data impose. In particular, the goal is to explore the synergies between model-based and data-driven approaches and to analyze novel strategies for extracting meaningful information from the available data, accompanied by investigation into the latest optimization techniques tackling the related large-scale problems.

Quality measure score predictor for imaging via SVR

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Accurate assessment of image quality is of utmost importance in various imaging applications, including medical diagnostics, remote sensing, computer vision, and denoising-deblurring tasks in general. In this presentation, we propose a novel approach using Support Vector machines for Regression (SVR) to predict quality measure scores specifically for imaging tasks. Several times in the literature, methods trained as SVR have been used as performance measure predictor, both in the context of imaging [1] and Deep Learning [2]. SVR, known for its ability to handle non-linear relationships and high-dimensional data, is leveraged to develop a reliable predictor for quality evaluations. On the other hand, variational models are a classical tool for many imaging problems, but they do have known limitations, as the absence of general guidelines for selecting the hyperparameters they depend on. Bilevel optimization schemes have been proposed in order to overcome this issue and learn a satisfying set of hyperparameters [3]. In particular, they offer a high level of interpretability while keeping the amount of data required low. We use our performance predictor, based on SVR, to set the hyperparameters of an optimization scheme obtained by unrolling a fixed number of FISTA-like iterations applied to the minimization of a suitable energy functional [4, 5]. Model-based data-augmentation strategies have been adopted to overcome issues related to the richness and the significance of the training dataset. The resulting SVR-based quality measure score predictor showed encouraging performances on an extensive numerical experimentation, validating its potential for accurate and efficient quality assessment in imaging applications.

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Some New Criteria for Automatic Parameter Selection in Variational Models for Poisson Noise Corruption

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Poisson noise is a pervasive cause of data degradation in many inverse imaging problems. Typical applications where Poisson noise removal is a crucial issue are astronomical and medical imaging. Both scenarios can in fact be characterized by a "low-light" condition, which is intrinsically related to the acquisition set-up in the former case, while in the latter it is somehow preferable so as to preserve the specimen of interest (microscopy) or keep the patient safer by irradiating lower electromagnetic doses (CT). However, the weaker the light intensity, the stronger the Poisson noise degradation in the acquired images and the more difficult the reconstruction problem.
Variational methods are an effective model-based approach for reconstructing images corrupted by Poisson noise. However, their performance strongly depends on a suitable selection of the regularization parameter balancing the effect of the regulation term(s) and the data fidelity term. One of the approaches still most used today for choosing the parameter is the discrepancy principle proposed in [1]. It relies on imposing a value of the data term approximately equal to its expected value and works quite well for mid- and high-photon counting scenarios. However, the approximation used in the theoretical derivation of the expected value leads to poor performance for low-count Poisson noise. The talk will illustrate three novel parameter selection strategies which are demonstrated to outperform the state-of-the-art discrepancy principle in [1], especially in the low-count regime. The three approaches rely on decreasing the approximation error in [1] by means of a suitable Montecarlo simulation [2], on applying a so-called Poisson whiteness principle [3] and on cleverly masking the data used for the parameter selection [4], respectively. Extensive experiments are presented which prove the effectiveness of the three novel methods.

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A Reduced Order Approach for Artificial Neural Networks applied to Object Recognition

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Computer Vision is a thriving field increasingly exploited in several scientific and engineering contexts in order to solve complex tasks such as the recognition and detection of objects inside pictures. A possible approach to deal with image processing problems is represented by Convolutional Neural Networks (CNNs). Such architectures well perform on complex tasks such as object recognition but may require a high number of layers to extract all the features of the problem at hand, leading to more parameters to be calibrated during the training phase. This naturally opens several computational issues in the learning procedure, as well as in the memory and space required by the model itself, especially in the case these networks have to operate in vision devices with limited hardware. A possible solution for the aforementioned problem is represented by the development of a dimensionality reduction technique for CNNs by employing Proper Orthogonal Decomposition (POD), a method widely used in the context of Reduced Order Modeling, or Higher Order SVD (HOSVD), to keep into account the intrinsic tensorial structure. The reduced network is then obtained by splitting the original one in two different nets connected by the reduction technique: the first one obtained by retaining a certain number of layers of the original model and a second one that deals with the classification of the features extracted by the previous part.
In our works [1, 2, 3] we propose several version of reduced networks to tackle two different problems: image recognition and object detection. For the first case, we provide the numerical results obtained by applying such method to benchmark CNNs, such as VGG-16 and ResNet-110, using CIFAR-10, CIFAR-100 and a custom dataset [1, 3]. For the object detection case, we present a possible generalization of the method proposed for Artificial Neural Networks to object detectors and in particular to SSD-300 or neural networks with a similar architecture [2, 3]. We then provide the results obtained by training our reduced model against the PASCALVOC dataset.

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Randomized Inversion Methods for EEG imaging

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Reconstructing the brain activity map from electroencephalographic (EEG) measurements requires solving an ill-posed and ill-conditioned inverse problem [1]. As a preliminary regularization step, we use the dipole sampling method [2, 3], which also allows us to reduce the dimensionality of the inverse EEG problem. Then, we solve the low dimensional problem using weighted Minimum Norm Estimate (wMNE) [4] and standardized LOw Resolution brain Electromagnetic TomogrAphy (sLORETA) [5] algorithms as inversion methods. We provide error estimates of the reconstruction error, i.e., the difference between the brain activity map obtained by solving the full EEG inverse problem and that one obtained by solving the low-dimensional problem. Numerical tests we performed on synthetic EEG data confirm the effectiveness of the randomized version of the wMNE and sLORETA algorithms.

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Estimating hyper-parameters for an inverse problem in brain imaging

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Electroencephalography (EEG) and magnetoencephalography (MEG) are non-invasive neuromaging techniques with one-millisecond temporal resolution. The M/EEG inverse problem consists in estimating the spatio-temporal distribution of the brain electrical activity, based on recordings of the magnetic/electric field at the scalp [1]. Standard approaches to solving the M/EEG inverse problem comprise Tikhonov regularization with an ℓ^2 penalty term and, more recently, spatio-temporal solvers promoting solutions that are sparse in the spatial domain and smooth in the temporal domain. However, the majority of available inverse methods tend to have a rather strong dependence on the value of the regularization parameter [2], which is typically difficult to know in practice.
In this talk, I will describe a hierarchical Bayesian framework for solving the M/EEG inverse problem, and two recent advances [3, 4] that allow to estimate hyperparameters from the data, making the method particularly robust against hyperparameter misspecification.

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MS13 - Approximation methods, functional equations and applications

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ABSTRACT

Numerical methods are the basis for approaching a wide variety of mathematical models arising from applications. The aim of this minisymposium is to gather researchers working on different kinds of

natural phenomena and physical processes, modeled by evolutionary problems such as ordinary differential equations, partial differential equations, fractional equations and Volterra integral equations. Particular attention will be devoted to the derivation of efficient numerical methods which are able to accurately follow the qualitative and quantitative behavior of the solution, possibly also by employing parallel strategies. Applications in several contexts will be considered, among which: enviromental models, image processing methods in medical field, image restoration, population and epidemic models, economic models, metastatic tumor growth models. Theoretical and practical contributions will be also welcome.

Bistability of a mathematical model for the control of an olive tree disease

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In this talk I will present a plant epidemic model accounting for interactions between some beneficial phyllosphere organisms and a phytopathogen fungus by means of a four dimensional Ordinary Differential Equation (ODE) system. The system possesses five equilibria that are suitably analyzed for feasibility and stability. Numerical simulations show potentially interesting bistable behavior, exhibited by three different pairs of equilibria, as well as persistent oscillations in some cases [1]. All three pairs of bistable equilibrium points, for the four dimensional model, have been analyzed by approximating the basins of stability, plus the bistable case for the three dimensional model where the beneficial phyllosphere organisms is not yet inserted in the olive system [2]. Knowing more about the bistable dynamics of the system allows the possible assessment of human intervention for control of the disease.

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Non local equations for image restoration: Space scale properties of the continuous and discrete approach with practical illustrations

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In this talk we describe how non-local evolutionary equations can play a key role in image processing/restoration. From the continuous model to the fully discrete one the theoretical framework is described in here, with special regard to the classical space scale axiomatic within the continuous and semi-discrete settings. The performance of these models in practical instances is shown, in fact we illustrate the theoretical results with their performance with medical images.
This talk is a part of results published in [1].

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Solving numerical problems arising in environmental modeling through parallel strategies

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This work focuses on the task of fitting data derived from environmental problems. Numerous procedures and methods have been documented in the literature to address this objective [3]; however, when dealing with real datasets, they all encounter significant computational complexity. In this study, we propose an innovative GPU parallel algorithm that is specifically designed for accurately fitting environmental and bathymetric data, utilizing the Kriging method [2]. By harnessing the capabilities of advanced parallel computing architectures, our implementation efficiently tackles large-scale problems [1]. Experimental tests have confirmed substantial improvements in terms of execution times and memory usage. These enhancements have been achieved by leveraging appropriate parallel numerical libraries and custom-designed parallel kernels within the CUDA environment.

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Analytical and numerical preservation properties of a modified SIR model with contact matrix: application to the diffusion of information

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In this talk, we aim to analyze a modified SIR (Susceptible-Infected-Recovered) model with contact matrix [1, 1]. Theoretical results concerning the positivity of the analytical solution, the conservation of the total population, and the stability of the equilibrium points are given. Moreover, the numerical preservation of these properties through by step by schemes based on Standard and non Standard Finite Difference methods [6], and on the Modified Patankar Euler method [1], is studied.
The above results are applied to the diffusion of information in social networks [3, 2]. Several numerical experiments on real data on social platforms, like Twitter, Instagram and Facebook, are shown in order to prove the effectiveness of the different numerical approaches.

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A Nyström-type method for Volterra integral equations based on equispaced nodes

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This talk deals with the numerical treatment of Volterra integral equations of the type

$$f(s) + \mu \int_0^s k(t,s) f(t)(s-t)^\alpha t^\beta dt = g(s), \quad s \in (0,1],$$

where $\alpha, \beta > -1$, $\mu \in \mathbb{R}$, f is the function to determine, the right-hand side g is defined on [0, 1], and the kernel k is defined on $\mathcal{D} = \{(t,s) : 0 < t < s \leq 1\}$,
A Nyström-type method based on Generalized Bernstein polynomials is presented [1].
Stability and convergence are studied in the space of continuous functions, and several numerical tests are presented to show the performance of the proposed approach.

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Fast Solvers for a Phase Field Corrosion Model

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A phase field model for simulating the deterioration of 304 stainless steel metal due to contact with a sodium chloride solution, has been quite recently introduced in [3].
This model consists of a system of two PDEs characterized by high stiffness that makes unpractical the use of explicit integrators, as they require extremely small time steps for stability.
In this talk we present some efficient solvers for the solution of the considered problem. These schemes are obtained by combining a standard finite difference approximation in space, and a time integrator that exploits the Kronecker-sum structure of the discrete Laplacian for the fast solution of the system of ODEs obtained.
Numerical tests on two benchmark problems are proposed to show the efficiency of the proposed methods, in comparison with other techniques from the literature based on the use of higher-order exponential methods [1, 2].
We will finally present a time fractional model for the anomalous diffusion of chloride ions in reinforced concrete [4] and a conservative numerical method for its solution [5].

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A network-constrain Weibull AFT model based on proximal gradient descent method

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In this work, we propose and explore a novel network-constraint survival methodology considering the Weibull accelerated failure time (AFT) model combined with a penalized likelihood approach for variable selection and estimation [2]. Our estimator explicitly incorporates the correlation patterns among predictors using a double penalty that promotes both sparsity and the grouping effect. In order to solve the structured sparse regression problems we present an efficient iterative computational algorithm based on proximal gradient descent method [1]. We establish the theoretical consistency of the proposed estimator and moreover, we evaluate its performance both on synthetic and real data examples.

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A Nyström method for Hammerstein integral equations on a closed interval

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The talk is about the numerical approximation of nonlinear integral equations of the Hammerstein type, defined on the closed real interval $[-1,1]$:

$$f(y) + \lambda \int_{-1}^{1} k(x,y)h(x,f(x))dx = g(y), \qquad y \in [-1,1], \tag{1}$$

where λ is a fixed real parameter, with $|\lambda| \leq 1$, g and k are known functions defined on $[-1,1]$ and $[-1,1]^2$, respectively, h, defined on $[-1,1]^2$, is assumed to be nonlinear in f, and f is the unknown in $[-1,1]$.

The Hammerstein integral equations appear in nonlinear physical phenomenons such as electromagnetic fluid dynamics, reformulation of boundary value problems with a nonlinear boundary condition (for instance see [2]).

There are several numerical methods for approximating the solution of (1). The most popular ones are collocation methods [4], Galerkin methods [3] and Nyström methods [1, 5], based on piecewise polynomial approximation.

Here we propose a numerical method of Nyström type based on a Gaussian quadrature formula. Equation (1) is discretized by the Nyström method and the nonlinear system is solved by an iteration scheme (it can be the Newton's method or the Broyden's one). This choice allows to use a global approximation approach and to treat the weighed case in a second step.

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On the numerical solution of some Volterra integral equations reformulating metastatic tumor growth models with treatment

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Modeling metastatic tumor growth with treatment is of paramount importance in developing and advancing knowledge about curing cancer. It is also important to introduce efficient numerical methods to solve the introduced models.
One possible approach to model metastatic tumor growth is via a size-structured partial differential equation (PDE) describing the evolution in time and size of the metastatic density, coupled with ordinary differential equations (ODEs) describing the evolution in time of the primary tumor (see [1, 3, 4], for the 1D and 2D models in the autonomous case, and [1, 3] for the 1D and 2D models in the non-autonomous case, as would be the case for modeling a therapy).
In the same fashion of [3], the 2D metastatic model introduced by Benzekry [1], which takes into account a combined cytotoxic/antiangiogenic treatment, is reformulated in terms of a linear Volterra integral equation (VIE) whose unknown are biological observables of interest as the total metastatic burden or the cumulative number of metastases (whose volume is larger than a certain size) at a fixed time.
In order to solve this VIE, we first transform it into an equivalent integral equation on the positive semi-real axis and, then, we apply a Nyström method using a proper truncated product quadrature rule based on Laguerre's nodes together with an additional point. The dimension of the linear system to solve is reduced due to the use of a truncated approximation process. Furthermore, one needs to solve only one linear system whatever is the number of the evaluation times. It will be shown how this numerical approach permits to reduce the computation times compared with the method already proposed in [2].

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Numerical methods over equispaced grids

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The use of equidistant points is crucial in many engineering and mathematical physics problems which are modeled by integral and/or differential equations. In this context, the involved functions are available only in a discrete set of equally spaced nodes. In these cases, the classical methods based on piecewise polynomial approximation offer a lower degree of approximation, while the efficient procedures based on the zeros of orthogonal polynomials cannot be used.
Here we present two different quadrature formulas over equispaced grids: the first one [3] is obtained by means of the sequence $\{B_{m,\ell}(f)\}_m$ of the so called Generalized Bernstein polynomials [5], where $B_{m,\ell}(f)$ is the ℓ-iterated boolean sum of the classical Bernstein polynomial $B_m(f)$; the second one [1] is based on the constrained mock-Chebyshev least squares operator $\hat{P}_{r,n}(f)$, recently introduced in order to defeat the Runge phenomenon that occurs when using polynomial interpolation on large sets of equally spaced points [2].
Finally, we consider a mathematical model in population theory for individual interactions at a distance, that is described by a reaction-diffusion-type equation with an integral term accounting for the intraspecific competition. The numerical scheme [4] for the computation of the solutions of a simplified model of such type is based on the line method, for which the partial differential equation describing the population evolution and diffusion is frozen at some selected space nodes. The integral accounting for the competition of all other individuals is discretized over the same set of points by means of one of the previously introduced quadrature rules. In this way, an ordinary differential system is thus obtained, on which the standard Runge-Kutta-Fehlberg 45 (RKF45) method can be applied.

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Improved methods for the enrichment and analysis of the simplicial vector-valued linear finite elements

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The simplicial vector linear finite elements are commonly used for numerically solving the stationary Stokes equations. They are known, however, to suffer from severe shortcomings in application to more complicated situations. An enriched finite element, that overcomes the aforementioned drawbacks, was proposed and developed by Bernardi and Raugel. It can be regarded as an advanced and generalized version of the conventional simplicial vector linear finite element, and it has been employed in a wide range of practical engineering computation fields. It uses polynomials as enrichment functions. However, the intractable linear dependence issue is always encountered when this type of enrichment functions is employed. In line with previous researches, the main contribution of this work is to present a general strategy for enriching the simplicial vector linear finite element by non-polynomial enrichment functions. This enriched finite element is defined with respect to any simplex, and can be regarded as an extension of Bernardi and Raugel element. A key role is played by a characterization result, given in terms of the non-vanishing of a certain determinant, which provides necessary and sufficient conditions, on the enrichment functions and functionals, that guarantee the existence of families of such enriched elements. We show that the enriched basis functions admit a closed form representation in terms of enrichment functions and functionals.

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Adapted numerical treatment of stiff PDEs models from applications

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Mathematical models expressed through Partial Differential Equations (PDEs) represent powerful a tool for the description and prediction of real phenomena in time and space. In the scientific literature, there are several numerical methods that have been constructed to solve these problems. However, PDEs describing a specific model may be endowed with a-priori known characteristics of fundamental importance, which are not always captured by the used numerical discretization, if this is not carefully chosen.

In this talk, starting from a numerical approach recently introduced in the scientific literature for solving stiff ordinary differential equations (Calvo et al. J. Comput. Phys., 436, 110316, 2021), which is based on an appropriate preconditioning of the problem to be solved, we derive new efficient, stable and accurate methods, called TASE (Time Accurate and highly-Stable Explicit) methods [1, 3, 5]. We will describe the derivation and consistency and stability properties of TASE methods, showing their efficiency and competitiveness with other well-known numerical schemes of the scientific literature for stiff initial value problems. Finally, we will consider three models of PDEs of interest related to the development of vegetation in arid environments (Eigentler et al. Bull. Math. Biol., 81, 2290–2322, 2019), to the corrosion of metallic materials (Mai et al. Corros. Sci., 110, 157–166, 2016), and to the movement of electrons in solar cell components (Maldon et al. Entropy, 22(2), 248, 2020). These models are characterized by a-priori known properties, such as positivity, oscillations in space, severe stiffness mainly induced by the diffusion term, which require the use of ad hoc temporal and spatial discretizations. With this in mind, we will adapt the TASE methods for the related numerical solution [2, 4], showing that they are able to efficiently deal with stiffness and to preserve any positivity and oscillations.

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Conservative Multistep Methods for Production-Destruction Differential Systems

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The mathematical modeling of various real life phenomena leads to positive and conservative Production-Destruction differential Systems (PDS) [2]. The enforcement of such properties for the numerical solution of PDS usually yields a severe restriction on the step-length of integration, motivating a growing interest in devising positivity-preserving and unconditionally conservative schemes [1, 3, 4, 5]. Here we extend the Patankar-type modification to multistep methods and prove that the resulting discretizations preserve, with no conditions on the step-length, not only the positivity of the solution, but the linear invariant of the continuous-time system as well. Furthermore we introduce an embedding technique for the Patankar weights denominators and provide results on arbitrarily high order of convergence.

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Resolution Approximation Methods for Image Processing Applications

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Resolution Approximation Methods (RAM) play a crucial role in many real-world applications where preserving the original image quality is essential. Depending on the specific applicative field, the approximation may focus on spatial and/or color (intensity) information [7], [6]. Over the years, several methods have been proposed for color (gray) images, and multiple research directions have been pursued to enhance the performance and robustness of RAM [1],[2], [3], [4] and [5].
This contribution explores some approaches for both spatial and color (intensity) resolution approximation, providing a comprehensive analysis of their benefits, drawbacks, and potential future advancements.

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A CUDA implementation for solving systems of Volterra Integral Equations

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The resolution of Volterra Integral Equations' (VIEs') systems falls into various applied problems requiring numerical solutions with improved properties related to accuracy and efficiency. One of the widespread application fields consists of image clustering, which can be improved by employing a pre-processing based on a system of VIEs [1, 2].
The resolution process of VIEs does not only require accuracy using appropriate numerical schemes but also an effort related to efficiency. Therefore, numerical schemes take advantage of Waveform Relaxation methods, since they unable one to parallelize the resolution of a system of VIEs, obtaining significant speed-up results.
In particular, parallel strategies consists of Multiple Instruction Multiple Data (MIMD) [4], applied through the Message Passing Interface (MPI) package, Multiple Instruction Single Data, or Single Instruction Multiple Data [4], obtainable with CUDA [3], an architecture for using GPUs for General Purpose [5].
The main aim of this presentation consists of showing how applying a Non-Stationary Waveform Relaxation method through CUDA helps the efficiency improvement in numerically solving systems of Volterra Integral Equations. In particular, the numerical experiments confirm both the maintaining of the convergence order of the numerical method and the significant increase of the speed-up rate as the system dimension growths.

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MS14 - Theoretical and numerical analysis of some classes of functional equations and applications

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ABSTRACT

Functional equations, of differential or integral type, arise in several models of the applied sciences and technology. The aim of the minisimposium is to show recent advances in theoretical study of some classes of functional equations and in the development of efficient numerical methods for their resolution. Moreover some possible applications to concrete problems will be highlighted.

Special polynomials and functions in the description of various generalizations of heat-equation

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A method to find general solutions for extended forms of d'Alembert and Fourier heat equations is presented. The use of pseudohyperbolic functions in connection with some special classes of Hermite polynomials, of higher and fractional order, consents to introduce advanced operational techniques to discuss solutions of various generalized forms of heat equations. Moreover, an appropriate combination of different techniques may provide a fairly useful tool to deal with the solution of evolution equations of higher order or fractional diffusive type. Finally, these methods are useful to obtain either numerical or analytical solutions.

A new Nyström type method for solving BVP problems on real line

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This talk deals with a new numerical method for solving Boundary Value Problems (BVPs) of the following type

$$\begin{cases} f''(x) - \mu a(x) f(x) = h(x), \\ f(-\infty) = f(+\infty) = 0, \end{cases} \tag{2}$$

where $\mu \in \mathbb{R}$, a and h are given functions satisfying suitable assumptions and f is the unknown solution.
Boundary-value problems on infinite intervals are of interests because are model for many problems arising from physical phenomena, such as the flow of a gas through a semi-infinite porous medium or non-Newtonian fluid flows.
In [2], following an idea in [1] and using the so-called Green's function

$$G(x,t) = -\frac{1}{2} \begin{cases} e^{-t}e^{x}, & -\infty < x \le t, \\ e^{t}e^{-x}, & t \le x < \infty, \end{cases}$$

the equivalent Fredholm integral equation

$$f(t) - \int_{\mathbb{R}} G(x,t)\widetilde{a}(x) f(x)\, dx = \int_{\mathbb{R}} G(x,t) h(x)\, dx, \tag{3}$$

where $\widetilde{a}(x) = (\mu a(x) - 1)$, has been derived from (2) and a Nyström type method has been proposed in order to approximate its solution. Such numerical method is constructed by approximating the unknown solution by the Lagrange polynomial based on the Laguerre zeros and the additional point $4m$. Its stability and convergence have been proved for functions $\widetilde{a}$ satisfying a smoothing property. Here we propose a new Nyström method for solving equation (3) having two advantages with respect to the one proposed in [2]. It employs an interpolation process based only on the Laguerre zeros and then it leads to compute simpler modified moments. Moreover, its stability and convergence require only that the function $\widetilde{a}$ belongs to a weighted space of continuous functions on $\mathbb{R}$. Numerical tests and comparisons with the method proposed in [2] will be presented.

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A boundary integral equation method and its applications

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Classically, the solution of the Dirichlet problem for Laplace equation is sought in the form of double layer potential. The alternative method consists in looking for the solution by means of a simple layer potential. In this talk, we present how to obtain these integral representation (see [1] for simply connected domains and [2] for multiply connected domains). The boundary integral equation method we use requires neither pseudo-differential operators theory nor hypersingular integrals, but it only hinges on the theory of reducible operators and the theory of differential forms. We also show the applicability of our method to different systems of partial differential equations (e.g., [3], [4], [5]).

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Airy functions in the description of generalized heat-type equations

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We discuss higher-order Airy functions emerging as solutions to an ordinary differential equation which generalizes the classical Airy equation. Higher-order Airy functions also emerge in the solution of higher-order heat-type equations when the order of the space derivative is an odd integer number. A fractional extension of such generalized Airy functions is obtained by studying a space-fractional heat equation involving a higher-order Riesz-Feller operator. While the solutions to the mentioned equations are oscillating functions which can be interpreted as signed measure densities, subordination via a Lèvy stable subordinator transforms the oscillating Airy functions into genuine probability density functions. In particular, the distribution of Lèvy stable processes is obtained.

Some Apostol-type Hermite degenerated polynomials

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This work presents a generalization of new classes of degenerated Apostol–Bernoulli, Apostol–Euler, and Apostol–Genocchi Hermite polynomials of level m, defined by the following generating functions.

$$\tau^{m\alpha}[\sigma(\lambda;\mu,b;\tau)]^{\alpha}(1+a\tau)^{\frac{\xi}{\mu}}(1+\mu\tau^2)^{\frac{\eta}{\mu}} = \sum_{\omega=0}^{\infty} {}_H\mathfrak{B}_{\omega}^{[m-1,\alpha]}(\xi,\eta;\mu,b;\lambda)\frac{\tau^{\omega}}{\omega!},$$

$$2^{m\alpha}[\psi(\lambda;\mu,b;\tau)]^{\alpha}(1+\mu\tau)^{\frac{\xi}{\mu}}(1+\mu\tau^2)^{\frac{\eta}{\mu}} = \sum_{\omega=0}^{\infty} {}_H\mathfrak{E}_{\omega}^{[m-1,\alpha]}(\xi,\eta;\mu,b;\lambda)\frac{\tau^{\omega}}{\omega!}$$

and

$$(2\tau)^{m\alpha}[\psi(\lambda;\mu,b;\tau)]^{\alpha}(1+\mu\tau)^{\frac{\xi}{\mu}}(1+\mu\tau^2)^{\frac{\eta}{\mu}} = \sum_{\omega=0}^{\infty} {}_H\mathfrak{G}_{\omega}^{[m-1,\alpha]}(\xi,\eta;\mu,b;\lambda)\frac{\tau^{\omega}}{\omega!},$$

where

$$\sigma(\lambda;\mu,b;\tau) = \left(\lambda(1+\mu\tau)^{\frac{1}{\mu}} - \sum_{l=0}^{m-1}\frac{(\tau\log b)^l}{l!}\right)^{-1}$$

and

$$\psi(\lambda;\mu,b;\tau) = \left(\lambda(1+\mu\tau)^{\frac{1}{\mu}} + \sum_{l=0}^{m-1}\frac{(\tau\log b)^l}{l!}\right)^{-1}.$$

In addition, we establish some algebraic and differential properties for these new classes of polynomials.

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MS15 - New trends in applicable approximation theory

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ABSTRACT

Approximation Theory is a branch of Mathematics that bridges pure and applied mathematics. It overlaps with both classical and modern analysis, as well as numerical analysis, linear algebra, and even various branches of applied mathematics.
Its origin dates back a very long time ago with the fundamental works of Bernstein, Chebyshev, Haar, Hermite, Kolmogorov, Lagrange, Markov, and others. However, nowadays, interest in studying various approximation techniques has grown significantly due to the development of computer technology and its applications in natural and engineering sciences. Therefore, there is a continuous impulse to develop new and better-performing approximation techniques, easy to compute and implement, and able to capture the particular features of the problem under consideration.
The aim of this minisymposium is to show the last developments and advances in approximation theory, highlighting connections between emerging mathematical research and applications.
The talks focus on several techniques of approximation which have practical applications to a wide range of mathematical problems written in terms of ordinary differential equations, partial differential equations, and integral equations. Some of the topics that will be treated in the talks include approximation by orthogonal polynomials, Shepard basis functions, radial basis functions, regularization techniques, and partition of unity schemes.

A μ-mode framework for tensor structured problems, with an application to evolutionary differential equations

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Many d-dimensional tasks in numerical analysis can be solved by applying repeatedly one-dimensional rules to all the directions, leading to the so called tensor product formulas. This is the case, for example, in the context of multidimensional function approximation using pseudospectral expansions, multivariate interpolation, and solution of evolutionary differential equations with tensor structure. In this talk, we present a common tensor framework from which it is possible to extract an *efficient-to-implement* solution, i.e. a BLAS-oriented formulation, of the d-dimensional task [2]. The key point consists in the suitable usage of the μ-mode product (also known as tensor-matrix product or mode-n product) and related operations (the Tucker operator, in particular). These concepts are widely known by the tensor algebra community, but their employment is mainly restricted in the context of tensor decompositions. The MATLAB/GNU Octave implementation of the needed tensor operations, collected in the freely-available package KronPACK[1], will be briefly discussed during the talk as well.
Also, we will present an application of the framework to the computation of exponential-like matrix functions, typically arising when solving numerically evolutionary differential equations using exponential integrators [1, 3]. Finally, we will conclude the talk with some numerical experiments on multidimensional problems, which globally show the effectiveness of the approach.

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On the constrained mock-Chebyshev least squares operator with applications

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The constrained mock-Chebyshev least squares operator is a linear approximation operator based on an equispaced grid of points [1, 2]. Like other polynomial or rational approximation methods, it was recently introduced to defeat the Runge phenomenon that occurs when using polynomial interpolation on large sets of equally spaced points. The idea is to improve the mock-Chebyshev subset interpolation, where the considered function f is interpolated only on a proper subset of the uniform grid, formed by nodes that mimic the behaviour of Chebyshev–Lobatto nodes. In the mock-Chebyshev subset interpolation, all remaining nodes are discarded. In contrast, in the constrained mock-Chebyshev least squares interpolation, they are used in a simultaneous regression, aiming to improve further the accuracy of the approximation provided by the mock-Chebyshev subset interpolation. We will discuss some theoretical aspects of the constrained mock-Chebyshev operator and some applications to numerical differentiation and integration [3, 4].

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On the application of anti-Gauss cubature rules to second-kind integral equations on the square

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This talk deals with the numerical solution of Fredholm integral equations of the second kind defined on the square. A Nyström-type method based on Gauss and anti-Gauss cubature rules is developed and analyzed in terms of stability and convergence, and an averaged Nyström interpolant is proposed to approximate the solution of the problem.
Numerical tests confirms the accuracy and the computational advantage of adopting such a Nyström interpolant, in comparison with the classical Nyström interpolant based on the Gauss rule.

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Multivariate Numerical Derivatives as an Integral Equation Solution

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We consider the problem of computing multivariate numerical derivatives from multidimensional data. This is an important problem in many fields of engineering and scientific studies, such as: image segmentation; edge detection; magnetic resonance imaging; computerized tomography; numerical solution of PDE; some examples can be found in [1] and [3].
It is well known that the computation of derivatives is an ill-posed problem, in fact, small errors on the data can produce large errors in the computed derivatives. Hence, many regularization methods have been proposed in order to reduce the propagation error in the computed derivatives. In particular, among the various methods proposed for the numerical differentiation problem there are: mollification methods; finite-element methods; variation methods, smoothing spline methods, Lanczos' methods, integral equation methods and radial basis functions approximation, see for example [2],[4],[5] and [6].
In this work, the estimation of the partial derivatives from multidimensional data is obtained by solving an ad-hoc integral equation, whose solution depends on data set. We study the robustness and the stability of the proposed method. Some numerical examples are used to show the feasibility and solidity of such method.

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A Spectral Approach for the Solution of Differential Equations

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Differential equations are a largely used kind of equations for the description of many scientific phenomena in terms of their mathematical models. For instance, studies of Physics, Chemistry, Biology or Economics rely on models consisting in ordinary or partial differential equations. Moreover, the more elaborate and interdisciplinary the phenomenon, the more complex the resulting model. Thus, any advance in the solution of differential problems gains great interest, especially from the applied sciences. In more detail, numerical methods for solving initial value problems for ordinary differential equations of first order play a central role in numerical analysis, and the best known are multistep methods [5] and Runge-Kutta methods [2]. On the other hand, boundary value problems associated with second order differential equations are a famous counterpart, for which several numerical methods have been developed, e.g., spline approximation methods [3], finite element methods [1], reproducing kernel methods [4]. For these second kind of problems, the ability of the related numerical methods to deal with partial differential equations is crucial.
In this work, we propose a numerical method to solve differential equation problems, based on a proper approximation of the derivative operator. Such an approximation is devised from the singular value expansion of the kernel of a proper integral operator, which reformulates the differential operator. The involved integral equation is a Volterra integral equation of the first kind. We present some ideas and preliminary numerical tests.

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Shape Parameter and Radius Search in Partition of Unity Interpolation

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The search of the shape parameter in Radial Basis Function (RBF) interpolation is a well-known problem in approximation theory. Moreover, the computational cost problem related to the size of the data solved by the Partition of Unity Method (PUM) [1, 2] leaves the determination of the subdomains' radii as an open problem. In this contribution, we propose the *Bayesian Optimisation* [4] as a tool for the simultaneous search of the optimal shape parameter and the radius in RBF-PUM interpolation. The process is a step-by-step self-update procedure that consists in modelling the error function with a Gaussian process that drives the choice of the parameter to evaluate, resulting in a consistent saving time with respect to classical techniques such as Leave One Out Cross Validation (LOOCV) [3].

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Polynomial approximation and numerical integration with exponential weights

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In the last years different weighted polynomial approximation processes have been introduced for functions defined on non-compact domains, e.g. open or unbounded intervals of the real line, and having exponential monotonicity at the endpoints (see [1, 2, 3] and the reference therein).
The aim of this talk is to discuss recent results on the topic and their application to quadrature rules and numerical methods for integral equations. Special attention will be devoted to the construction of new function spaces, the study of orthonormal polynomials with respect to non-classical weights and the convergence of related approximation processes.

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Riesz Representation Theorem as a tool for regularized solution of integral equations

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First kind integral equations arise in many applications. A typical situation is when one needs to identify certain parameters of a physical system confined in a specified domain. Some sensing devices used in such settings allow different configurations, leading to overdetermined systems of integral equations with discrete data in the presence of boundary constraints. It is well-known that Fredholm integral equations of the first kind are often ill-posed problems. When the right-hand side is discretized, e.g., when it consists of experimental measurements, the difficulties related to ill-posedness are enforced, as the problem admits infinitely many solutions. We describe a numerical method for computing the minimal-norm solution. The algorithm stems from the Riesz representation theorem and the theory of reproducing kernel Hilbert spaces (RKHS) [1, 2]. Since the resulting linear system is strongly ill-conditioned, we construct a regularization method based on a truncated expansion of the minimal-norm solution in terms of the singular functions of the integral operator defining the problem. Numerical experiments, both synthetic and deriving from an application in applied geophysics, are presented to show that the new method is extremely effective when the sought solution is smooth, but produces significant information even for non-smooth solutions.

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On approximating fictitious heat sources arising in an inverse heat transfer problem

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By considering a paradigmatic heat conduction problem on a domain with a single cavity, we prove that the presence of the void can be fully replaced by a fictitious heat source with support contained in the void region [1]. We illustrate the effectiveness of this approach in a situation where the source term can be analytically recovered from the values of both temperatures and heat fluxes taken on the boundary of the cavity.
The practical importance of this result is that e.g. in real-world applications we often deal with a limited knowledge, due to practical inaccessibility, of the inner physical changes occurring in a heat-conductive physical system and their estimation through thermographic inspection is an important inverse problem. Our result provides a strategy to map such a nonlinear geometric inverse problem, e.g. a hidden corrosion problem [2], onto a more manageable one, that involves the identification of forcing terms given the knowledge of external boundary data [3]. Moreover, the demonstration that the support of the fictitious forcing term corresponds to the region of the cited void assures the possibility, at least theoretically, to get an accurate estimate of the void region from an adequate knowledge of the temperature field. To set the stage for a systematic study of the inverse problem, we present algebraic computations, based on a finite-element discretization of the domain, that give an approximation of the fictitious source from the available measurements. We show the relevance of a sparse-recovery constraint [4], in particular with an additional nonnegativity constraint [5], and how the degree-of-accuracy of the reconstruction varies with respect to the decrease in the number of available temperature-measurement points. Finally, we show that the algebraic reconstruction could be favorably used as a prior to locate the unknown fictitious forcing term, e.g. in a bayesian learning method.

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On approximating discrete measures

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Approximating a continuous measure by a discrete one is a common practice. Generally, the aim is to develop Gauss-type quadrature rules for integrals which involve nonclassical measures. The idea is to exploit such approximation to obtain the recursion coefficients of a set of discrete orthogonal polynomials and construct a Gauss rule on their zeros. Such quadrature scheme asymptotically approximates a Gauss formula for the continuous measure. We will discuss various methods for approximating the measure and propose a new algorithm for the computation of the recursion coefficients. Numerical experiments will compare the new technique to the existing ones. The perspective of research is to apply such Gaussian rules to the solution of integral equations.

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Community Detection and Interpolation on Graphs

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Graphs are powerful tools for representing spatial data, while graph theoretical techniques may be used to translate the classical scattered data problem into a signal interpolation problem on the nodes [3]. However, when the data increases, and hence the graph becomes larger, the computational cost may not be sustainable. A possible way to overcome this issue is finding graph communities and then using Partition of Unity Methods (PUMs) as auxiliary tools [1].
In this contribution, we consider approximation methods based on local generalized translates of a Graph Basis Function (GBF) giving rise to a low-cost GBF-PUM global interpolation scheme [2].

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Discontinuity detection from scattered data by kernel based techniques

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Accurate interpolation of non-regular two-variate functions from a given set of scattered data is a challenging problem that occurs in many applications going from signal processing to geophysics. By non-regular function, we mean that the function or its partial derivatives are discontinuous along some planar curves of the given domain. The choice of the interpolation model plays a crucial role in the quality of the reconstruction. If the basis of the interpolation space does not reflect the properties of the underlying function, artifacts will usually appear in the final reconstruction. In order to get a good approximation, we need to precisely define the locations of such curves. In this talk, we discuss a kernel-based adaptive strategy to extract the needed information from the given data.

MS16 - Kinetic equations: numerical methods and applications

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ABSTRACT

Kinetic equations naturally arise when examining a statistical description of a large system of interacting particles (or agents*) evolving over time. These equations can describe a wide range of phenomena, playing a fundamental role in classical physical problems and industrial applications, e.g., in plasma physics, granular gas motion, semiconductor design, or geophysics and meteorology problems. More recently, this type of mathematical modeling has been extended to systems of interacting particles to describe socio-economic and biological phenomena, such as financial markets, road traffic, the movement of crowds, flocks of birds, the control of opinions, the spread of cancer cells and infectious diseases or the formation of biological networks.*

The development of numerical methods to solve this type of equations results very challenging due to the large number of equations involved, the resulting complexity of the solutions and of the algebraic structure of the model, and the inherent high dimensionality of the problems, associated with the well-known curse of dimensionality*. In this scenario, accuracy and computational complexity must be carefully balanced.*

In this minisymposium, several recent developments of numerical methods for kinetic equations and related applications will be presented, spanning from plasma physics and swarm dynamics, to life sciences and opinion formation. The minisymposium also promotes the activities of the GNCS Project "Numerical methods for multiscale differential problems: high-order schemes, optimization, control".

A kinetic perspective on genetic algorithms in optimization

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Genetic algorithms are optimization methods inspired by the natural selection mechanism in populations of individuals. In this context, individuals, or particles, represent possible solutions and they interact with one another via crossover and mutation dynamics to find a global solution to the optimization problem. Despite their popularity, such derivative-free heuristics typically lack rigorous mathematical understanding.
In this talk, we review recent work on the mathematical modeling of genetic algorithms via Boltzmann-type equations. In particular, we show how the derived kinetic description allows for a theoretical analysis of the algorithm convergence properties in the case where the selection among the population is guided by the Boltzmann-Gibbs distribution associated with the objective function.

A data-driven kinetic model for opinion dynamics and contacts

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In recent years, kinetic models and Boltzmann-type equations have emerged as powerful tools for describing and analyzing the collective behaviors of systems of interacting agents, with various possible application fields. Our model for opinion dynamics contributes to this growing body of literature on the use of kinetic models and Boltzmann-type equations in many fields which may seem far from statistical physics and gas dynamics. We describe the evolution of opinions starting from the microscopic level, assuming that each agent has associated two real values: its number of followers on a social media platform and its opinion. First of all, we model the evolution of the social following of the agents, since we assume that the number of followers is not influenced by the opinion. We assume that opinions are continuous variables that lie on the bounded interval $[-1, 1]$, and that the agents update their opinions after the interaction with others. The strength of such interaction depends on the number of followers of each agent and on the distance between their opinions. We also suppose that there is a certain amount of randomness in the interaction, modeling external factors such as the possibility to access to information. We derive the kinetic equation that describes the time evolution of the distribution of opinions in presence of social media contacts in the population, and we study its properties using analytical and numerical methods. We show that our kinetic model captures important features of opinion dynamics, such as the emergence of consensus and polarization, according to the choice of different interaction kernels between the agents. We also show that, using data extracted from a real social media, it is possible to reconstruct the interaction kernel in order to fit the actual trend of the opinion distribution of the agents on certain topics.

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Hydrodynamic traffic flow models including random accidents: A kinetic derivation

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We will talk about a kinetic derivation of a second order macroscopic traffic model from a stochastic particle model. The macroscopic model is by a system of hyperbolic partial differential equations (PDEs) with a discontinuous flux function, in which the traffic density and the headway are the averaged quantities. A numerical study illustrates the performance of the second order model compared to the particle approach. We also analyse numerically uncertain traffic accidents by considering statistical measures of the solution to the PDEs.

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A kinetic study on cell migration: the twofold influence of the extracellular matrix

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In several physiological and pathological situations, cells perform directed motion in response to external stimuli by sensing the environment with their membrane protrusions. This gives rise to direct migration toward specific biochemical or biophysical cues. In this work, we focus on the influence of the extracellular matrix, developing a non-local model for cell migration where a single cue has a twofold way effect on movement. Precisely, we analyze how this single cue can affect the polarization and speed of motion of the cells, looking at the interplay between contact guidance and steric hindrance. Starting from a microscopic description of the stochastic mechanism of cell re-orientation, we take advantage of classical tools of kinetic theory to formally derive the corresponding kinetic equation for cell collective motion that implements exactly the microscopic dynamics. Then, we obtain the related macroscopic equation in the appropriate regime on the basis of the observed experimental parameters. Finally, we test our model in several scenarios, comparing the outcomes of both the microscopic, kinetic, and macroscopic models with experimental results and also showing the potential applicability of this framework in the case of cell movement in heterogeneous environments [1].

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Kinetic description of swarming dynamics with transient leadership

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The study of the collective and synchronized behaviour of animals, like bird flocks, fish schools and insect swarms, plays a central role in Mathematical Biology. Here the focus is on a model that describes the collective motion of birds in which spontaneous sudden changes of direction happen without the influence of predators, [1]. The main idea is that each bird can be a turn initiator becoming a leader whose influence acts on its nearest neighbours that are supposed to be in the followers status. Once that an agent becomes a leader it initializes a change of direction which is propagated along the whole flock. However, the leaders influence is assumed to be limited in time. Indeed, the interest is on the dynamics of *switching leaders* or *transient leadership*: each agent can change its label in time from leader to follower and vice-versa. The model can also include food sources which are visible only by the agents in the leaders status. Starting from the microscopic model, we derive a kinetic description of the agents distribution which combines an update of the positions and velocities based on binary interactions rules with a dynamic change of labels between the followers and leaders status, [2], [3]. We show how to solve the problem numerically with a Monte Carlo algorithm to simulate the labels evolution and a Nanbu algorithm to simulate the interactions. To approximate the topological ball, we substitute the classical exhaustive search with a k-nearest neighbour search in order to reduce the computational cost from quadratic to logarithmic. We conclude by presenting different numerical tests to validate the obtained results.

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Kinetic models on interactions within communities

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We present a novel approach that combines a differential framework for analyzing bivariate opinion formation dynamics with a compartmental model for the spread of fake news. By employing mean-field analysis techniques, we demonstrate that the resulting Fokker-Planck system can accurately capture the bimodal distributions of opinions commonly observed in polarization dynamics. To ensure realism, we customize our numerical simulation to interface with existing data obtained from online social network databases.

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Kinetic and Macroscopic Description of Self-Organizing Multi-Agent Systems with Continuous Leader-Follower Transition Dynamics

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The emergence of leaders and followers is typical of many self-organization phenomena ranging from wound healing to the dynamics of flocks of birds. In this talk, I will present a new kinetic model for describing self-organization in multi-agent systems in the presence of a leader-follower dynamics. In particular, the agents will be characterized by their position, by their velocity and also by a continuos parameter quantifying the degree of leadership. The kinetic model will be derived by an appropriate microscopic stochastic model and will be non–local in the physical space in order to account for long –range interactions. I will discuss a technique for deriving macroscopic equations from the resulting Bolztmann-Povzner equation. Numerical simulations of the microscopic and macroscopic models will be presented.

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Particle stochastic-Galerkin methods for uncertainty quantification of plasma equations

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Uncertainty is a fundamental aspect of physical, biological, and socio-economical systems, and should be considered in the corresponding mathematical models, formulated through PDEs, to provide a more data-oriented representation of these phenomena. This is a particularly interesting problem in the kinetic framework. As a matter of fact, kinetic equations play an important role in the description of several kinds of phenomena involving a large number of interacting particles. Among all, plasma models are studied at the kinetic level by the Landau equation and have gained a lot of interest due to the important applications related to fusion reactors and ongoing projects such as ITER, JET, and SPARC.

The construction of numerical methods for such equations with random inputs is a challenging problem, thanks to the high dimensional structure of the equations, involving both phase space variables and stochastic parameters, and the formation of multiscale structures that must be captured by the numerical schemes. Furthermore, a numerical solver must be able to preserve the structural physical properties such as the non-negativity of the distribution function, the main conservations of invariant quantities, the entropy dissipation, and the equilibrium states.

Recently, a new class of numerical methods that combine a particle-based approximation of the distribution function in the phase space together with a stochastic Galerkin expansion of the particles in the random space has been proposed. These methods are spectrally accurate in the space of the random parameters, thanks to the sG formulation, and conserve the structural properties of the equation, because of the particle nature.

The schemes have been presented for the homogeneous Boltzmann equation in [2] and then extended to the Vlasov-Poisson-BGK system with random inputs in [1]. Current ongoing works are focussing on the homogeneous Landau equation.

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A kinetic theory approach to modeling prey-predator ecosystems with expertise levels

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A kinetic model for an ecological system composed of four different populations is proposed. Based on a prey-predator framework characterized by individuals experience, a system of kinetic nonlinear equations is formulated by using standard tools. Conservative and nonconservative scenarios are studied. In particular, in the latter proliferative/destructive parameters and external action are not neglected. For each case, long-time evolution of the system is analyzed. Numerical simulations show that this model behaves in a way consistent with other similar ecological models formulated by classical dynamical systems involving ordinary differential equations with lumped dependent variables. Furthermore, for each simulation, stationary solutions, if they are gained, are shown. Finally, since oscillatory behaviours appear for some values of the parameters of the ecological system, a first numerical bifurcation analysis is performed.

Asymptotic-preserving IMEX methods: bridging scales in hyperbolic and kinetic equations

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Many problems in physics and engineering involve multiple scales that, if not properly addressed, lead to severe numerical limitations on discretization parameters. In this talk, we will discuss the time discretization of multiscale time-dependent PDEs using Implicit-Explicit (IMEX) methods, with a special focus on hyperbolic and kinetic problems and their asymptotic-preserving (AP) properties [4, 6]. First, we will review the classical approach within Runge-Kutta methods, which involves partitioning the transport and source terms. This approach is suitable for numerically solving scaling limits that are dominated by a compressible fluid-dynamic behavior. Next, we will analyze the case of diffusive and/or low Mach number limits. We will show how to deal with the additional difficulties caused by stiffness in the characteristic velocities of the system, which can lead to a parabolic-type behavior. Finally, we will present recent generalizations, including the development of methods that allow for a unified treatment of different asymptotic limits [3], methods that combine a linearly-implicit treatment of stiff terms within the IMEX paradigm [5], as well as extensions of these ideas to multi-step methods [1, 2].

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Study on the consistency of POD-based ROM applied to SWE solved with augmented Riemann solvers

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The shallow water equations (SWE) are widely used to model many non-stationary free surface flows, but they do not have an analytical solution, so it necessary to use numerical methods to solve them. The upwind augmented Roe's method has been reported to produce robust and stable solutions when applied to the SWE [1]. Augmented Riemann solvers are designed to preserve equilibrium in presence of source terms [2]. Other numerical corrections than the well-balancing are necessary to fix some unphysical numerical solutions that may appear in realistic scenarios, such as the entropy and the wet–dry front problems. Reduced-order models (ROMs) based on the proper orthogonal decomposition (POD) are used to save computational costs without loss of accuracy. They need to be trained using a set of high-fidelity solutions computed with the full-order models (FOMs). The main objective of this work is focused on concept of consistency [3] of the ROMs when trained with FOMs other than the ones from which they were developed. We are interested in studying whether it is necessary or not to consider numerical corrections such as the well-balancing, the entropy fix or the wet-dry treatment when designing the ROM and which properties of the FOM are preserved by the ROM [4].

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MS17 - Unfitted boundary methods

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ABSTRACT

The interaction between two coupled evolutionary differential problems need to be accounted in a large variety of physical systems. This interaction may include the description of the evolution of the interface (shared boundary) between the two coupled systems. Some examples of these problems are fluid/structure interaction problems, evolution of multiphase fluids (i.e. droplets, emulsions, foams, etc.), phase-change processes, mixed-dimensional PDE. Due to the a-priori unknown displacements or deformations of such shared boundaries, unfitted boundary methods emerges as suitable techniques for avoiding time-consuming remeshing procedures. In particular, unfitted boundary methods are extremely convenient, since the two coupled evolutionary problems can be discretized on a fixed grid, covering the whole computational domain, thus including points that rely also inside the closed boundaries. Note that, numerical methods relying on boundary-fitted grids would need time-consuming mesh regeneration/deformation and the consequent projection of the solution at a certain time onto a new grid, so that leading to possible loss of accuracy.

The scope of the present symposium is to bring together different experiences and expertise in the field of modeling and methodologies for unfitted boundary problems. This symposium will explore recent developments and trends in the design of accurate and efficient methods for coupled multiphysics problems. Among others, topics of interest include micro- and nano-transport, fluid-structure interaction, volcano thermo-poroelastic deformation and bio-inspired approaches for mesoscales computations.

Dealing with spatial discontinuities in unsaturated flows

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In this work we present some tools for handling discontinuities due to heterogeneities in soil structure, when modeling water flow in unsaturated soils. We start from the advection-diffusion Richards' equation for modeling this phenomenon, and we treat the discontinuities by resorting to Filippov theory to the semi-discretized model arising from the transversal method of lines. Both 1D and 2D spatial domains are considered, and numerical schemes are proposed accordingly, as in [1, 2].

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Parallel-in-Time Solver for the All-at-Once Runge–Kutta Discretization

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We derive fast and robust parallel-in-time preconditioned iterative methods for the all-at-once linear system arising upon discretization of time-dependent PDEs. The discretization we employ is based on a high-order Runge–Kutta method in time, combined with suitable Finite Element in space, for a number of time-dependent PDEs. This gives raise to a huge saddle-point linear system, to be iteratively solved. We develop an optimal preconditioner whose block structure allows for parallelism in the time variable, as long as one is able to provide an optimal solver for the system of the stages of the method.
We thus propose a preconditioner for the latter system based on an SVD of the (real) Runge–Kutta matrix $A_{\mathrm{RK}} = U\Sigma V^{\top}$, assumed to be invertible, which provides a nice eigenvalue distribution of the preconditioned saddle point matrix, under the assumption that the related matrix $U^T V$ has eigenvalues with non negative real part [1].
The proposed approach is intrinsically parallel. Application of the preconditioner requires, however, the solution of a block bidiagonal linear system, which is performed by making use of the `xbraid` subroutine in the framework of the multigrid-in-time approach developed in [2]. We show the numerical efficiency of our SVD-based preconditioner by solving the system of the stages arising from the discretization of the heat equation and the Stokes equations, with a sequential time-stepping. Finally, we provide numerical results of the all-at-once approach for both problems, showing the excellent speed-up achieved on a the *Marconi100* supercomputer up to 4096 processors.

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Very high order methods on non-polygonal domains: The Reconstruction Off-site Data (ROD) method

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Realistic problems involve complex domains with curved interfaces or wedge. A straightforwards substitution of the physical domain by a polygonal numerical one leads to at least, a second order error (or worst). Several techniques have been developed to address the boundary issue such as the isoparametric method [3], the NURBS method [10], the ghost point ot ghost cell method [7], the cut finite element method [4, 5, 12] and many more.
Recently, methods based on a definitely separation of the physical and numerical domains such as the ROD [6] or the Shifted Boundary methods [1, 2, 13] have emerged. Basically, we transfer boundary condition prescribed on the real boundary into an equivalent boundary condition onto the grid nodes or mesh edges of the numerical domain where the discretization is implemented.
We present the ROD method principle and its usage in different frameworks such as the finite difference [6, 11], the finite volume [8, 9] and more recently the Discontinuous Galerkin method [14]. We provide some examples to show that we recover the optimal order of convergence together with a very good stability.

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Weak- and Strong–coupling approaches for implicit schemes in the dynamic immersed boundary framework

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Modeling the transport of deformable capsules under different flow regimens is crucial in a variety of fields, including oil rheology, blood flow and the dispersion of pollutants. In this work a mixed finite element/finite difference numerical framework for fluid-structure interaction problems is proposed and critically analyzed. The two solutions are obtained on two separate meshes interacting via a transfer function for entrusting, on the fluid side, no-slip conditions over the immersed structure; while, on the structure side, external hydrodynamics stresses. Specifically, the evolution of fluid conserved quantities is obtained through the solution of the Boltzmann equation in the BGK approximation on a 3D Cartesian lattice endowed with 19 discrete velocity directions. The Boltzmann equation is enriched with a forcing term demanded for the fluid/structure coupling. Zou-He conservative bounce-back procedure is used for enforcing Dirichlet known-velocity conditions on external boundaries while a dynamic-Immersed Boundary approach defines no-slip conditions over the immersed structure. The latter being integrated in time with a P-$(EC)^k$ β-Newmark scheme. A finite element approximation is adopted for the immersed structure evolution. Such structure is considered as a zero-thickness smooth closed two-dimensional manifold responding to an in-plane linear elastic strain and a bending resistance. The two solutions are coupled by following both, weak and strong coupling approaches. These strategies are compared and thoroughly analyzed in term of stability, accuracy and computational burden. This approach is employed to detail transport, dynamic, and deformation of micrometric capsules into microfluidics chip and capillaries [1, 2].

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Finite-difference ghost-point methods for Poisson equations with curved boundaries

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Elliptic equations in arbitrary domain (possibly with moving boundary) are central to many applications, such as diffusion phenomena, fluid dynamics, electromagnetism, charge transport in semiconductors, crystal growth, monument conservations and many others.
Among the different techniques, unfitted boundary methods have been increasingly popular in the last decades thanks to their flexiblity and enhanced efficiency for moving complex-shaped domains, since no meshing procedures is needed (unlike fitted boundary methods).
A popular approach is based on ghost-point methods, where grid point values are defined outside the domain (ghost values) by a proper highly accurate extrapolation of boundary conditions. Usually, every ghost value is defined in terms of only internal values, leading to a decoupled ghost point method. However, in some complex-shaped domains or in presence of general boundary conditions, sometimes this approach is not efficient or require impractical implementation techniques.
In this paper we present a coupled ghost-point method for arbitrary domains and general boundary conditions [3]. The approach leads to a large linear system (where the unknowns are both ghost and internal values) to solve. The methodology can be easily extended to high-order accuracy and it is reasonably practical for parallelization purposes. The linear system is not symmetric, nor diagonally dominant. However, a suitable multigrid approach is proposed, based on a Boundary Local Fourier Analysis to optimize the relaxation parameters to smooth the solution along the tangential direction of the boundary [2]. In this way, the optimal multigrid performance is recovered and boundary effects (that usually degrade the multigrid efficiency) are avoided.
The method is also applied to other classes of problems: incompressible fluid-dynamics [1], linear elasticity, hyperbolic equations, convection-diffusion problems [4].

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Finite element discretization of fluid–structure interaction problems with Lagrange multiplier: how to deal with the coupling term

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We consider a fictitious domain formulation with distributed Lagrange multiplier for fluid-structure interaction problems [1]. The evolution of the structure is modeled by Lagrangian description on a reference domain, which is mapped, at each time step, to the actual position of the solid body. The fluid is described by an Eulerian model and its mesh is extended also in the region occupied by the structure: the coupling is weakly enforced making use of a Lagrange multiplier. In particular, the coupling term is defined on the solid reference domain and it involves both fluid and solid variables. At discrete level, this definition requires integration of functions defined on non matching meshes: the procedure can be carried out with two different techniques [2]. The first technique consists in implementing an exact composite quadrature rule on the intersection between fluid and solid mesh, whereas, with the second technique, we can just integrate on the solid mesh introducing an additional source of error. We discuss how results are affected by the choice of assembly technique presenting quadrature error estimates for the inexact integration case and several numerical tests.

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Numerical modeling of landslides run-out phase with an efficient parallel well-balanced scheme

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Hydrogeological instability is among the effects of climate change with major impact on people and built environments security. Among instabilities, landslides are responsible for significant human and economic losses worldwide [1].
Landslide dynamic is characterized by a broad range of velocity-scales, from the steady creeping slip to a catastrophic avalanche passing through the intermittent rapid slip. During these phases, the landslide undergoes different mechanical behaviours. In particular, during the triggering phase, the landslide behaves roughly like a rigid body and the driving process is the pore-pressure diffusion that causes the intermittent slipping of the involved material. Once the landslide is initiated, it follows various behaviours. In particular, can propagate following a behaviour similar to a homogeneous visco-plastic material, as is the case of mudflows, or following more complex behaviours where the solid and liquid phases interact and have significantly different velocities, as is the case of debris flows.
We propose a scalable adaptive multi-core numerical framework, which is based on the two-step Taylor-Galerkin (TG2) method [3] recasted to be valid on quadtree meshes [3], thus able to deal with the presence of hanging nodes. The TG2 scheme is then enriched with the presence of an implementation of the Path-Conservative (PC) method as the work [4] but valid in case of continuous finite element spaces, in order to be able to deal with non-conservative products present in the model equations and ensuring well-balancing property. The method is applied to the solution of single- and two-phase depth-integrated models and is demonstrated to reproduce well academic tests which are not based on the PC procedure. Following deeper validation purposes, we even provide comparisons with other tools already available in the literature for the case of realistic simulations.

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Spectral methods for a class of nonlinear convolution-based peridynamic models

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The peridynamic equation consists in an integro-differential equation of the second order in time able to model fractures and damages in the context of nonlocal continuum mechanics.
We study numerically a nonlinear peridynamic model both in one and two-dimensional domain by implementing high-order spectral methods. Indeed, spectral methods are suitable in such context as the presence of a convolution product in the equation allows us to exploit the advantage of the FFT algorithm. We make a comparison on the implementation of Fourier and Chebyshev polynomials and use a volume penalization technique in order to overcome the limitation of working on periodic domains due to the Fourier approach. The performance of our approach is validated with the study of the convergence with respect to the spatial discretization.
A theoretical convergence result is also provided and the obtained convergence estimate is in accordance with numerical tests. We test the performance of the methods with respect to the time integrator. In particular, we consider the Störmer-Verlet scheme, the implicit Newmark-β method and the 2D-Chebyshev collocation method.

Structural schemes for stationary equations

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In this presentation, we propose a new class of compact schemes (based on [1], [2], [3]) for finite differences numerical methods, to provide high order accurate approximations of a smooth solution [4].
The discretization involves nodal approximations of the function together with the first and second derivatives also considered as unknowns of the problem. Then the method definitively splits the discrete problem into a set of Physical Equations (inner and boundary equation) and a set Structural Equations (linear relations between the unknowns), independent of the physics of the problem. The construction of structural equations comes from the kernels of matrices we elaborate by assuming exact resolution of polynomial functions.
We provide an analys of the accuracy, stability and spectral resolution for the most common structural equations. Numerical tests have been carried out to address both the stability and accuracy issues for popular linear and non-linear problems.

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Numerical ghost-point models for geophysical observables

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We present a second-order accurate ghost-point finite-difference numerical method in a 2D axisymmetric unbounded domain for solving the Poisson equation and the elastostatic equation coupled with the thermo-poro-elastic extension of Hooke's law [3], in which geometries of arbitrary shape are defined by level-set functions.
The method considers a smooth transformation of the coordinates to map an unbounded domain discretized with a quasi-uniform mesh into a bounded one discretized with a uniform mesh. In this way, the equations on the internal points are discretized with the usual finite-difference discretization using a 9-point or a 5-point stencil for the elastostatic or Poisson equation, respectively. The boundary conditions are instead imposed through a ghost-point technique that is described in [1] and [4], which allows to define the field variables on the points outside the domain that are close to the boundary.

The proposed method was then applied in volcanology to model gravity changes and ground deformations induced by thermo-poro-elastic sources. It takes into account the real topography of the volcano and the non-homogeneous distributions of the medium elastic properties and of the pressure, temperature and density variations at the source. The coordinate transformation avoids inaccuracies introduced by finite truncation of the domain and allows gravitational potential and deformations to vanish at infinity [2].

Many methods, such as the finite element ones, require the definition of the mesh if the geometry is modified. This approach instead considers the source immersed in a Cartesian grid [1] avoiding the recalculation of the mesh. The method is computationally efficient when it is necessary to perform a large number of simulations for the geophysical observables inversion problems which seek to recover the shape of the source.

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MS18 - Analysis and numerics of wave propagation phenomena

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ABSTRACT

The Minisymposium is devoted to differential equations that model wave propagation phenomena, formulated either in the frequency or in the time domain. The development and analysis of numerical methods for the approximation of their solution is a challenging task and have undergone an explosive interest in recent years for the scientific community. The meeting will focus in particular on discretization techniques for computing accurate, efficient and robust solutions of the mentioned problems by means of variational domain methods or boundary integral based ones. The main goal is to bring together experts in the field of numerical analysis, belonging to different international research groups, to discuss on the most recent advances and current open challenges on fast and innovative strategies for real-life applications.

Space-time continuous and coercive formulation for the wave equation

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Space-time methods for evolution PDEs regard time as an additional dimension, as opposed to semidiscretisation techniques such as the method of lines. Some advantages in pursuing these methods include the possibility of implementing local time-stepping and space-time adaptivity and the fact that the approximate solution of the PDE is defined at every point in the space-time domain (and not on time slices).
For the second-order wave equation, a stable discrete formulation on tensor-product elements has been proposed in [2], but a stable space-time variational formulation that allows the use of general discretisations is not available.
To derive such a formulation, we propose integration by parts testing against a Morawetz multiplier (i.e. a specially crafted test function) and obtain a bilinear form that is continuous and coercive (sign-definite) as required by the Lax-Milgram theorem. This strategy follows the approach previously adopted for Helmholtz problems in [1]. The formulation is set in a function space endowed with a norm that is stronger than the usual one on $H^1(\Omega \times (0,T))$, and because of this, any conforming discretisation is required to be $C^1(\overline{\Omega \times (0,T)})$. Coercivity holds for problems where impedance boundary condition $\partial_t u + \theta \partial_n u$ are imposed on $\partial\Omega \times (0,T)$ when Ω is star-shaped with respect to a ball and also in scattering problems with a star-shaped Dirichlet scatterer. Lax-Milgram theorem implies the well-posedness of the variational formulation on any discrete space $V_h \subset C^1(\overline{\Omega \times (0,T)})$, and by Cea's lemma explicit error bounds can be computed. Numerical experiments confirm the theoretical results.

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Space-time discontinuous Galerkin methods for wave propagation in coupled poroelastic-elastic media

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Poroelastic-elastic problems model elastic waves impacting a porous material and consequently propagating through it. The numerical simulation of these phenomena provide a fundamental tool for the assessment of a wide range of scientific applications in the field of acoustic, aeronautical and biomedical engineering, as well as computational seismology [2]. In this talk, we present and analyze a space-time finite element discontinuous Galerkin method on polytopal meshes (PolyDG) for the numerical discretization of coupled poroelasticity-elasticity wave propagation problems. The mathematical model consists of the low-frequency Biot's equations in the poroelastic medium and the elastodynamics equation for the elastic one. To realize the coupling, suitable transmission conditions on the interface between the two domains are weakly embedded in the formulation. The coupling conditions considered in our work are a consistent generalization of [3], since we also take into account the effect of partial filtration at the interface.

In order to accurately simulate multiphysics wave phenomena in heterogeneous domains, the numerical scheme should deal with an accurate geometrical description of the arbitrary complex interfaces possibly without compromising the efficiency in terms of computational cost. Therefore, we propose an arbitrary-order PolyDG method [1] for the space discretization of the coupled problem that, thanks to its high-level of flexibility, can be employed in real applications. The discretization in space is then coupled with a discontinuous Galerkin time integration scheme, resulting in a full space-time dG discretization. We present a complete stability analysis for both the continuous and the semi-discrete formulations, and we derive *hp*-error estimates for the semi-discrete formulation in a suitable energy norm. The method is applied to a wide set of numerical test cases to verify the theoretical bounds. Examples of physical interest are also presented to investigate the capability of the proposed method in relevant geophysical scenarios.

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On the Energetic Galerkin Boundary Element Method applied to 3D Elastodynamics

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We consider a boundary integral reformulation of 3D time-domain elastodynamic (vector) wave problems, defined in unbounded domains external to an open polyhedral screen, endowed with a Dirichlet type boundary and null initial conditions. For the resolution of the corresponding Boundary Integral Equation, we use the space-time energetic Galerkin Boundary Element Method (introduced for the first time in [1]) with double analytical integration in time variable. The resulting weakly singular double integrals in space variables are then evaluated by inner analytical and outer numerical integrations [2]. In the presented numerical examples, graded meshes are used to recover the quasi-optimal approximation convergence rates known for screens and for polygonal domains in 3D [3] and the singular behaviour of the solutions from corners and edges.

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A hyperbolic model of thermal conductivity in nanosystems

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In the general context of continuum mechanics, a very important role is played by the so-called balance laws. From the theoretical point of view, a balance law is just the statement of the causes of the contents time-changes of a certain extensive physical quantity over a given domain. From the practical point of view, each balance law is expressed in terms of a partial differential equation (i.e., the so-called balance equation) which is usually written in a local form in such a way that it has to be valid in any point of a given domain.
According to the second law of thermodynamics, the entropy production has to be always non-negative in any point and at any time, whatever the thermodynamic process is [1], [2]. Since all solutions of the balance equations have to comply with the second law, that unilateral constraint is mainly used to determine the forms either of the constitutive relations [3], or of the evolution equations of the state-space variables.
In this talk we propose a non-local and non-linear thermodynamical model of heat transfer at nanoscale beyond the well-known Maxwell-Cattaneo theory. The compatibility of the proposed model with second law has been proved. The model is subsequently used to investigate the propagation of a heat pulse in one-dimensional nanosystems in the linear case. The predicted results are compared with those arising from the Maxwell–Cattaneo theory in order to point out the possible influence both of the non-local effects, and of the relaxation effects of the higher-order fluxes. Some problems related to initial data and boundary conditions are also discussed.

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A CFL-Free Space–Time Isogeometric Method for the Acoustic Wave Equation

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Space–time Finite Element Methods (FEMs) for wave propagation problems in the time-domain were introduced in [2]. Since then, many studies on space–time methods for transient waves have been proposed, triggered by the practical advantages of space–time schemes if compared to standard time-stepping techniques. Space–time discretizations benefit from numerical solutions defined throughout the time interval, optimal mesh adaptation to moving fronts in the space–time domain, efficient treatment of moving boundaries, space–time parallelisation and space–time multilevel preconditioning.

Isogeometric Analysis (IgA) is an evolution of the classical FEM that is meant to simplify the interoperability between computer aided design and numerical simulations. Among the others remarkable properties of IgA, space–time isogeometric schemes require much less degrees of freedom if compared to space–time finite element discretizations. Indeed, in the discretization of a space–time problem on a d-dimensional space domain, denoting with n_{sub} the number of subdivision in each dimension and p the polynomial degree, the total number of degrees of freedom is almost $p^{d+1}(n_{\text{sub}}+1)^{d+1}$ for hp-FEM, while it is only $(n_{\text{sub}}+p)^{d+1}$ in the case of IgA that employs splines with maximal regularity.

Despite their appealing properties, naive space–time isogeometric discretizations of the wave equation can easily result in a CFL (*Courant–Friedrichs–Lewy*) condition, which is required to ensure stability. In this talk, we will show an unconditionally stable high-order space–time isogeometric discretization of the linear acoustic wave equation [1]. The proposed numerical scheme is based on a stabilization technique that extends the one devised in [3] to high-order *and* smooth space–time IgA. As a result, we get a novel space–time isogeometric method that benefits from optimal convergence rates and desired energy properties without any constraint on the time mesh-size.

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Dirichlet-to-Neumann Coupling for Mixed-Dimensional Time-Dependent Wave Problems

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A reoccurring theme in computational mechanics in recent years is the need to reduce the size of large discrete models. One type of such a reduction is spatial dimensional reduction, which one may perform in cases where the solution in some region of a high-dimensional (highD) computational domain, say two-dimensional (2D), behaves in a low-dimensional (lowD) way, say one-dimensional (1D).

The motivation in constructing a mixed-dimensional (say 2D-1D) model comes from the fact that solving the problem in its highD form everywhere may require a very large computational effort. The idea is thus to partly reduce the spatial dimension of the problem, in order to obtain a hybrid model which is much more efficient. One field of application where mixed-dimensional coupling is of special interest is that of the dynamics of elastic structures. Typically, the LowD model consists of the slender parts of the structure that have rod- or beam- or plate- or shell-like behavior, and which constitute most of the structure volume, while the HighD parts are the small regions that have to be modeled as 3D elastic bodies.

There are several scenarios where this could be the case. Most significant is the scenario where the solution in a certain region behaves in a way that is weakly (or hardly) dependent on a certain coordinate, relative to the other coordinates. Another possible scenario is when we are interested in the solution within a geometrically slender region. In this case we might be interested in the lateral average of the solution within this region rather than in its lateral distribution. Alternatively, we might already know the nature of the lateral distribution of the solution within this region and wish to know the axial distribution. In these cases, the lateral dimension is the dimension we would eliminate, resulting in a mixed-dimensional model.

In the present work, we consider the 2D-1D coupling and 3D-2D coupling of models, to form a single hybrid 2D-1D and 3D-2D model, for the time-dependent linear scalar wave equation and for elastodynamics. The mixed-dimensional coupling is done using the Dirichlet-to-Neumann (DtN) map associated with the LowD part of the problem. We shall discuss two ways in which the DtN coupling can be done: in one of them the HighD and lowD problems exchange information in each time step, whereas in the other the two problems are solved independently. The well-posedness of the hybrid problem as well as the coupling error are discussed, and numerical examples are presented.

Space-time ultra-weak discontinuous Galerkin method for the Schrödinger equation

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We present a space–time ultra-weak discontinuous Galerkin discretization of the linear Schrödinger equation. We prove that the method is well-posed and quasi-optimal in mesh-dependent norms for very general discrete spaces. Four different choices of discrete spaces are considered:

(i) a non-polynomial Trefftz space of complex wave functions [1];

(ii) the full polynomial space [2];

(iii) a quasi-Trefftz polynomial space [2];

(iv) a polynomial Trefftz space [3].

Several numerical experiments validate the accuracy and advantages of the proposed method for each discrete space.

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On numerical modelling of an upper hybrid resonance in cold plasma

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Harmonic wave propagation in cold plasma is described by Maxwell's equations with a tensor of dielectric permittivity that depends in particular on particle density, which, in general, varies in space. We consider the 2D TE mode, which further can be rewritten as a second order PDE with varying coefficients. Due to vanishing of a coefficient in front of the principal term, the model becomes degenerate; in physics this causes resonant plasma heating. Mathematically, this problem had been intensively studied by B. Després and co-workers, cf. e.g. [2, 1] and references therein, who, in particular, remarked that the resonances are related to singular solutions of the problem.
We consider a simplified problem, namely, a second-order PDE, where the coefficient in the principal part changes its sign along an interface Σ, cf. [3]. The physical, singular solutions are not covered by a 'natural' variational framework in which this problem is posed, but appear when considering the limiting absorption principle (LAP).
In this talk, we discuss validity of the LAP for the simplified problem. Next we show how it yields a natural decomposition of the solution to the problem into a regular (continuous across the interface Σ) and singular (with a logarithmic and jump singularity) parts.
We next present a numerical method to solve this problem, based on a modification of the variational formulation from [3]. We discuss in particular the question of equivalence of the new formulation with the original limiting absorption problem and finish the exposition with several numerical experiments.

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A Hausdorff-measure boundary element method for acoustic scattering by fractal screens

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Sound-soft fractal screens can scatter acoustic waves even when they have zero surface measure. We formulate such scattering problems as singular integral equations and we approximate them using the boundary element method (BEM). Each BEM basis function is supported in a fractal set, and the integration involved in the formation of the BEM matrix is with respect to a non-integer order Hausdorff measure rather than the usual (Lebesgue) surface measure. Using recent results on function spaces on fractals, we prove convergence of the Galerkin formulation of this "Hausdorff BEM" for acoustic scattering when the scatterer is a compact d-set for some suitable Hausdorff dimension d. For a class of fractals that are attractors of iterated function systems (IFS), we prove convergence rates for the Hausdorff BEM and superconvergence for smooth antilinear functionals, under certain natural regularity assumptions on the solution of the underlying boundary integral equation. We also propose numerical quadrature routines for the implementation of our Hausdorff BEM, along with a fully discrete convergence analysis, via numerical integration estimates and inverse estimates on fractals, estimating the discrete condition numbers. Finally, we show numerical experiments that support the sharpness of our theoretical results and our solution regularity assumptions, including results for scattering in $\mathbb{R}^2$ by Cantor sets, and in $\mathbb{R}^3$ by Cantor dusts.

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Skeleton integral equations for acoustic transmission problems with varying coefficients

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In our talk we will derive an integral equation method which transforms a three-dimensional acoustic transmission problem with variable coefficients and mixed boundary conditions to a non-local equation on the two-dimensional boundary and skeleton of the domain. For this goal, we introduce and analyze abstract layer potentials as solutions of auxiliary coercive full space variational problems and derive jump conditions across domain interfaces. This allows us to formulate the non-local skeleton equation as a direct method for the unknown Cauchy data of the original partial differential equation. We develop a theory which inherits coercivity and continuity of the auxiliary full space variational problem to the resulting variational form of the skeleton equation without relying on an explicit knowledge of Green's function. Some concrete examples of full and half space transmission problems with piecewise constant coefficients are presented which illustrate the generality of our integral equation method and its theory.

Fast Time Domain Boundary Element Method using 3D Adaptive Cross Approximation

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We consider the time domain Boundary Element Method (BEM) for the homogeneous wave equation with vanishing initial conditions and given Dirichlet and/or Neumann boundary conditions. The generalized convolution quadrature method (gCQ) developed by Lopez-Fernandez and Sauter [2] is used for the temporal discretisation. The spatial discretisation is done classically using low order shape functions and a collocation approach.
Essentially, the gCQ requires to establish boundary element matrices of the corresponding elliptic problem in Laplace domain at several complex frequencies. Consequently, an array of system matrices is obtained. This array of system matrices can be interpreted as a three-dimensional array of data which should be approximated by a data-sparse representation. The Adaptive Cross Approximation (ACA) can be generalized to handle these three-dimensional data arrays [1]. The basic idea is the same as for the original algorithm. Adaptively, the rank of the three-dimensional data array is increased until a prescribed accuracy is obtained. On a pure algebraic level it is decided whether a low-rank approximation of the three-dimensional data array is close enough to the original matrix. Hierarchical matrices are used in the two spatial dimensions in combination with the usual ACA. The third dimension of the data array represents the complex frequencies. Hence, the algorithm makes not only a data sparse approximation in the two spatial dimensions but detects adaptively how much frequencies are necessary for which matrix block.
In the presentation this methodology is recalled and applied either to the H-matrix as a whole or for each block within the H-matrix. Some examples will show how the method performs.

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Isogeometric approximation of the scalar wave equation

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In recent years several there has been an increasing attention to high order simulations of acoustic and elastic wave propagation. While our previous works focused on approximations based on spectral and spectral elements methods, we then extended our study to Isogeometric (IGA) methods that allow not only the standard p- and hp- refinement of hp- finite elements and spectral elements, where p is the polynomial degree of the C^0 piecewise polynomial basis functions, but also a novel k- refinement where the global regularity k of the IGA basis functions is increased proportionally to the degree p, up to the maximal IGA regularity $k = p - 1$ [1].
In this presentation we consider the numerical approximations of the acoustic wave equation with absorbing boundary conditions, that are introduced in order to simulate wave propagation in infinite domains, by truncating the original unbounded region into a finite one. The spatial discretization is based on IGA Galerkin [2] and Collocation [3] in cartesian and curvilinear 2D regions, while the time discretization is based on explicit or implicit Newmark schemes. We illustrate a detailed experimental study of the two IGA methods with regard to spectral properties of the IGA mass and stiffness matrices [5], stability, accuracy and convergence of the IGA schemes [2, 3, 4] with respect to all the discretization parameters, namely the local polynomial degree p, regularity k, mesh size h, and the time step size Δt of the Newmark schemes. Finally we show some preliminar numerical results on the application of an additive overlapping Schwarz preconditioner to both IGA Galerkin and Collocation approximations, testing its performance with GMRES or preconditioned conjugate gradients iterative methods.

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MS19 - Nonlinear PDEs in Quantum Mechanics and Applications

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ABSTRACT

The fundamental role of nonlinear partial differential equations in Quantum Mechanics is by now universally recognized. Within this context, nonlinear Schrödinger and Dirac equations provide effective models in many situations, from microscopic systems as Bose–Einstein condensates to electronic properties of high–tech materials as graphene. Recently, the development of the analysis of nonlinear PDEs has been pushed in new and challenging directions by major experimental advancements in condensed and solid matter physics. Such a strong impulse from this variety of applications triggers a wide horizon of theoretical investigations, contributing as well to foster the interconnection of several branches of mathematical analysis.

The aim of the minisymposium is to bring together recognized experts in the study of nonlinear PDEs in Quantum Mechanics alongside with young mathematicians working on the topic. The major goal is twofold: to promote the exchange of ideas and methods among people in the community with different expertises, and to encourage the diffusion of new problems with a potential relevance on future high–impact technological applications. Among the main topics that will be represented in the minisymposium are the analysis of nonlinear dispersive equations, with a prominent interest in models involving singularities and/or taking place on non–standard domains, and the study of universal properties of quantum many–particle systems.

Mathematics for Atomtronic: nonlinear hybrid systems

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Atomtronics is the complex of technologies that exploit ultracold matter instead of electron in order to transmit information. At present, it is at an initial stage, however mathematical models of atomtronic devices is necessary for the sake of designing them and of circumscribing their field of applicability. A problem that can already be rigorously invstigated is the existence of ground states for such devices, that can act either as obstacles to the transmission or as energy reservoirs. We give results for a simple model of cavity with antenna, called hybrid since it joins elements of different space dimensionality.

Regularized zero-range Hamiltonian for 3 bosons in 3d: construction and approximation

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Hamiltonians with zero-range interactions are well suited to describe systems of quantum particles at low energy where the details of the interactions become irrelevant and the only significant physical parameter is the scattering length. Unfortunately, as soon as the number of particles is larger than three the standard realizations of such Hamiltonians in three dimensions (known as TMS Hamiltonians), are affected by an instability known as Thomas effect: they are only symmetric and all their self-adjoint extensions are unbounded from below.
In [1] we consider a system of three identical bosons interacting through zero-range interactions appropriately regularized by an effective three-body force. This model, first suggested in [3], was recently revived in [2]. We prove that the Hamiltonian describing the system is self-adjoint and bounded from below thus preventing the emergence of the Thomas effect. Furthermore, we show that it can be obtained as the norm resolvent limit of approximating Hamiltonians with rescaled non local interactions (separable potentials) and with a suitably renormalized coupling constant.

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The Dirac equation with concentrated nonlinearity: stability and instability of solitary waves

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In this talk it will be analyzed the nonlinear Dirac equation with Soler-type nonlinearity concentrated at one point and present a detailed study of the spectrum of linearization at solitary waves.

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On the well-posedness for NLS with a point interaction

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In this talk I will discuss some results on the solution theory for the time-dependent NLS equation with a point interaction. After introducing a natural scale of adapted Sobolev spaces, I will show how to characterize the sub-critical non-linearities at fixed (possibly fractional) regularity. By exploiting suitable dispersive properties of the linear flow, a well-posedness result will eventually follow by Kato-type methods. The last part of the talk will be devoted to open problems and perspectives.

Complete ionization for a two-dimensional non-autonomous point interaction model

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The talk will discuss the two-dimensional Schrödinger equation with a non-autonomous point interaction of delta type. After a mention to the global well-posedness of the associated Cauchy problem, we establish the asymptotic behavior of the *survival probability* of the bound state of the free problem in the case of a monochromatic periodic non-resonant interaction. Such probability is proved to vanish, thus showing that the model is subject to a *complete ionization* phenomenon, and its decay is proved to be $\mathcal{O}((\log t/t)^2)$ up to lower order terms. This is a work in collaboration with W. Borrelli and R. Carlone.

MS20 - Mathematics for Machine Learning

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ABSTRACT

Machine learning (ML) is one of the hot topic of nowadays research in the areas of Applied Mathematics. ML connects statistical, probabilistic, analytical and computational aspects arising from data. The aim of ML is to find hidden insights used to build intelligent applications and valid patterns. Therefore, the mathematics behind ML is mandatory to comprehend the fundamental principles upon which it is possible to set up more complicated real-life systems. The purpose of the mini-symposium is to provide a discussion for researchers in order to present new mathematical concepts for understanding the procedures of the ML and future trends.

Bounds and limitations on generalization capabilities of Graph Neural Networks

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Graph Neural Networks (GNNs) have emerged in the past years as a powerful tool to learn tasks on a wide range of graph domains in a data-driven fashion; based on a message passing mechanism, GNNs have gained more and more popularity for their intuitive formulation, strictly linked with the Weisfeiler-Lehman (WL) test for graph isomorphism to which they have been proven equivalent [1, 3]. From a theoretical point of view, GNNs have been proved to be universal approximators and their generalization capabilities (namely, bounds on the VC dimension [2]) have been recently investigated for GNNs with piecewise polynomial activation functions [4]. The aim of our work is to extend this analysis on VC dimension of GNNs to other commonly used activation functions such as sigmoid and hyperbolic tangent, using the framework of pfaffian functions theory; moreover, we carry on an in-depth analysis on the generalization capabilities of GNNs, considering different frameworks to evaluate their (in)nability to learn the so-called *identity effects*, i.e. the power of determining if an object is composed by two identical patterns or not [5]. The theoretical analysis is supported by an extensive experimental study.

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Graph-Informed Neural Networks for Physics-Informed Learning of Partial Differential Equation Solutions

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The possibility to embed mathematical models in Deep Learning models for solving complex physical problems attracted the attention of many scientists in recent years. Concerning the solution of differential equations, Physics-Informed Neural Networks (PINNs) proved to be particularly successful [1]. A PINN is a Neural Network (NN) trained for learning the solution of a differential problem by using a loss function defined by the differential equations of the problem and the boundary conditions. The main advantage of this approach is that training data (typically obtained running expensive numerical simulations) are not required for training the surrogate NN model. On the other hand, error analysis for PINNs can be hard due to the highly nonlinear nature of the NNs; then, getting information about the solution's approximation quality can be a difficult task.
Graph-Informed Neural Networks (GINNs) [2] are NNs based on Graph-Informed (GI) layers, i.e., layers embedded with the adjacency matrix of the graph structure characterizing the given data. In this talk, we present an approach where we train a GINN as a PINN for learning not the solution of a Partial Differential Equation (PDE) problem directly but a linear combination of Radial Basis Functions (RBFs) that approximates that solution. Specifically, given a set of points in the domain, we build a graph connecting those points that are near to each other (given a threshold distance value), and we consider these points as centers of Gaussian RBFs; then, we exploit the properties of GI layers for building a GINN having the task of learning both the RBF's width parameters and the coefficients of an RBF-linear combination approximating the solution of the PDE problem. The learning procedure (i.e., the training of the GINN) follows the PINN principles, minimizing a loss function defined by the PDEs and the boundary conditions of the problem. The idea behind this method is to build a new type of PINN of simpler usage, control, and analysis.
In this presentation, we illustrate the first experimental results of the proposed method on some PDE test problems, and we describe the possible potentialities of this new approach.

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Optimizing penalty hyperparameters in nonnegative matrix factorization with bi-level strategy

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Hyperparameters are parameters explicitly defined by the user to control the data-learning process in a machine learning context. They can have a significant impact on the data knowledge extraction process. Optimizing hyperparameters turns out to be a very interesting open question [1, 2]. Recently, data mining applications have used matrix factorization (MFs) to capture information embedded in large datasets. A MFs method can be considered an optimization problem in which penalty terms are used to enforce constraints that emphasize useful properties [4]. Tuning the hyperparameters affecting the weight of these additional constraints is particularly challenging in this unsupervised learning scenario and, to the best of our knowledge, the literature panorama does not provide a general framework that addresses this choice optimally due to the variety of fields involved in this problem. In this talk, we want to emphasize the role of hyperparameters in the context of penalized nonnegative matrix factorizations (NMFs) and the importance of selecting appropriate values for them. Inspired by the bi-level formulation used in the supervised scenario [3], we approach the selection of hyperparameters from an optimization standpoint, incorporating their choice directly into the unsupervised algorithm as part of the updating process. We provide some existence and convergence results of numerical solutions for the associated optimization problem. We also design a novel algorithm that incorporates hyperparameter tuning into the updates of the nonnegative matrix factors, and we test it on synthetic and real datasets.

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Real kernel methods *vs* complex kernel methods in machine learning and signal theory

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We build on work by P. Bouboulis & S. Theodoridis, [1], and pursue their program of recovering the kernel methods (as employed in signal analysis and machine learning theory) from *real* RKHS and kernels, to the *complex* domain.
We[2] solve the maximum problem

$$\sup \Big\{ \sum_{j=1}^{p} \big|f(z_j)\big|^2 \,:\, \|f\|^2 \le E \Big\}$$

in the complex RKHS of holomorphic L^2 functions $f : \Omega \to \mathbb{C}$, for any bounded domain $\Omega \subset \mathbb{C}^n$ and any finite set of points $z_1 \,, \cdots \,, z_p \in \Omega$. The result is applied to the space $L^2H(\mathbb{B}^n)$ of holomorphic L^2 functions on the unit ball $\mathbb{B}^n \subset \mathbb{C}^n$. The problem of producing sampling expansions starting from complete orthonormal systems $\{\phi_\nu\}_{\nu\ge 0} \subset L^2H(\Omega)$ is taken up by refuting [based on counterexamples, such as the Bergman kernel $K(z,\,\zeta)$ for the unit ball $\Omega = \mathbb{B}^1$] K. Yao's hypothesis (cf. [3]) that $\phi_\nu(z) = c_\nu\, K(z,\,\zeta_\nu), \quad z \in \Omega, \quad \nu \ge 0$, for some sequence of points $\{\zeta_\nu \,:\, \nu \ge 0\} \subset \Omega$ and some $\{c_\nu \,:\, \nu \ge 0\} \subset \mathbb{C}$, and instead by approximating each ϕ_ν uniformly on Ω by a linear combination of reproducing kernels. The means to said approximation are provided by the Faber-Kaczmarz-Mycielski algorithm $\mathcal{A}(h)$ with

$$h(z,\,\zeta) = \frac{K(z,\,\zeta)}{K(\zeta,\,\zeta)}\,, \quad z,\,\zeta \in \Omega,$$

learning (cf. [2]) from the data $\big\{\big(\zeta_k\,,\,\phi_\nu(\zeta_k)\big)\big\}_{k\ge 0}$ and producing an approximating sequence

$$\big(\phi_\nu\big)_k(z) = \sum_{j=0}^{k-1} e_j\big(\phi_\nu\big)\; h(z,\,\zeta_j), \quad k \ge 1,$$

where $e_j(\phi_\nu)$ is the error committed by $\mathcal{A}(h)$ at time j.

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A Nonmonotone extra-gradient Trust-region method with noisy oracles

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Trust-region (TR) methods are a well-established class of iterative numerical methods for optimizing nonlinear continuous functions. In each iteration, TR methods minimize an approximation (model) of the objective function, often a quadratic model, within a trust-region. In this article, we propose and analyze a nonmonotone TR method for unconstrained continuous optimization problems

$$\min_{x\in\mathbb{R}^n} \phi(x),$$

where $\phi : \mathbb{R}^n \to \mathbb{R}$ is (twice) differentiable with Lipschitz continuous derivatives, but neither the objective function nor its associated derivatives are assumed to be computable accurately. This is the case, for instance, when solving the unconstrained optimization problems arising in the training of deep neural networks, where the application of subsampling strategies yields noisy approximations of the finite sum objective function and its gradient. Our approach involves additional sampling in order to control the resulting approximation error, i.e., to construct an adaptive sample size strategy. Depending on the estimated progress of the algorithm, this can yield sample size scenarios ranging from mini-batch to full sample functions. We provide convergence analysis for all possible scenarios and show that the proposed method achieves almost sure convergence under standard assumptions for the trust-region framework. We report numerical results showing the performance of the proposed optimizer in the training of deep residual networks for image classification tasks. Our results show that the proposed algorithm outperforms STORM, a progressive batching stochastic second-order TR algorithm proposed in [1].

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Gaussian processes based data augmentation and expected signature for time series classification

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During the last twenty years rough path theory has emerged as a key idea to understand integration for general irregular paths [1]. Recently rough paths have proved to be an effective tool in the machine learning field [3]. The signature is a fundamental notion that describes a path in terms of algebraic objects (iterated integral). The various properties of the signature of a path, such as the capability of characterising a path or the existence of a universal approximation theorem, suggest that the signature transform can be extremely useful for analysing or classifying time series.
In this work we propose a new time series classification model based on the signature transform. The model combines two main ideas. The first is a stochastic data augmentation based on a Gaussian Processes regression model [2]. The second idea is to capture the relevant features of paths by means of the expected signature, computed over the ensemble obtained in the phase of data augmentation. In particular, the model takes a time series $x = (x_t)_{t\in I}$, over a set of times I, as input, and generates a new set of time series, $\{y^i = (y^i_s)_{s\in T} : i \le K\}$ on a richer set of times T, i. e. $I \subset T$. The generation of the new set of series is performed by sampling from a Gaussian distribution with mean and variance learned by the model itself. The expected signature is thus estimated by averaging over a normalized version of the signature of each y^i. Then the computed expected signature is used as input to a linear layer in order to get the prediction.
Signature normalization has a strong theoretical explanation: Chevyrev and Oberhauser [4] have proved that the expectation of a normalized version of the signature is able to characterize the law of a large family of stochastic processes. In our numerical context normalization turns out to be crucial to stabilize the estimate of the expected signature.
Our model presents several advantages, such as its scalability and adaptability. It integrates seamlessly in more complex architectures and it can be easily modified in order to solve also time series regression problems. The model has been tested on several datasets and it has been compared with other models proposed in the literature on the subject.

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MS21 - Mathematical Modelling in Biology

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ABSTRACT

The understanding of biological systems such as cells, tissues and organs is increasingly taking advantage of tools from quantitative sciences, which can provide powerful instruments to unravel complex mechanisms. A paramount example in this respect is represented by the emerging field of mechanobiology, which aims at analysing how mechanics affects the tissue, cellular and subcellular processes, and involves the interaction of mathematics, physics, engineering, and chemistry. At the same time, the study of pathological conditions, such as neurodegenerative diseases, tumours, cardiovascular and musculoskeletal disorders, benefits from the interaction of quantitative models and medical observations. The contribution of mathematical models in all these fields can indeed provide a twofold support to the research process: by unveiling fundamental mechanisms underlying complex biological phenomena and by supporting the clinical translation. In this context, the aim of this Mini-Symposium is to

showcase recent advancements in the rapidly evolving field of mathematical modelling in biology and biomedicine. In particular, the Mini-Symposium is divided in three parts, each focused on a specific topic.

Part I: Tumour Modelling

The first session of the Mini-Symposium will focus on the mathematical modelling of tumour mechanics *and its application to precision and personalised medicine. Specifically, we will focus on the description of cancer growth and its response to therapies. We will also focus the attention on other phenomena such as tumour angiogenesis, i.e. the formation of the tumour own vascular network. The proposed models will make use of theoretical tools, such as multiple scale expansions, phase field modelling and poroelasticity, coupled with computational tools that allow quantitative predictions using patient-specific data.*

Part II: Cell Adhesion, Active Motion and Reorganisation

The second part of this Mini-Symposium will be specifically focused on cell adhesion, active motion and reorganisation. *Cells' ability to migrate and reorganise onto two dimensional substrates and inside three dimensional environments plays an essential role in many physiological and pathological processes, including embryonic development, wound healing, immune response, cancer progression and metastasis formation. In the second session we will present some notable examples of how mathematical models can shed light on this complex processes, across the different spatial and temporal scales.*

Part III: Continuum Models of Soft Tissue Mechanics

Finally, the third part of this Mini-Symposium will be focused on continuum models for soft tissue mechanics. *Organs and tissues perform fundamental tasks that ensure the accomplishment of vital functions for the entire organism. However, during lifetime, several pathological conditions may arise and compromise the functionality of living tissues. Among those, cardiovascular diseases and musculoskeletal alterations can dramatically impair life quality and expectancy. The mathematical and numerical modelling of both physiological and pathological conditions of living tissues, along with the mechanisms involved in restoring their correct functioning, will be the focus of the third session.*

Mechanobiology of glioblastoma cells under osmotic stress

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We investigate the mechanobiological features of cells cultured in monolayers in response to different osmotic conditions [1]. In-vitro experiments have been performed to quantify the long- term effects of prolonged osmotic stresses on the morphology and proliferation capacity of glioblastoma cells. The experimental results highlight that both hypotonic and hypertonic conditions affect the proliferative rate of glioblastoma cells on different cell cycle phases. Moreover, glioblastoma cells in hypertonic conditions display a flattened and elongated shape. The latter effect is explained using a nonlinear elastic model for the single cell. Due to a crossover between the free energy contributions related to the cytosol and the cytoskeletal fibers, a critical osmotic stress determines a morphological transition from a uniformly compressed to an elongated shape.

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Mathematical modelling of axonal cortex contractility

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The axonal cortex is comprised of a regular arrangement of F-actin and spectrin, which can contract due to the presence of myosin II motors. This active tension plays a crucial role in determining the shape of axons in a physiological context. Recent experiments [2] have demonstrated that axons adjust the contraction of the cortex when subjected to mechanical deformations, exhibiting a non-trivial coupling between the hoop and the axial active tension. However, the underlying mechanisms behind this phenomenon are still not well understood. In this study, we present a continuum model of the axon based on the active strain theory [1]. By using the Coleman-Noll procedure, we shed light on the coupling between the hoop and the axial active strain through the Mandel stress tensor. We conduct a qualitative analysis of the system assuming incompressibility and establish the existence of a stable equilibrium solution. In particular, our results suggest that the axon regulates the active contraction to maintain a homeostatic stress state. Additionally, we employ numerical simulations using a more suitable compressible constitutive law and compare the results with experimental data, demonstrating a remarkable quantitative agreement.

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Mechanics of diffusion-mediated budding and implications for virus replication and infection

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Budding allows virus replication and macromolecular secretion in cells through the formation of a membrane protrusion (bud) that evolves into an envelope. Envelope formation requires the transport of transmembrane (spike) proteins across the membrane, thus, is a diffusion-limited process [1],[2]. This seminar proposes a simple model to describe budding in the context of virus replication, discovering size limitations and size-dependent kinetics [3]. The optimal virus size, giving fastest replication, is validated against experiments for Coronavirus, HIV, Flu, and Hepatitis. Moreover, the model can predict the size polydispersity of a virus population, here tested against Coronavirus. Finally, the model is extended to describe infection via endocytosis and membrane fusion. This model provides a useful tool to correlate the statistical distribution of the geometrical features of a virus population with the nanoscale properties of the virion. AAA

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Modeling brain tumour growth and deformation of cerebral ventricles: a patient-specific mechanical approach

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Brain tumours pose significant medical challenges due to their unpredictable location and varying degrees of malignancy. Malignant brain tumours, in particular, are known for their aggressive behaviour, presenting obstacles to effective treatment. The growth of a brain tumour can result in a mass effect, causing compression and displacement of surrounding healthy brain tissue. This can lead to changes in ventricle volume, resulting in increased intracranial pressure and potentially severe neurological complications [1]. Additionally, the compression of adjacent healthy areas may also occur, further compromising their normal function and contributing to the overall impact of the tumour. The current standard of care for brain tumours involves surgical resection as the primary treatment, followed by radiation therapy and chemotherapy, whenever feasible [2].
In this study, we propose a multiphase mechanical model for brain tumour growth that quantifies deformations and solid stresses caused by the expanding tumour mass. Our model considers the influence of brain fibres on the tumour's anisotropic growth patterns, accounting for the irregular and heterogeneous nature of brain tumours. To construct realistic three-dimensional brain geometries and capture the shape of the ventricles, we incorporate patient-specific MRI and DTI data. By investigating the intricate interactions between brain tumours and the surrounding brain tissue, our model yields valuable insights into the extent of ventricular compression caused by tumour growth. Additionally, it elucidates the impact on the adjacent healthy brain area affected by tumour growth. The numerical results obtained using the software *FEniCS* show the model's effectiveness in capturing the complex dynamics of brain tumour growth and its mechanical impact on surrounding brain tissue. This work contributes to advancing our understanding of tumour progression and have the potential to guide the development of targeted therapies tailored to individual patients.

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Multiscale modelling of fluid transport in vascular tumours subjected to electrophoresis anti-cancer therapies

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Applied electric field treatment has experimentally shown to improve drug delivery in a variety of vascularised tumours, however, there are lack of realistic mathematical models with direct measurements. Real world physical systems such as fluid transport in biological tissues have multiscale nature, exhibiting different chemical and physical behaviour on particular levels. Upon zooming in a hierarchical system one can see a variety of distinct arrangements, where the peculiarity in mechanical behaviour should be taken into account to realistically model the overall behaviour. From a mathematical standpoint, it is challenging to resolve multiscale systems at reduced computational costs, as it is practically impossible to fully undertake the microscale material with its geometric complexity. We use the asymptotic homogenisation technique to acquire an effective differential problem that is to be solved on the macroscale only, whilst retaining information about the microstructure by encoding the micro variations in the homogenised coefficients. We investigate the effect of an applied electric potential on the flow of Darcian-type fluid occurring in two different phases, namely the tumour and healthy regions. We derive a novel mathematical model by generalising [1], which reads as a Darcy's type system of PDEs. The new model can be used to predict the effect of an applied electric field on cancerous biological tissues, paving a new way of improving current electrochemotherapy protocols.

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Parameter estimation in cardiac biomechanical models based on physics-informed neural networks

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Due to their predictive character and capacity to support the interpretation of clinical data, biophysical models of the cardiovascular system are being developed at an increased rate in the scientific community [1]. High-resolution, accurate multi-physics mathematical models are computationally expensive, and their personalisation requires the fine calibration of a huge number of parameters, making it difficult to apply them in clinical settings. In order to generate reliable and efficient surrogate reduced-order models that are capable of reconstructing displacement fields and estimating patient-specific biophysical properties, a novel methodology is presented in this talk. The method is based on the integration of physics-informed neural networks methodologies [2] with high-resolution three-dimensional cardiac biomechanical models. The physics of the problem is represented by a mathematical model based on partial differential equations, and the proposed learning algorithm encodes information from displacement data, which can be routinely acquired in the clinical setting, and combines it with the physics to regularise the problem and improve its convergence properties. Several benchmarks are provided to demonstrate the accuracy and robustness of the proposed method and great potential for the accurate and efficient identification of patient-specific physical properties.

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A multiscale description of combined therapy effects on tumor progression

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Gliomas are malignant brain tumors arising from mutations in the glia cells of the central nervous system. Their growth and migration inside the brain is a highly complex phenomenon, influenced by a multitude of intrinsic and extrinsic factors, which are responsible for the typical features of tumor aggressiveness and invasiveness. Although research advances have allowed significant progress in the comprehension and treatment of gliomas, these tumors are characterized by a poor prognosis, and recurrence remains the main cause of mortality. Here, we propose a multiscale framework for the description of glioma progression in response to different combined therapies affecting both the tumor cells and the brain vasculature. Precisely, we propose a kinetic model for glioma and endothelial cell evolution, where individual cell dynamics, accounting for receptor binding kinetics, are integrated into the mesoscopic equations for the description of cell population dynamics. Both at the individual and the population level, the effects of three main types of therapeutic treatments, i.e., radio-, chemo-, and anti-angiogenic therapy, on both cell types are taken into account. The derived macroscopic setting is then tested in several scenarios with the main aim of showing the effects that different treatment protocols can have on the evolution of the neoplasia [1].

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Numerical Methods for Fisher-Kolmogorov Equation with Application to Prionic Proteins' Spreading in Neurodegeneration

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The spreading of prionic proteins is at the basis of brain neurodegeneration. To study the numerical modelling of the misfolding process, we introduce and analyze a discontinuous Galerkin method for the semi-discrete approximation of the Fisher-Kolmogorov (FK) equation. We employ a PolyDG method for space discretization, which allows us to accurately simulate the wavefronts typically observed in the prionic spreading [1]. For this problem, we prove stability and a priori error estimates for the semi-discrete formulation. After a numerical verification, we carry out realistic simulations of α-synuclein in a three-dimensional patient-specific brain geometry reconstructed from magnetic resonance images. Moreover, we simulate the spreading in a two-dimensional brain slice in the sagittal plane with a polygonal agglomerated grid.
Starting from medical images we also construct reduced-order models based on graph brain connectome, which are helpful if the problem needs to be solved many times, for example in uncertainty quantification algorithms. In the FK equation, the reaction coefficient can be modelled as a stochastic random field, considering the many different underlying physical processes, and overcoming its non-measurability. We infer probability distribution by means of the Monte Carlo Markov Chain method applied to clinical data of Amyloid-β concentration. The resulting model is patient-specific and can be employed for predicting the disease's future development. Forward uncertainty quantification techniques (Monte Carlo and sparse grid stochastic collocation) are applied to quantify the impact of the reaction variability on the progression of protein accumulation within the next 20 years [2].

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Mathematical Model of Fluid Flow in a Lymph Node

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Lymph nodes (LNs) are organs scattered throughout the lymphatic system which play a vital role in our immune response by breaking down bacteria, viruses, and waste; the interstitial fluid, called lymph once inside the lymphatic system, is of fundamental importance in this process as it transports these substances inside the lymph node. The main mechanical features of the lymph node include the presence of a porous bulk region (lymphoid compartment, LC), surrounded by a thin layer (subcapsular sinus, SCS) where the fluid can flow freely.

Lymph nodes are critical sites for the filtration and processing of lymph fluid, which contains a variety of immune cells, antigens, and other molecules. Understanding the fluid dynamics within lymph nodes is crucial for elucidating the mechanisms of immune response and for the development of therapies for lymphatic disorders. Despite its importance, as far as we know, only few models in the literature attempt to describe the behavior of lymph from a mechanical point of view or mimicking the LN mechanical properties in a LN-on-a-chip model.

In this talk we will describe a mathematical model obtained using the asymptotic homogenization technique that describes the fluid flow inside a lymph node, taking into account its multiscale nature. We will describe how this model can be used to describe the flow pattern, pressure distribution, and shear stress within a lymph node.

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An optimization based 3D-1D coupling approach for the simulation of tissue perfusion and chemical transport in evolving vascular networks

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A new numerical approach is proposed for the simulation of the exchanges between an evolving capillary network and the surrounding tissue [1]. In particular we take into account the interplay between blood perfusion and substance delivery during tumor-induced angiogenesis. Thanks to proper modeling assumptions, which guarantee the well-posedness of the problem, the capillaries are reduced to their centerline, hence lowering the computational cost of solving the discrete problem. The interaction between the capillaries and the surrounding tissue is thus described by a 3D-1D coupled problem. The actual novelty of our approach lies in the solving strategy, which resorts to the reformulation of the equations into a PDE-constrained optimization problem [2]. Two auxiliary variables are introduced, approximating the value of the unknowns on the capillary wall, and a properly designed cost functional is minimized constrained by the 3D-1D set of equations. The resulting strategy appears to be highly robust and flexible in handling geometrical complexities. No conformity between the 3D mesh and the 1D partition of the capillary centerlines is required, thus making the method particularly suitable for the simulation of evolving vascular structures. Indeed, the 3D mesh does not need to be adapted to newly generated capillary sprouts and the blood perfusion and substance exchange problems can be easily solved at any stage of the network growth. Thanks to the chosen formulation, interface variables are directly available, without the need of post processing, and the exchanged flux can easily be computed, according to Starling's law. While fluid pressure and chemical concentration are described by the optimization based 3D-1D coupling, the proposed model accounts also for the diffusion of a chemotactic growth factor (VEGF), modeled by a 3D equation with a singular sink term. The capillary growth depends on the concentration and the gradient of VEGF, and is regulated by some proper branching and anastomosis rules.

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Energetic and Fibre Reorientation Models to Describe Cell Cytoskeletal Reorientation under Cyclic Stretching

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During their life cycle, cells are constantly exposed to a wide range of stimuli coming from the surrounding microenvironment. These cues are fundamental to drive a broad variety of cellular processes and behaviours: the importance of chemical signals is well known, but experiments have shown that a significant role is also played by mechanical prompts. As a pivotal example, there are several types of cells, like muscle cells in the heart, fibroblasts, or lung cells, that display the ability of reorienting their cytoskeleton following a cyclic deformation. Several experiments clearly demonstrated this fact [2, 3], though the mechanisms driving the process are not fully clarified.
In this talk, after a brief review of significant experimental observations on the topic [2], we present some models in the framework of Continuum Mechanics that we developed to describe cell reorientation under cyclic stretching of the substrate. We firstly discuss an energetic approach where the cell layer is treated as a nonlinear elastic body, and the preferential orientation is predicted by finding the directions that minimize the elastic energy [4]. Then, we generalise this approach and describe the remodelling of cell cytoskeletal fibres [1]. We will discuss the main features of our mechanical models, comparing our results with biological data from the literature.

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T cell therapy against cancer: A predictive diffuse-interface mathematical model informed by pre-clinical studies

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T-cell therapy is emerging as an effective treatment against solid cancers. Developing *in silico* models to predict T cell behaviour and efficacy would help therapy optimization and clinical implementation. In this talk, we present a model for the responsiveness of mouse prostate adenocarcinoma to T cell-based therapies [1]. Our mathematical model is based on a Cahn-Hilliard diffuse interface description of the tumour, coupled with Keller-Segel type equations describing immune components dynamics. The model is fed by pre-clinical magnetic resonance imaging data describing anatomical features of prostate adenocarcinoma. We perform numerical simulations based on the Finite Element Method to describe tumor growth dynamics in relation to local T cells concentrations. When we include in the model the activation of tumor-associated vessels, we observe an increase in the number of T cells within the tumor mass and the model predicts higher therapeutic effects (tumor regression) shortly after therapy administration. The simulation results are in good agreement with reported experimental data [2]. As our diffuse-interface mathematical model is able to quantitatively predict the T cell *in vivo* behavior, it represents a proof-of-concept for the role that *in silico* tools may play in the optimization and personalization of immunotherapy against cancer.

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Modelling Cell Reorientation under Stretch

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The active response of cells to mechanical cues due to their interaction with the environment has been of increasing interest, since it is involved in many physiological phenomena, pathologies, and in tissue engineering. In particular, several experiments have shown that, if a substrate with overlying cells is cyclically stretched, they will reorient to reach a well defined angle between their major axis and the main stretching direction. The aim of this talk will be to investigate the interplay between mechanics and cell organization. It will be shown that cells organise their internal structure to minimize an elastic energy that then drives this reorientation process. Viscoelastic effects will then be included to explain the dependence of the appearance of the phenomenon as a function of oscillation frequency. Finally, randomness is taken into account and discussed on the basis of a Fokker-Planck equation.

Mathematical modelling of brain tumour growth: reduced order modelling and parameter estimation

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The physical parameters driving the growth and the recurrence of Glioblastoma Multiforme (GBM) are highly specific to each patient. For this reason,finding a mathematical model that allows an accurate parameter estimation from neuroimaging data becomes of fundamental importance if we want to propose a computational framework that could help clinicians with decision-making. In general, parameter estimation requires a high computational cost, often unsuitable for clinical use if not assisted with techniques to reduce the complexity of starting problem.
In this talk, we propose a diffuse interface model of GBM growth based on mixture theory, which consists of a Cahn-Hilliard equation coupled with a reaction-diffusion equation to describe the evolution of the nutrient for cancer cells. The specificity of each patient is modelled via a set of numerical parameters, which dictate the peculiar growth of the tumour and whose prediction is the final objective of the proposed methodology. Starting from a full-order discretization of the proposed model based on the finite element method, we obtain a reduced-base model (ROM) through the proper orthogonal decomposition technique (POD). For the solution of the PDEs system, we use `FEniCSx`, a powerful computing platform, while its reduction is computed thanks to the Python library `RBniCSx`. By means of a neural network-based approach, we build a map between the parameter space and the solution in the reduced space that describes the concentration of the tumour over time. As a tool to estimate patient-specific parameters, we propose an approach based on a second neural network trained to predict the parameters of the model based on the tumour distribution in two separate time instants. In this way, the computational effort focused on the training phase, that requires the FOM to be solved several times starting from the same initial condition, is balanced by the rapidity in the estimation of the parameters once the information on the actual evolution of the tumour at a second time instant is available. Such an approach may be exploited in clinical practice to deduce the parameters of the model from imaging data.

Actin based motility unveiled: how chemical energy is converted into motion

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The chemo-mechanical motor of several biological systems is a polymerization process that converts chemical energy into mechanical work. The chief component in this activity is actin, a multi-functional protein forming filament in the cell cytoskeleton that is capable of generating protrusive forces when polymerization occurs in close proximity to a barrier or to a load. External impulses of a chemical or mechanical nature trigger a chemical reaction, which converts the monomeric form of actin, G-actin, into a polymerized branched-filamentous form, F-actin [1]. Upon polymerization, the cross-linked network acts against the plasma membrane, a pathogenic bacterium or an endosome, pushing them forward and promoting directional motility. In a recent publication [2], we have suggested that the *volumetric expansion* exerted after the phase change from monomeric to a cross-linked network of actin filament ultimately converts chemical energy into motion.
At the leading edge of cells, in fact, actin is organized in a bidimensional dendritic array of branched filaments. Branched actin filaments are generated beneath the plasma membrane by external signal responsive WASP-Arp2/3 machinery and kept functioning by a set of regulatory proteins. Those binding proteins control actin turnover and filament elongation, mediate the initiation of new filaments as branches on pre-existing filaments and promote (de)branching and (de)polymerization, thus regulating the mechanical response of moving cells.
In this note, a thermodynamically consistent continuum-mechanics formulation will be proposed, stemming from continuity equations that account for actin chemical kinetic. The model manifests itself in macroscopic descriptors of biochemical and biological details of the relevant processes, thereby resulting in sufficient generality to be appropriate for several biological systems.

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Nematic elastomers, relaxation dynamics and active nematic gels

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In this talk, we show how the theory of nematic elastomers can serve as a fruitful modelling paradigm for other, only remotely related, materials. The key idea is to decouple macroscopic and microscopic degrees of freedom, via a deformation gradient decomposition. While the observed deformations are macroscopic, microscopic degrees of freedom are taken into account in a coarse grained way by introducing material reorganization and relaxation. In particular, when relaxation times are much faster than deformation times, one recovers nematic liquid crystals theory (Ericksen-Leslie). This enables us to explain some subtle features of acoustic propagation in nematic liquid crystals [1], where both crystallike and fluidlike features emerge. At the intermediate level, we recover polymer dynamics and viscoelastic behaviour [2]. Furthermore, this theory also provides a modelling framework for active nematic gels, which is both natural and thermodynamically consistent. By contrast with standard theories, activity is not introduced as an additional term of the stress tensor, but it is added as an external remodelling force that competes with the passive relaxation dynamics and drags the system out of equilibrium [3]. Viscoelastic effects, defect dynamics and self-ordering, typical in biologically active materials, are naturally described by the theory and do not have to be included as external ingredients [4].

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MS22 - BEMs for advanced applications

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ABSTRACT

Since its early days, the Boundary Element Method (BEM) has been conceived as an accurate, scalable and reliable tool in computational science and engineering. In particular, in the last three decades, the number of its applications to cutting edge academic/industrial fields has impressively grown up.
This Minisymposium is devoted to both theoretical and numerical aspects of BEMs and its main goal is to bring together experts in the field to discuss on the most recent advances and current open challenges for this approximation technique and related methods, especially in view of advanced applications.

Integral formulation for 2D hydraulic fractures

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In a recent publication the problem of quasi-static crack propagation in brittle materials has been framed into the theory of standard dissipative processes [3] and through variational formulations the crack front quasi-static velocity has been characterized as the minimizer of constrained quadratic functionals. An implicit in time crack tracking algorithm, that computationally handles the constraint via the penalty method, was developed and implemented in [4].
Although the theoretical setting is sound, the derived crack tracking methods suffered from a major drawback that limited the interest in the approach to its theoretical content. In [5] a viscous regularization of the fracture propagation in brittle materials as a standard dissipative process was formulated. Rate-dependency provided a simple and accurate approximation of the crack front velocity, thus allowing to formulate effective crack tracking algorithms.
Such idea is applied here to hydraulic fracture processes [2]. The problem is governed by a differential equation for the fluid response (the so-called lubrication equation) and by a hypersingular boundary integral equation for the elastic domain where quadrature formulas in [1] have been used.
Although limited to a simple benchmark geometry, the novel set of integro-differential equations here proposed are capable to model the evolution of the lag and of the crack advancing in a straightforward way.

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An H-matrix based acceleration of Iga-BEM for 3D Helmholtz problems

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The design of a suitable, efficient, and accurate numerical method to solve wave problems is encountered in many academic and industrial applications. Without prejudice against the time-domain methods, which are important for many classes of wave problems, our focus is the frequency-domain approach in which the waves are assumed to propagate at a single frequency. In this case the governing wave equation reduces to a time-harmonic form known as the Helmholtz equation. In approximating the solution to this equation, the Boundary Element Method is classically formulated by expressing the solution elementwise in the form of a piecewise polynomial variation. Thus, the problem is reduced to seeking the amplitudes of these polynomial basis functions. Very recently, an Isogeometric Boundary Element Method (IgA-BEM) has been proposed in literature for the numerical solution of Helmholtz problems on 3D domains admitting a multi-patch representation of the boundary surface [3]. While being powerful and applicable to many situations, this approach shares with standard BEMs a disadvantage which can easily become significant in the 3D setting. Indeed, when the required accuracy is increased, it can soon lead to large dense linear systems, whose numerical solution requires huge memory, resulting also in important computational cost. In this talk, we propose a fast IgA-BEM based on the hierarchical matrices (H-matrices) [4] technique, that allows us to approximate the fully-populated matrices by data-sparse ones, by using the Adaptive Cross Approximation (ACA) algorithm [1]. Furthermore, the reduction of the computational time to solve the linear system comes from a GMRES solver, used with the fast H-matrix/vector product [2]. The numerical efficiency and accuracy of the method are assessed from numerical results obtained for benchmarks problems with exact solutions.

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Time-domain boundary elements for elastodynamics

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We discuss recent and on-going progress for boundary element methods in linear elastodynamics, with a focus on locally refined meshes and complex boundary conditions. We present well-posed boundary integral formulations for the time-dependent Lamé equations for problems in polyhedral domains, as well as mixed or nonlinear (contact) boundary conditions. The solutions of such boundary problems exhibit singularities due to the geometry, change of boundary condition, or nonlinearity. We discuss theoretical and computational progress on their numerical approximation by boundary element methods in the time domain. In particular, stable formulations and a priori and a posteriori error estimates for approximations on locally refined meshes will be considered.

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A 3D finite element - boundary element coupling method in time domain for the scalar wave equation

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We consider a transmission problem, where the homogeneous wave equation on a bounded Lipschitz domain Ω is coupled with another homogeneous wave equation on the exterior $\Omega^c = \mathbb{R}^3 \backslash \Omega$. We derive a variational formulation based on the Poincare-Steklov operator. We use a tensor product ansatz and derive an efficient time stepping scheme, precisely the Marching-on-in time (MOT) scheme. Finally, we present an a priori error estimate and conclude the presentation with different numerical examples.

Fast boundary element methods for the wave equation

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Time-domain boundary element methods (BEM) have been successfully applied to dynamic problems in acoustics, electromagnetism and elasticity. BEM feature the advantage that only the boundary of the volume have to be meshed, which leads to far less degrees of freedom. However, the storage and computational requirements are huge, since the system matrices are dense. This is particularly problematic in the dynamic setting as each time step or frequency involves the computation of BEM matrices. In this talk, we propose a novel low-rank approximation scheme, which effectively reduces both storage and computational costs to almost linear in the number of degrees of freedom. The algorithm is based on hierarchical matrix compression in the spatial coordinates and uses adaptive cross approximation in the time variable. By collecting the BEM matrices for all time-steps in a three-dimensional tensor, we are able to exploit the structure of the low-rank approximation to accelerate the time evolution of the method. Finally, we showcase the efficiency and performance of the new algorithm in numerical examples.

MS23 - Effective Solvers and Reduced Order Models for CFD Problems: Advances and Perspectives

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ABSTRACT

This minisymposium focuses on recent advances and future perspectives in the development of effective numerical solvers and reduced order models (ROMs) for computational fluid dynamics (CFD) and fluid-structure interaction (FSI) problems, with application to aerospace, automotive, civil engineering, environmental science, energy systems, and biomedicine. The high computational cost typically associated with simulations of such problems often limits their practical applications.

The minisymposium addresses the challenges and opportunities associated with the development and application of these techniques, emphasizing the need for accurate and reliable simulation results, the importance of computational efficiency and scalability, and the need for the effective integration of these methodologies into existing computational workflows.

A broad range of topics related to effective solvers and reduced order models for CFD problems is covered, including but not limited to advanced numerical techniques empowered by high performance computing algorithms, novel reduced order modeling techniques, error estimation and control, model order reduction exploiting machine learning (ML) and other artificial intelligence (AI) techniques, model-based and data-driven approaches for uncertainty quantification (UQ) and sensitivity analysis (SA), and applications to large scale real-world problems in the aforementioned fields.

The minisymposium aims to bring together researchers from academia and industry working on CFD problems to share their expertise and ideas, foster collaborations, and promote the development of efficient and accurate numerical techniques for solving complex fluid dynamics problems.

Multiphysics modeling of the cerebrospinal fluid by discontinous Galerkin methods on polytopal grids

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Modeling the dynamics of Cerebrospinal Fluid (CSF) in the brain involves various physics, such as CSF filtration through cerebral tissue and its flow in three-dimensional neuron-free regions like the ventricles and the subarachnoid space. Moreover, CSF generation is closely connected to blood perfusion in the brain. In this work, we propose a multiphysics model that incorporates dynamic Multiple-Network Poroelastic (MPE) equations for tissue poromechanics [3] and Navier-Stokes equations for 3D CSF flow. The MPE model considers multiple scales of blood vessels and the extracellular component of CSF, while interface conditions describe physiological mass and stress exchange [2].
For the space discretization of the model, we introduce a discontinuous Galerkin method based on polytopal grids to accurately represent the extremely complex geometry of the interface between the two physical domains. We present an a priori analysis of this method, extending [1, 3] to account for interface terms. Time discretization combines the Newmark β-method with the θ-method. We perform verification tests in simplified and realistic geometries and a three-dimensional patient-specific simulation based on magnetic resonance images.

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Optimal Transport-inspired Deep Learning Framework for Slow-Decaying Problems: Incorporating Sinkhorn Loss and Wasserstein Kernel

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Reduced order modeling has emerged as a powerful technique to speed up the investigation of complex systems described by partial differential equations (PDEs).
Traditional linear methods, such as proper orthogonal decomposition (POD), have limitations in capturing complex nonlinear phenomena and suffer from information loss. Nonlinear reduction techniques, including deep learning (DL) frameworks, have gained popularity for addressing these challenges. DL-based ROMs offer the ability to better span the nonlinear manifold associated with parameterized PDEs.
In this work, we propose a novel DL-based ROM framework that leverages the powerful tools of Optimal Transport (OT) [2] theory and Kernel Proper Orthogonal Decomposition (kPOD) [3]. OT provides a principled way to measure the distance between probability distributions, which is a fundamental problem in many areas of science and engineering. Our framework exploits the OT-based distance metric, known as the Wasserstein distance, to construct a custom kernel that captures the underlying hidden features of the data. The dimensionality reduction is carried out nonlinearly using KPOD, which exploits the kernel trick to implicitly employ a high-dimensional space known as the *feature space*.
To train our models, *i.e.,* to recover the forward and backward mapping from the latent space to the full order solution, we exploit an autoencoder architecture, where the encoding layer is forced to learn the reduced representation. The training of the proposed architecture is performed using the Sinkhorn algorithm [1], a computationally efficient method for solving the OT problem. Specifically, we use the Sinkhorn loss as a regularization term to encourage the learned representations to be invariant to the input domain. Our numerical investigation shows promising results, achieving state-of-the-art performance when compared to existing DL-based ROM methods.

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Computational Fluid Dynamics in aeronautics: challenges for the implmementation of non-intrusive p-ROM in industry

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Aeronautical industries, driven by the stricter environmental regulations are facing major design challenges. The zero-emission prototype and the needs of more advanced propulsive technologies imply intensive use of Computational Fluid Dynamics (CFD) to cut design and optimization cost. The availability of a large database of solution made with CFD legacy code, makes interesting the use of ROM non-intrusive techniques, that with an approach data-driven can help in cutting the total computational cost and go through a greener HPC world. In the CFD simulations four key factors must cohoperate (and hence they can bring to an error in the prediction of the flow field [1]): the numerical discretization chosen, the model, the mesh built for the given discretization, the geometry. The Reynolds-Averaged Navier-Stokes (RANS) model in the context of finite volume method has still nowadays a great success in the turbomachinery community. In this work, we will not consider modelling error and neither geometry error. In order to reduce the discretization error, the error-based remeshing trechinques have demonstrated their interest in recent industrial applications [2]. In addition to it, nonlinear registration-based model reduction [3] procedure for rapid and reliable solution of parameterized steady conservation laws can reduce the overall design loop and computation cost. Classical industrial problems are really challenging for model reduction techniques due to the presence of non-linear terms in the equations and to the presence of parameter-dependent coherent structures, such as shocks, that cannot be adequately represented through linear approximation spaces (e.g POD). In this work we will present a method that minimizes the discretization error by using automatic remeshing techniques coupled with point-registration. In addition to this we will enumerate the implications for the implementation of these methodology in an industrial framework.

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A library for risk detection for Abdominal Aortic Aneurysm: automatic pipeline and preliminary results

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When an abdominal aortic aneurysm (AAA) is detected, the current criterion for surgical intervention is the maximum diameter criterion. This empirical criterion does not take into account the overall geometry of the aneurysm and the effects of blood flow in the development of pathology. On the other hand, several hemodynamic risk indicators have been tested in the literature on a large population of patients with satisfactory results in risk estimation. However, their use is far from popular in the clinical world because they often require long hemodynamic simulations and the results are not readily available. We propose a method based on model order reduction using machine learning (ML) techniques to provide clinicians with a simple, immediate tool that can immediately classify a new patient in terms of risk indicator, thus speeding up and simplifying the diagnostic process. The initial 3D geometry will be provided by the start-up company NUREA, starting with the patients' CT scans, which will be used to reconstruct a 3D digital twin of the aortic tree using the PRAEVAorta software. From the initial patient cohort, our pipeline consists of three steps. In the first step, digital twins are cut below the renal arteries and at the iliac bifurcation ([1]) to isolate the aneurysm sac. The contour of the aorta is then parameterized using Fourier series. The second step is to perform hemodynamic simulations on each parameterized aneurysm. The tool used is Simvascular ([2]). Previously calibrated inlet and outlet boundary conditions are provided for the simulation in order to obtain as realistic a result as possible. Finally, the risk indicators defined on the aneurysm wall are extracted and related to the parameterized geometry in the third step. In particular in this last phase the entire data set is then treated with model reduction techniques, specifically Proper Orthogonal Decomposition, with the aim of defining a solution space. The classification for the incoming out-of-sample aneurysm geometries is then realized with a non-supervised approach (Gaussian Mixture Models)

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A high-order Discontinuous Galerkin discretisation of the diffused-interface five equation model for two-phase compressible flow simulations

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A diffused-interface approach based on the Allen-Cahn phase-field equation is developed within a high-order Discontinuous Galerkin framework [1]. The interface capturing technique is based on the appropriate combination of explicit diffusion and sharpening terms in the phase-field equation, where the former term involves the computation of the local interface normal vectors. Due to the well-known Gibbs phenomenon encountered in high-order discretisations of steep profiles such as shocks and/or interfaces, the accurate evaluation of the interface normal vector requires special consideration. To this end, the numerical strategy proposed in this work uses an additional smooth level-set function, which is advected by the same velocity field of the phase-field, to compute the interface normal vectors [2]. It is shown that for appropriate choices of numerical fluxes and parameters of the model, the phase-field remains bounded without any need for explicit regularisation or mass redistribution. The proposed diffused-interface technique is implemented within a five equation model for the simulation of fully compressible two-phase flows. In order to preserve isolated interfaces, a quasi-conservative discretisation of the five equation model is employed [3]. A series of numerical experiments of increasing complexity are presented in order to assess the accuracy and robustness of the developed methodology, including two-phase flows involving viscous effects, gravitational forces, and surface tension. Overall, the proposed methodology is shown to preserve fundamental features of two-phase flows such as the boundedness of the phase field, accurate computation of the interface normal vectors, small mass conservation errors and exact resolution of contact discontinuities, without, at the same time, giving up the significant benefits offered by high-order spatial discretisations.

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MS24 - Modern Techniques for Biomedical Data Analysis

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ABSTRACT

The last few years have shown the ever-increasing need for personalised and sustainable health solutions, supported by rapid clinical trials with reduced animal experiments and fast and accurate diagnostic tools. This need has led to the development of multidisciplinary methods in which mathematics and statistics play a fundamental role by providing: (i) digital twins for patient-specific therapeutic solutions (e.g. AI-based techniques for generating synthetic biomedical data, or personalised drug dosage); (ii) time series analysis techniques to estimate biophysical parameters of interest from indirect measurements (e.g., estimation of brain activity from non-invasive measurements); (iii) machine learning techniques to extract information from high-dimensional experimental data (e.g., genomic data, PET images, MRIs); and (iv) learning nonparametric systems of differential equations from noisy data (e.g. in the case of longitudinal healthcare data obtained during hospital visits).

In this symposium we will explore these topics, providing a cutting-edge view of the latest mathematical and statistical techniques for biomedical data analysis. We will discuss the latest development of digital twins of healthcare patients in combination with machine learning technologies for the generation and validation of synthetic data in oncohaematology. Next, we will propose the use of chemical reaction networks for optimising drug dosage in oncology using efficient Newton-based approaches, and discuss the use of spectral graph wavelet packets to compress, denoise and reconstruct functional MRI signals of extremely large graphs, simulating neuronal connections in the human brain. We will then investigate the use of unsupervised techniques for the automatic calculation of transition frequencies from the theta to alpha brain rhythm, and its application to neurological diseases. Then, we will discuss nonparametric differential equation learning for noisy and sparse longitudinal data, in the specific context of antibiotic resistance data obtained during hospital visits. Finally, we will introduce and discuss the latest development of statistically robust radiomics features in neuro-oncology.

The innovative work presented in this symposium cuts across several domains of the application of mathematics to biological data and uses a variety of methodological tools (machine learning; graph theory; optimisation; time series analysis) to bring forth multidisciplinary insights. Considering that multidisciplinarity is a core value of applied mathematics, we believe this symposium will be of great interest to SIMAI members.

An efficient Newton-based approach for computing steady states of chemical reaction networks modelling cancer cells

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Chemical Reaction Networks (CRNs) are powerful tools that can be used, e.g., for describing the interactions that occur between proteins inside human cells. A properly designed one is suitable for illustrating the complex nature of cancer and helping in computing the effects of protein mutations and specific targeted drugs on healthy cells [1].

From a mathematical viewpoint, CRNs can be modelled as systems of autonomous ordinary differential equations, whose steady state solutions yield the cells proteins concentrations at equilibrium. Finding them and observing their variations in the presence of mutations, drugs, or both is fundamental for determining which drugs to administer in order to restore the healthy state of the cell. The most common approach for computing steady states consists in simulating the system's dynamical evolution in time, but, since this is a very time-consuming method, especially when the CRN size increases, here I propose a different approach. It involves recasting the steady state computation problem as a root-finding one, and solving it by applying an algorithm that combines the Newton approach with the gradient descent direction and exploits a specific Armijo rule for the step selection. The non-negativity constraints are assured by a suitable operator at the end of each step [2].

I'll show how such scheme, that converges to steady states under specific assumptions, outperforms the dynamic method in terms of both speed and precision.
Moreover, starting from a CRN introduced for modeling the G1-S transition phase of colorectal cells, the method is validated in simulations mimiking both physiological and mutated status and also in the presence of targeted drugs applied individually or together in a combined therapy [3].

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Wavelet packets and graph neuronal signal processing

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Nowadays graphs became of significant importance given their use to describe complex system dynamics, with important applications to real world problems, e.g. graph representation of the brain, social networks, biological networks, spreading of a disease, etc..

In this work, [1], we introduce a novel graph wavelet packets construction, to our knowledge different from the ones known in literature. We get inspired by the Spectral Graph Wavelet Transform defined by Hammond et all. in [2], based on a spectral graph wavelet at scale $s > 0$, centered on vertex n, and a spectral graph scaling function, respectively. Moreover after defining the wavelet packet spaces, and the associated tree, we obtain a dictionary of frames for $\mathbb{R}^N$, with known lower and upper bounds.

We will give some concrete examples on how the wavelet packets can be used for compressing, denoising and reconstruction by considering a signal, given by the fRMI (functional magnetic resonance imaging) data, on the nodes of voxel-wise brain graph $\mathcal{G}$ with 900.760 nodes (representing the brain voxels) defined in [3]-[4].

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Clustering algorithms for automatic computing the transition frequency from theta to alpha brain rythm: theory and validation

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Neurodegenerative diseases, such as Alzheimer, Parkinson and Lewis Body dementia (DLB), are commonly widespread all over the world. Recognising their early stages can be fundamental for patients. For this aim, the use of neurophysiological biomarkers derived from electroencephalographic (EEG) data are of great importance because of the low cost and non-invasiveness of EEG, which records, over time, the electric field produced on the scalp by the neural currents flowing in the brain. Thus, features extracted from EEG time-series such as Grand Total Score, EEG coherence, spectral power densities and connectivity measures, are nowadays used [1, 2].
Another useful, though often overlooked, EEG biomarker is the transition frequency (TF) from theta to alpha frequency band. Recently Vallarino et al. proposed a new technique to compute TF, called Transfreq which exploits only a resting state recording. They propose four different clustering techniques, based on mean-shif and k-means, to study spectral profiles associated to the EEG channels according to their content in alpha and theta bands.
In this talk I will revise the mathematical details beyond Transfreq algorithm and its performance by showing the obtained EEG biomarkers, especially TF, on: (i) a dataset of patients affected by Alzheimer disease, where the computed TF shows a significant correlation with the Mini-Mental State Examination (MMSE) score, a measure of cognitive impairment; (ii) a dataset with patients affected by DLB and healthy controls, where the spectral EEG features clearly show a shift towards lower frequencies of brain activity in DLB patients.

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Generation and Validation of Synthetic Data in Oncohematology

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Hematological malignancies (commonly referred to as blood cancers), collectively rank as the fifth most prevalent cancer category in economically developed countries [2] and present significant complexity diversity in terms of etiology, treatments, and outcomes.
Advancements in the field of oncohematology rely on the availability of high-quality and diverse datasets for research and clinical applications. By integrating information from multiple sources, such as clinical records, omics data and medical imaging, researchers can gain new insights and develop innovative diagnostic and prognostic models [1, 4], ultimately improving patients care.
However, due to privacy concerns and limited accessibility of patient data, obtaining such datasets can be challenging, especially in the context of rare malignancies. This has led to synthetic data generation techniques emerging as a promising solution [3]. Generating synthetic data involves creating artificial datasets that emulate the statistical properties and characteristics of real patient data, ensuring the preservation of valuable information while safeguarding patient privacy.
To validate the generated synthetic data, various statistical and machine learning techniques are employed, including comparing synthetic data to real data in terms of distributional properties, predictive accuracy, and clinical utility. However, generating (and validating) data that preserves inter-dependencies between different data sources is still an open problem that requires further investigation.
This talk will explore how synthetic data generation can impact oncohematology research by overcoming limitations related to data access and privacy, while still extracting meaningful insights that have the potential to enhance our understanding of complex diseases, facilitate the development of novel therapeutic approaches, and improve patient outcomes. Additionally, practical and ethical considerations related to the use of synthetic data will be discussed.

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ODE Learning Problem with Adjoint State Method

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Learning latent Ordinary Differential Equations (ODEs) from scarce and noisy data is a recently emerging topic in the machine learning community ([1], [3], [5]). In this context, the aim is to learn a non-parametric system of ODE from (noisy) time series data. Differential equations play a crucial role in many fields of applications, ranging from fluid dynamics to engineering, from acoustic to biomedical applications.
In our approach we define the ODE system as $\dot{u}(t) = f(u(t), m) = \Phi(u(t))^T m$ where u is the time-dependent state variables vector, Φ is a set of basis functions evaluated in the solution u of the system and m is the vector of unknown parameters to be estimated on which we impose sparsity condition in order to find the only functions in the basis Φ which describe our data. One nevralgic problem is to compute the gradient of objective functional with respect to parameters m: in our work we exploit the Adjoint-State-Equation method [6].
In this talk I will firstly present the underlying mathematical foundations of this method. Then I'm going to show the performances of this method on several known simulated differential systems such as FitzHugh-Nagumo, Lotka-Volterra or Lorenz. The obtained results and performances will be compared with other state-of-the-art methods such as SINDy [1], PINN-SR (with polynomial and Fourier candidate functions) [3], npODE [4] ([2], [5]).

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Reproducibility of radiomics in neuro-oncology

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Radiomic studies have shown promise in improving clinical decision-making and personalized medicine. The ability of radiomics to provide quantitative imaging features for tumor characterization and treatment assessment makes it an especially attractive application in neuro-oncology [5]. However, concerns about the generalization of such studies' results have emerged in the last years, to the point where radiomics is experiencing a reproducibility crisis [4]. In this talk, we illustrate and review the main sources of heterogeneity in methodologies, including imaging acquisition protocols, feature extraction algorithms, and statistical analysis techniques, which has led to variability in reported radiomic signatures, hindering reproducibility [3]. Standardization efforts related to the harmonization of imaging acquisition protocols, the development of reporting guidelines, and data sharing initiatives will be discussed [2]. Final comments on the process of translating radiomic data into clinically useful tools for guiding clinical care will also be provided [1].

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MS25 - Scientific Computing and Data Science in Biomedicine

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ABSTRACT

*C*omputational modeling provides a crucial contribution to the understanding of physical mechanisms in the field of biomedicine. To address the intrinsic complexity of physiological and pathological processes and their multiscale and multiphysics nature, suitable mathematical models must be developed and reliable, efficient, and robust numerical methods must be devised to simulate such phenomena. Moreover, to enable clinical translation, very efficient and cost-effective methods are required for model personalization. Recent approaches merging Data Science and Scientific Computing represent a promising research direction to reconstruct quantities of interest with high resolution and enable near-real-time model predictions. These methods (based, e.g., on Gaussian Processes or Neural Networks) provide reliable surrogates of considered models by leveraging large amounts of data and at a lower computing cost than traditional physics-based models. In addition, novel approaches combining physics-based and data-driven methodologies like Physics-informed Machine Learning proved effective in solving inverse problems in electrophysiology and fluid dynamics. This mini-symposium will bring together applied mathematicians developing numerical/data-driven methods in computational medicine, supporting future collaborations and expanding the international research network in these emerging fields.

Blood dynamics in the left heart to study mitral regurgitation and two mitral valve repair techniques: an image-based computational fluid dynamic study

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Mitral valve prolapse is a heart valvular disease characterized by a displacement of a leaflet into the left atrium during the systolic phase. The main complication is mitral valve regurgitation (MVR), a condition leading to the formation of a regurgitant jet in the left atrium during the ventricular contraction. Nowadays there are two different surgical repair techniques to restore a correct mitral valve function: the Carpentier's technique [1] and the neochordae technique [2].
Computational methods in realistic cardiac geometries represent a non invasive way to provide blood dynamics information and help the surgeons to better understand the left heart physio-pathology and to model and predict the outcomes of surgical interventions.
In this respect, we used Computational Fluid Dynamics (CFD) with prescribed motion where the displacement of the left heart internal walls (left atrium, left ventricle and aortic root) and valves (aortic and mitral valve) is provided by dynamic imaging. In particular, we applied such method to study MVR to highlight phenomena may arise as a result of this pathology such as the occurrence of turbulence, remodeling, risk of hemolysis and washout of atrial blood flow. Moreover, we used CFD with imposed motion to compare the two different surgical repair techniques of the mitral valve in order to quantify their effects on the atrial and ventricular blood flow and to highlight possible differences on some haemodynamic indexes (such as wall shear stresses, relative residence time, turbulence formation) with the aim of providing potentially clinical useful information.

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Lattice-Boltzmann Methods for blood and perivascular fluid flow with pulsating vessel walls

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The treatment efficacy of neurological disorders, realized through methods such as the convection-enhanced drug-delivery, is influenced by the precise drug distribution within the brain tissue. Perivascular spaces constitute a conduit for fast flow propagation due to their high hydraulic conductivity, thus favoring an increased drug-migration into the surrounding tissue, away from the targeted area for treatment [1]. Therefore it is crucial to gain more insight into the mechanisms driving perivascular flow in order to enhance treatment planning and to optimize drug delivery in the brain.
One of the key-factors facilitating solute transport in perivascular spaces is the pulsation of arterial walls [2]. Hence, our goal is the simulation of perivascular fluid flow together with the blood flow-induced pulsatile movement of vessel walls. We realize this using the Lattice-Boltzmann Method (LBM), which provides a computationally efficient way for complex fluid flow simulations. In particular, we numerically treat the elastic pulsation of vessel walls and its influence on the fluid mechanics and flow-behavior of blood or perivascular fluid, while considering conservation of mass and momentum. The primary challenge lies in the employment of fluid-structure interaction in LBM to accurately model the vessel expansion and contraction from both, the arterial and perivascular side. To this end, we couple free and porous flow using the homogenized approach from [3] with varying porosity to reproduce wall pulsation. Subsequently, we aim to explicitly include the moving interface by expanding the approach of [4] to more general vessel geometries, such that an eventual adaptation to realistic 3D settings is facilitated.
Since our long-term objective is the simulation within real, patient-specific geometries and for real-world clinical scenarios we additionally seek to maintain a manageable computational complexity for the transition from 2D to 3D.

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A Finite Element Study of Cardiac Electrical Activity in a Human Cardiac Tissue with Multiple Myocardial Ischemia

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The heart electrical conduction system propagates the electrical impulse originated from the sinoatrial node (SA) called cardiac pacemaker, situated in the left atrium, due to which heart muscle starts to contract, and then this signal travels to the whole heart, and the contraction of entire heart muscle takes place. The basis of the electrical activity is the action potential, which is facilitated by ionic channels and the ionic cell transporters that enable the movement of ions across the cardiac cell membrane. Myocardial ischemia takes place when the blood flow to the heart and oxygen supply to the heart is abnormal. It is one of the leading causes of sudden death. Due to this myocardial ischemia metabolism and electrophysiological changes appear which results in the alteration of cardiac electrical activity. In this talk, a modified human ventricular TT06 cell level model (ODEs) coupled with the tissue level (PDE) is considered to analyze the influence of Hypoxia on the cardiac electrical activity of a human cardiac tissue (HCT). The apriori finite element error estimate of this PDE- ODE system for the numerical scheme is found to be as $o(h^2 + k)$. A HCT (domain) is modeled in such a way that it consists multiple ischemic subregion (subdomain). A modified Human ventricular TT06 ionic model coupled with the tissue level model is solved using FE and BEFD methods to analyze the cardiac electrical activity in Human Cardiac Tissue with Multiple Myocardial Ischemia. 61% decrease in the vicinity of two ischemic regions leads to 13% drop in action potential duration(APD) in the neighboring healthy region. Increasing the number of ischemic regions from 1 to 4 leads to a 39% drop in APD.

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Modeling a biophysically detailed atrial fiber architecture in cardiac computational models

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A crucial aspect of cardiac computational models (CCM) revolves around accurately representing the arrangement of myocardial fibers, also known as myofibers, which are essential for the characterization of cardiac tissue. The collective organization of myofibers plays a pivotal role in both the propagation of electric signals and the mechanical contraction of the heart [1]. Therefore, it is imperative to incorporate accurate cardiac fibers in CCM. Due to the difficulty of reconstructing cardiac fibers from medical imaging, a widely used strategy for generating a surrogate fiber architecture for CCM relies on mathematical models known as Rule-Based-Methods (RBMs), which provide a surrogate of myocardial fibers field. Existing atrial RBMs predominantly rely on semi-automatic rule-based approaches that manually prescribe fiber orientations in specific atrial regions or on atlas-based methods, where fibers from a reference geometry are mapped onto a target geometry. These approaches often necessitate manual intervention and are tailored to specific morphologies. Recently, Laplace-Dirichlet-RBMs (LDRBMs) designed specifically for the atrial chambers have shown promise by accurately representing atrial fiber features in diverse morphologies [1]. However, these novel algorithms may overlook important fiber bundles, and they have primarily focused on bilayer morphology while considering only the left and right atria separately. Furthermore, many recent LDRBMs lack rigorous validation against the same cardiac geometry used for imaging data acquisition. In this study, we introduce an enhanced novel atrial LDRBM capable of prescribing a highly detailed biatrial and volumetric fiber architecture. Additionally, we validate this new method by comparing the atrial LDRBM fibers with a dataset of Diffusion Tensor Magnetic Resonance Imaging (DTMRI) fibers [2], investigating the differences between using the novel atrial LDRBM and the DTMRI fibers in electrophysiological simulations. Lastly, we propose a detailed volumetric bi-atrial human fiber atlas based on high-resolution DTMRI data using the novel LDRBM approach.

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An electromechanical-torso model for the generation of the electrocardiograms

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The electrocardiogram (ECG) is one of the most commonly-used non-invasive diagnostic technique to gain insights into the electrical behavior of the heart, and detect a broad range of cardiovascular diseases. Being able to compute realistic ECGs, however, is not an easy task due to their high sensitivity on physical, numerical and geometrical parameters. Moreover, the myocardial contraction determines a change in the heart shape and, thus, a corresponding displacement of the electrical sources responsible for the ECG generation. However, the influence of the heart deformation on the ECG have often been overlook in *in silico* models.
In this work we aim at accounting for such deformations proposing a new 3D-0D closed-loop electromechanical-torso model, coupling an electromechanical model for the heart [1] and a generalized Laplace equation to simulate the torso electrophysiology. The displacement of the heart-torso interface surface due to the myocardial contraction, is achieved in the torso domain by means of a lifting method, whereas the corresponding effect on the torso electrophysiology is included by incorporating mechano-electric feedbacks in the generalized Laplace equation. Differently from previous work [2], we solve the EMT model on static *reference configurations* of the cardiac and torso domains, thus avoiding online remeshing at each time step of the numerical simulation. Moreover, we implement a suitable segregated-intergrid-staggered numerical scheme to handle the different space-time scales required by the different core models involved [1].
Numerical tests are carried out on a realistic 3D in-silico biventricular geometry and on a realistic torso. Both healthy and pathological conditions, e.g. ventricular tachycardia, are simulated considering either static of moving domains. Fairness of the comparison is ensured by prescribing the same numerical and parameters setting in all simulations.

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MS26 - Bayesian and Monte Carlo methods in applied science and industry

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ABSTRACT

In the last decades, Bayesian methods have proven to be useful in an increasingly wide range of applications in both science and industry. One of the main reasons for this is that such methods allow to account for uncertainty in all situations where complete information is not available.
This typically happens in inference problems, where the aim is to infer information on some quantity that can only be measured indirectly, and in prediction problems, where the aim is to characterize the possible evolutions of a system with their respective probabilities. More recently, Bayesian methods are also more and more used to build stable Machine Learning models by accounting for uncertainty on hyperparameters.
From a computational point of view, Monte Carlo methods represent a key tool for computing solutions to Bayesian problems since closed form solutions can be provided only in a minority of cases.
In this symposium we provide an overview of recent applications of Bayesian and Monte Carlo methods in different fields ranging from seismicity to neuroscience, weather prediction, microscopy and machine learning.

Bayesian approach to Fluorescence Correlation Spectroscopy

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Fluorescence Correlation Spectroscopy (FCS) is a commonly employed technique for studying molecular dynamics in biological samples [1]. By analyzing the correlation function of fluorescence fluctuations within a defined observation volume, it provides valuable insights into the underlying molecular processes. FCS provides estimations of dynamic properties, such as diffusion coefficients, through fitting methods applied to the auto/cross-correlation function. As a result, this technique is built upon a theoretical mathematical model and it heavily relies on a high signal-to-noise ratio (SNR). To achieve a sufficient SNR, long-time sequences must be acquired, which can present limitations, particularly in live cell imaging contexts. We therefore explore innovative Bayesian approach to overcome these fit issues. The Bayesian approach allows us to obtain an entire probability distribution instead of a single prediction. Classical methods [2] predict a fixed number of diffusive coefficients. Our method, instead, allows for obtaining a prediction on the number of different diffusion coefficients and a probability distribution on the diffusion coefficients themselves. In this way, it is not necessary to fix the number of diffusion coefficients in advance. In addition, if there are *a priori* information available about the diffusion process, they can be easily incorporated into the model and lead to improved estimation of the probability distributions. This approach has been tested both on simulated data, from which is possible to quantify the error, and in controlled experiment. A comparison with state of the art analysis has been performed in terms of error and acquisition time.

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Priors for Bayesian Deep Learning

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The impressive success of Deep Learning (DL) in predictive performance tasks has fueled the hopes that this can help addressing societal challenges by supporting sound decision making. However, many open questions remain about their suitability to hold up to this promise. In this talk, I will discuss some of the current limitations of DL, which directly affect their wide adoption. I will focus in particular on the poor ability of DL models to quantify uncertainty in predictions, and I will present Bayesian DL as an attractive approach combining the flexibility of DL with probabilistic reasoning. I will then discuss the challenges associated with carrying out inference and specifying sensible priors for DL models. After presenting a few of my contributions to address these problems [1, 2, 3], I will conclude by presenting some interesting emerging research trends and open problems.

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A Bayesian approach to uncover temporal variations in seismicity

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In this study we statistically analyze some earthquake sequences of Central Italy to identify possible temporal variations in the probability distributions of seismic parameters, such as magnitude and spatial location of the epicentres. The data suitable for this analysis are taken from the Italian Seismological Instrumental and Parametric Database (ISIDe), compiled by INGV since 1985. In addition to the probability distributions commonly used to fit these data types (e.g. tapered Pareto, generalized gamma), the q-exponential distribution is also considered: it is the solution of a maximum entropy problem in the frame of nonextensive statistical mechanics, useful for describing complex, non-linear dynamic systems in many applications of environmental and social sciences, including seismology. Bayesian inference is performed by processing data on sliding time windows, such that each window has a fixed number of events and shifts at each new event. An indicator of the activation state of the system is identified in the variations of the estimated parameters of the models in the time windows [1]. Another criterion is based on the best fitting distribution in each time window, which is selected by comparing the evaluated values of the posterior marginal likelihood [2]. We found that the best fitting distribution varies over time jointly with seismic phase variations.

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A Weather Generation Model To Evaluate The Impact Of Meteorological Variability On Crop Growth

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We describe the development of a stochastic weather generation model in the context of a collaboration with REMTEC srl (`https://remtec.energy/`), an italian company that develops innovative solutions in the field of agrivoltaics. Agrivoltaics is a recent technique consisting in installing photovoltaic panels above cultivated fields, thus resulting in simultaneous use of the land for power generation and agriculture.
REMTEC srl was initially interested in developing a system for quantitative assessment of the impact of weather variability on variability in crop growth. The company was already in possession of a deterministic growth model for wheat which, given soil parameters and daily values of a set of weather variables, computes the temporal evolution of relevant biological parameters [4], therefore we developed a stochastic model capable of generating random time series of weather variables to be fed to the deterministic model. The statistical model is trained on the historical data of a given region of interest (downloaded with open source API from ERA5 [1]) to simulate random series of arbitrary length of different weather variables, taking care to preserve interannual and seasonality trends, autocorrelation and cross-correlation structures and marginal distribution functions.
Then, having observed that in particular years wheat benefited from shading, the aim became to develop a tool that could be used at any moment, using part of simulated data and part of real data available up to that time, to evaluate the impact of panel shading on crop growth and suggest to the user how to orient the panels day by day with the idea of letting the light filter in when the plant needs it most otherwise maximise energy production. With this purpose we had to determine how the shadow affects all meteorological variables, taking care that the shadow moves throughout the day and is not the same at all points in the cultivated field.
Stochastic weather generators have been an active field of research in the last decades [3]. Our main contribution was the use of copula models that allowed us to simulate multivariate stationary processes with non-Gaussian variables. The R package *anySim* [2] helped us to build an appropriately parametrized auxiliary Gaussian model such that the ICDFs map the Gaussian vector to obtain correlated random variables with desired marginal distributions and correlation structures.
The model has been integrated in an app (for both Windows and Mac) that allows the user to choose the sowing date and the soil parameters, and run the desired number of simulations.

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Two for the price of one: parameter and hyper-parameter estimation in Bayesian inverse problems through SMC samplers

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In the Bayesian approach to inverse problems one is interested in the approximation of the so-called posterior distribution, i.e. the distribution of the unknowns given the measured data. Analytical solutions for the posterior distribution are often not available, therefore Monte Carlo approaches are required in order to get an approximation. To make the matter worse, one often faces the correct setting of scalar hyper-parameters that define the model; for instance the noise standard deviation for additive Gaussian noise inverse problems.

In this work [1] we show how to build a specific class of Monte Carlo algorithms, named Sequential Monte Carlo (SMC) samplers, to provide an approximation of both the parameters and a scalar hyper-parameter at a negligible additional computational cost compared with the approximation of only the parameters.
SMC samplers are based on the iterative approximation of a sequence of distributions that smoothly reaches the target one. The main idea is to exploit the iterative nature of SMC samplers to sequentially approximate posterior distributions conditioned on different values for the hyper-parameter. Through this procedure, we provide both the approximation of a set of conditional posterior, allowing an Empirical Bayes approach, and the hyper-parameter marginalization, therefore allowing a Fully Bayesian Approach.

We show numerical results in a real world inverse problem, i.e. the MagnetoEncephaloGraphy (MEG) [2]. This medical imaging technique aims to reconstruct and localize brain sources given the magnetic field measured outside the scalp in a totally non-invasive way.
The results show that the proposed method gives multiple benefits: allows performing prior sensitivity analysis on the hyper-parameter, allows to recycle particles at all the relevant SMC iterations and guarantees an approximation of both the parameters and the hyper-parameter; all these features at a negligible computational cost.

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MS27 - Anomalies Emerging in Mathematical Modeling and Probability

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ABSTRACT

The aim of this special session is to present new perspectives on anomalies emerging in different areas of mathematics, including mathematical analysis and probability. We are interested in anomalous operators and structures, including fractional derivatives and fractal domains, that, nowadays, more and more frequently arise in the mathematical modeling of real world phenomena.
We tailored our proposal in order to offer a space of discussion of results ranging from the purely analytical approach to more probabilistic and applied frameworks. The scope is indeed to drive the audience from original results on fractional differential operators (possibly on fractal domains), to their probabilistic interpretation and, finally, to their applications.

The delayed Brownian motion killed on a moving threshold and its anomalous diffusive behaviour

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With the term *anomalous diffusion*, one generally refers to a process $X(t)$ describing the position of a particle such that its mean square displacement $\mathsf{E}[(X(t) - X(0))^2]$ is a nonlinear function of time, in opposition with *diffusion* processes in which such a linearity is required. The prototype diffusion process is clearly the Brownian motion, while there are several different models of anomalous diffusion, each one constructed in a different way. Among these, a quite interesting example is given by the Brownian motion *delayed* by the inverse of an independent subordinator [2], that arise as a limit of continuous-time random walks can be used to describe particle trapping phenomena in several situations. When such a process is *free*, the anomalous diffusion property is clear, and follows from a simple conditioning argument. In case, instead, the process is killed upon exiting a certain fixed open set, then the non-diffusive behaviour is also reflected in the tail of the exit time [3]. In both cases, different behaviour of the mean square displacement is also mirrored by the fact that, being non-Markov, the process does not have a backward Kologorov equation, but its one-dimensional (marginal) distribution can be characterized be means of a time-nonlocal partial differential equation. If we consider, however, the process killed upon touching a time-variable boundary, things become much more difficult. To overcome the general lack of strong Markov property, some non-restrictive hypotheses on both the subordinator and the threshold are considered. In this talk we will discuss the link between the considered process and a time-nonlocal partial differential equation with a suitable Dirichlet condition on the moving boundary and we will provide the asymptotic behaviour of its mean square displacement, showing that under suitable hypotheses this is still an anomalous diffusion. This talk is based on a joint work ([1]) with Prof. Pierre Patie from Cornell University and Prof. Bruno Toaldo from University of Turin.

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Anomalous diffusion on irregular structures

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A wide class of phenomena present anomalous diffusion (see, for example, [6]).
The aim of the talk is to propose mathematical models to investigate anomalous diffusion on irregular structures from an analytical point of view.
In particular, we present some results obtained in [1], [2], [3], [4] and [5].

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Managing Crowded Museums: Visitors Flow Measurement, Analysis, Modeling, Control, and Optimization. Two case studies

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We present an all-around study of the visitors flow in two important Italian museums, namely the **Galleria Borghese** in Rome [1], and the **Peggy Guggenheim Collection** in Venice [2], in which we have performed a real-data acquisition campaign. We have tracked visitors by means of an IoT system based on Raspberry Pi receivers, displaced in fixed positions throughout the museum rooms, and on wearable Bluetooth beacons given to the visitors. We have also counted visitors by means on an *ad hoc* application for smartphone. The resulting dataset was analyzed by means of an artificial neural network, clustering techniques and other statistical methods in order to get behavioral insights, including the most common paths followed by the visitors. On these bases, we built the transition matrix describing, in probability, the room-scale visitor flows and then a graph-based stochastic model for generating real-like visitor trajectories, thus resulting in an actual digital twin of the museum. Finally, the digital twin was used in combination with an optimization algorithm to enhance the museums fruition while respecting the numerous logistic and safety constraints.
After these studies, both museums actually changed their ticketing strategy and entrance/exit management.

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Path dynamics of time-changed Lévy processes: a martingale approach

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Lévy processes time-changed by inverse subordinators have been intensively studied in the last years. Their importance in connection with non-local operators and semi-Markov dynamics is well-understood, but, in our view, several questions remain open concerning the probabilistic structure of such processes. The time-changed Lévy processes are particularly useful to describe complex systems with fractional and/or anomalous dynamics. The purpose of our work is to analyze the features of the sample paths of such processes, focusing on a martingale-based approach. We introduce the fractional Poisson random measure as the main tool dealing with the jump component of time-changed càdlàg processes. A central role in our analysis is then played by fractional Poisson integrals associated with the jumps of the process. We investigate these integrals involving fractional random measures and the martingale property of their compensated counterpart. This allows to obtain a semi-martingale representation of time-changed processes analogous to the celebrated Lévy-Ito decomposition. Finally, an approximation scheme of such processes will be discussed.

Local and nonlocal singular Liouville-type equations

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In this talk, I will discuss existence and classification results for solutions to local and non-local singular Liouville-type equations in $\mathbb{R}^n$. In dimension one, the problem has applications in mathematical modelling of galvanic corrosion phenomena for ideal electrochemical cells consisting of an electrolyte solution confined in a bounded domain with an electrochemically active portion of boundary. In higher dimension, Lioville equations have applications to prescribed curvature problems in conformal geometry: solutions correspond to constant Q-curvature metrics on the Euclidean space, with a singular point at the origin. I will present some results obtained in collaboration with A. DelaTorre, A. Pistoia [2], A. Hyder and L. Martinazzi [1] concerning existence and qualitative properties of solutions.

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MS28 - Contributed Talks on Biomedical Modeling

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A mathematical study of the influence of hypoxia on tumour growth, phenotypic heterogeneity and radiotherapy

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In the study of cancer evolution and radiotherapy treatments, scientific evidence shows that a key dynamic lies in the tumor-abiotic-factors interaction. In particular, oxygen concentration plays a central role in the determination of the phenotypic heterogeneity of the cancer cell population, both from a qualitative and geometric point of view. This project focuses on the analysis of the influence of hypoxia as an environmental stressor promoting the selection of aggressive phenotypes and affecting therapeutic efficacy.

In this talk, we present a continuous mathematical model to study the influence of hypoxia on the evolutionary dynamics of cancer cells. The model is settled in the mathematical framework of phenotype-structured population dynamics and it is formulated in terms of systems of coupled non-linear integro-differential equations. Numerical simulations are performed using Galerkin finite element methods, with the aim to test different vessel dispositions, allowing to represent various biological situations.

Then, the effects of radiotherapy treatment are included, considering various therapeutical protocols, differentiated per doses and timing. The computational outcomes show that the mutual interactions between the tumor mass and the oxygen distribution can result in a geometric characterization of tumor niches differentiated by phenotypic characteristics that determine a heterogeneous response to radiotherapy. The analysis of the study results provides suggestions about possible therapeutic strategies to optimize the radiotherapy protocol in light of the phenotypic and geometric inhomogeneities of the tumor.

The study constitutes the first step in the development of a mathematical tool for the delineation of patient-specific protocols which, in the perspective of personalized medicine, aim not only at the reduction (and in the best cases at the eradication) of the tumor mass, but also at the optimization, in case of relapse, of the phenotypic composition of the tumor so that resistance to subsequent treatments can be avoided as possible.

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Review of the Infrared Small Target Detection Methods

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In order to reduce the influence of image background edges on the accuracy of infrared small target detection algorithm, this paper proposes an infrared small target detection method based on edge enhancement via weighted contrast measure(EEWCM). Firstly, the edges of the image are extracted using the improved Canny edge detection algorithm, then the edge image is linearly and parametrically superimposed with the original image, and finally the small target is detected using multidirectional derivative-based weighted contrast measurement(MDWCM). The improved Canny edge detection algorithm uses wavelet transform and bilateral filter to replace the Gaussian filter in the traditional Canny algorithm, and uses the Otsu algorithm instead of the double threshold algorithm, which improves the problem that the traditional Canny algorithm tends to lose edge information and has poor adaptability. In this paper, 500 images with complex air-ground background were selected from the dataset and recognized using five algorithms including ASPCM, DLCM, DECM, WDLCM and MDWCM, where the average SCR of the images after processing by each algorithm, the FAR recognized and the time consumed by each algorithm were concluded.

The system processes the image in a total of four steps. Firstly, the edge detection algorithm based on improved Canny operator is used to detect the edges of the image, and the grayscale map of the identified background edges is extracted separately. The process includes smoothing the original image using wavelet transform and bilateral filtering to eliminate the noise and other disturbing information that interferes with the stability of the image structure after grayscale and binarization processing to reduce the error rate; using Sobel algorithm to calculate the gradient of the image and its intensity to estimate the edge intensity and direction at each point; according to the gradient direction, the gradient amplitude is non-extreme value suppressed to eliminate edge false detection, the local maximum point is obtained and kept as the candidate edge point, and the gray value of the non-extreme point is set to zero; the Otsu algorithm is used to determine the double threshold value and connect the edges. In summary, the overall strategy model of the edge detection algorithm based on the improved Canny operator .

In infrared images, small aircraft targets are usually high bright spots with significantly higher grayscale values than the surrounding background. The target detection algorithm builds the model and identifies high bright spots in images based on the grayscale gradient characteristic between the small target and the surrounding background.

Finally, 500 images with complex air-ground background were selected from the dataset and recognized using the five algorithms. The experimental results show that MDWCM has the best image denoising ability, and the FAR is lower than that of MDWCM and others.

Kinetic systems with nonlocal interactions and small inertia

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In this talk, we investigate a multi-dimensional kinetic system considering inertial effects. Both smooth and singular self-interaction potentials are considered and smooth assumptions on cross-interaction potentials are required. We prove existence and uniqueness of measure solutions considering initial data in a Wasserstein space of probability measures. Then, the small inertia limits are investigated for both the smooth and singular case, proving convergence results towards the corresponding macroscopic first order systems.

Agent-based and continuum models for spatial dynamics of infection by oncolytic viruses

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The spatial dynamics between cancer cells and oncolytic viruses is still poorly understood. We present here a stochastic agent-based model describing infected and uninfected cells for solid tumours, which interact with viruses in the absence of an immune response. Two kinds of movement, namely undirected random and pressure-driven movements, are considered: the continuum limit of the models is derived and a systematic comparison between the systems of partial differential equations and the individual-based model, in one and two dimensions, is carried out. Furthermore, we study the one-dimensional traveling waves of the two populations, with the uninfected proliferative cells trying to escape from the infected cells.
In the case of undirected movement, a good agreement between agent-based simulations and the numerical and analytical results for the continuum model is possible. For pressure-driven motion, instead, we observe a wide parameter range in which the infection of the agents remains confined to the center of the tumour, even though the continuum model shows traveling waves of infection; outcomes appear to be more sensitive to stochasticity and uninfected regions appear harder to invade, giving rise to irregular, unpredictable growth patterns. The agreement between the discrete and continuum models can be recovered by increasing the number of agents, but this may compromise the biological meaning of the parameters.
Our results suggest that the presence of spatial constraints in tumours' microenvironments limiting free expansion has a very significant impact on virotherapy. Some of these situations allow us to qualitatively reproduce patterns observed in experiments *in vitro*, suggesting that stochastic events may play a central role in the use of oncolytic virotherapy.

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A filtering monotonization approach for DG discretizations of hyperbolic problems

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We introduce a filtering monotonization approach for Discontinuous Galerkin (DG) approximations of hyperbolic problems [1]. In particular, we present a technique which reduces the spurious oscillations that naturally arise in presence of discontinuities when high order spatial discretizations are employed. This goal is achieved using a filter function that keeps the high order scheme if the solution is regular and switches to a monotone low order approximation otherwise, following an approach proposed for the Hamilton-Jacobi equations by other authors [2]. The method has been implemented in the framework of the *deal.II* numerical library [3], whose mesh adaptation capabilities are also used to increase the resolution in the regions of interest and to reduce the region in which the low order approximation is adopted. The potentialities of the proposed filtering approach are shown in a number of numerical test cases. Ongoing work on the application of such techniques to global atmosphere dynamics benchmarks will be also discussed.

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Numerical characterization of arrhythmic propensity in atrial fibrillation patients

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Atrial fibrillation is the arrhythmia with the highest morbidity and mortality rate worldwide. It manifests with episodes of higher duration and frequency, characterized by focal or re-entrant drivers caused by the superposition of electrical or structural anomalies. The intra- and inter-patient variability of these latter complicates the gold standard therapeutic approach, consisting in electrically isolating with radio-frequency ablation pathological areas.
To tailor the treatment to the individual patient (i.e., to identify optimal patient-specific ablation targets), we develop a computational approach aimed at quantifying the arrhythmic propensity of the tissue. Specifically, we post-process electroanatomical data collected via a mapping catheter to infer patient-specific conduction velocities in sinus rhythm and during pacing from the coronary sinus. We integrate these data within a coupled system of partial- and ordinary differential equations capable of representing the dynamics of transmembrane potential and ionic species concentrations that characterize cardiac electrophysiology. The numerical discretization of this model enables reproducing in silico scenarios of induction and sustainment of re-entrant mechanisms typical of atrial fibrillation [2].
Numerical simulations show how severe slow conduction corridors are associated with localized re-entrant circuits' anchoring (thus, with a high arrhythmic propensity). In addition, areas of high heterogeneity present unstable rotational activity due to head-tail interactions. These results suggest that the distribution and severity of slow conduction corridors allow the stratification of atrial fibrillation patients [1] and the design of new personalized ablation strategies.

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Industrial Session

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IS1 - Graph Theory and Urban Science

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ABSTRACT

The birth of Graph Theory is very often dated back to 1736, and more specifically to the publication of Leonhard Euler's paper Solutio problematis ad geometriam situs pertinentis (cf. Commentarii Academiae Scientarum Imperialis Petropolitanae, 8 (1736), 128-1409), in which he introduced the Eulerian graphs via the famous Königsberg bridges problem. Presently, Graph Theory is considered a flourishing discipline with many beautiful theorems of interest for both pure and applied mathematics, and a wide range of applicability in several branches of scientific and technical disciplines and topics. In this context, in this mini-symposium, we discuss various tools and techniques integrating graph theory in the field of urban and territorial planning to study territorial relations and complex dynamics. One approach is the use of graph theory for modeling and visualizing the morphological relationships between different urban components at different scales. Additionally, we present advances in extending the space syntax algorithm improving its spatial analysis robustness further. A specific application perspective is focused on configurational analysis for cities of 15-minute size. In addition to these methods, we are also adopting machine learning to evaluate complex spatial phenomena and to regionalize environmental features. This allows us to better understand the patterns and trends in land use practices. Finally, we are applying spatial multi-criteria analysis and geographical informative systems to deliver scenario analysis in the sector of green-hydrogen energy production plants settlements plan. By combining these different tools and techniques, we promote a more comprehensive understanding of land use patterns and infrastructural networks. Our work is intended to inform policy makers providing effective contributions for sustainable and resilient cities development.

GeoAI: a novel approach to analyze complex spatial phenomena

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The increasing availability of geospatial data, especially in urban context, has led to the rise of Artificial Intelligence (AI) as one the biggest opportunities for geospatial information management over the next years. Geospatial Artificial Intelligence (GeoAI) is a new trend in geospatial computing which uses interdisciplinary methods, ranging from computer science, statistics and geography to extract knowledge from spatial data and understand complex spatial dynamics [4]. In particular, Machine Learning (ML) techniques aim to seek out generalizable predictive or recursive patterns in datasets and statistics, which is a core component to drawing a noticeable insight from raw-data. The aim is to make planning choices targeting spatial development most akin to places and maximize positive impacts on territory. However, the insights gathered from the data analysis could be influenced by personal know-how and intuition and may differ depending on the size, shape, and aggregation of the geographic units analyzed. The topic of statistical aggregation, better-termed Regionalization, is an unsupervised ML algorithm that identifies a spatially constrained clustering problem [1]. The objective is to identify a set of statistical units that exhibit a high level of similarity concerning several attributes - the clustering problem - but are also spatially contiguous by taking into account the connectivity graph. This is a spatially explicit models used to regionalize urban and territorial features that outperform the more general computer science models when applied to spatial data [3]. This issue has been recognize as NP-hard problem [2], while others authors published multiple contributions where different formulations and solutions have been analytically demonstrated and suggested [5].

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Urban science and graph - Part II

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In this industrial talk, will be discuss the relations between graph theory in the field of territorial planning to analyse dynamics in inner areas.

Graphs and Urban Science

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In this general and introductory talk we will focus on relations between Graph Theory and Urban Science.

An image segmentation approach for space syntax and urban mobility

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Space syntax is a set of techniques for analyzing spatial layouts and human activity patterns in buildings and urban areas, together with a set of theories linking space and society [1]. As Space is described in terms of discrete spatial elements that relate to human behavior it is usually represented with graphs and analyzed with graph theory techniques. Space Syntax theory, in fact, relates the social significance of space to the configuration of spatial structures. Configuration, in turn, refers to the set of topological relations among spatial elements that interdepend in a spatial system. These relationships can be objectively analyzed using various centrality measures, included among which are integration and choice. Space Syntax models, particularly the 'movement economy' and the 'centrality as a process' theories, underline the influence of configurational properties on the distribution of pedestrian movement and, consequently, on the location of economic activities [2]. Yet, the perspective embodied in space syntax theories does not consider the influence of morphological and compositional aspects of the urban environment on the distribution of individual and social practices and on the distribution of economic activities. As a result, this contribution addresses this limitation and investigates the utilisation of image segmentation algorithms to weigh the configurational variables of integration and choice according to the morphological aspects of built areas and to the design of the street space.

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Urban science and graph - Part I

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In this industrial talk, will be discuss the relations between graph theory in the field of urban and territorial planning to study territorial relations and complex dynamics.

Assessing the feasibility of Green Hydrogen Infrastructure deployment: a Spatial Multi-Criteria Analysis approach

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The global shift towards sustainable and low-emission alternatives is essential in the ongoing energy transition, and green hydrogen has emerged as a promising solution [3]. This study aims to evaluate the possibility of implementing Green Hydrogen Infrastructure (GHI) in urban areas using a Spatial Multi-Criteria Analysis methodology. Various factors, encompassing technical, economic, environmental, and social aspects, are taken into consideration to identify appropriate sites for hydrogen production, storage, and distribution facilities. To analyze spatial data and visualize the relationships between criteria and potential locations, the Analytic Hierarchy Process (AHP) is integrated into a Geographic Information System (GIS) [1][2]. Real-world case studies of energy-intensive industries, specifically "Siderpotenza S.p.A." in Potenza (Basilicata, Italy), "Italcementi" in Matera (Basilicata, Italy), and "Cementeria Costantinopoli" in Barile (Basilicata, Italy), are employed to validate the methodology. The analysis incorporates the distinctive characteristics of each urban area, including existing energy infrastructure, renewable energy potential, and local hydrogen demand. The results offer valuable insights into the optimal sites for establishing green hydrogen facilities, considering factors such as proximity to renewable energy sources, transportation networks, and potential synergies with existing industries. This research enhances our understanding of the feasibility and potential advantages associated with the implementation of green hydrogen in urban contexts. By considering multiple criteria and employing spatial analysis techniques, it provides valuable information for policymakers, urban planners, and stakeholders involved in the transition towards a sustainable and decarbonized energy future.

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IS2 - Mathematical Problems in Robotics and Control

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ABSTRACT

The term Industry 4.0 was used to denote the fourth industrial revolution, which includes the actions needed to create smart factories. In smart factories, novel types of robots are to be used, e.g., collaborative robots, to bring them out of the safety cages and make them work close to human operators, and multi-robot systems, to enhance the abilities of single–robot systems. Many of such systems are intended to work in partially structured environments by leveraging on learning capabilities. At the same time, novel automation systems are to be developed, which are necessary to manage the increased complexity of the shop floor and, by leveraging on the availability of powerful communication and data management technologies, achieve full factory integration. In this context, mathematics has become an essential part of robotics and automation, since it allows the development of algorithms and models that enable robots to perform complex tasks in an increasingly autonomous way as well that allow to develop effective control strategies at the shop floor and factory levels.
These algorithms and models are used in many different areas, including computer vision, machine learning, motion control, path planning and modeling and simulation, in order to develop new applications and technologies:

- *Modeling and simulation provide several benefits in robotics, e.g., to generate large amounts of training data for machine learning algorithms, reduce time and costs of the engineering design cycle, provide a fully controlled virtual testing and verification environment and developing more intelligent robots. On the other hand, the development of complex automation systems needs powerful and effective tools to model and simulate discrete-event systems, e.g., automata and Petri nets.*
- *Machine learning algorithms use mathematical techniques such as data analysis and regression to identify patterns in data and develop predictive models. Nowadays, these models are widely used in robots to improve their world representation abilities, which are, in turn, needed to let them work autonomously in partially structured environments.*
- *Robot control and planning problems use powerful mathematical tools, e.g., from optimization theory and computational geometry, to ensure effective and safe task execution. Also, control of discrete-event systems calls for adoption of, e.g., mathematical programming and formal languages theory.*
- *Robotics and automation systems need novel and sophisticated sensing devices to achieve autonomy and efficiency. E.g., computer vision adopts mathematical techniques to process images captured by cameras. Some examples are image classification and object detection in the object manipulation field, robot tracking, pose estimation and object grasping.*

The proposed mini-symposium is aimed at providing a selection of crucial mathematical problems related to the above described research topics. The keynote talk will provide an overview of the current trends in robotics and automation, while each talk will focus on a specific application and the related mathematical problems.

Multi-Agent Systems in Robotics

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Applications of networked multi-agent systems, such as networks of sensing devices, distributed surveillance systems or cooperative multi-robot systems, require that each agent shares a suitable amount of information with the mates [1]. A key problem in this domain is to design control and/or estimation algorithms by exploiting only local communications among the neighbouring agents [2]. Thus, in the last two decades, huge research efforts have been devoted to develop distributed control and estimation approaches, with applications in several domains, such as robotics, smart distribution grids, logistics and transportation systems.
This talk is focused on the application of multi-agent systems in the domain of robotics, with special emphasis on multi-robot systems. First, an overview of dynamical networked multi-agent systems is provided, where distributed control and estimation approaches for dynamical networked multi-agent systems are briefly reviewed. A distributed estimation algorithm is illustrated in detail as a paradigmatic example [3].
Then, in order to illustrate the main theoretical and application issues related to distributed control of networked multi-agent systems, a specific problem is examined in detail: namely, the centroid and formation control of teams of mobile robots [4]. Special emphasis is put on the mathematical tools used to develop the theory, some open problems, especially related to the performance analysis, as well as on future and ongoing research on this subject.

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Petri net models for the analysis of warehouse systems

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Designing a warehouse is a very challenging task and involves a large number of decisions. Three levels of warehouse design can be distinguished: strategic level, tactical level, and operational level [1, 2]. These levels address long-term, medium-term, and short-term decisions, respectively. This talk focuses on the operational level, which has been investigated since 1990 and performs the short-term optimization of handling sequences. For example, the decisions at this level concern resource assignment, goods allocation in storage locations, order sequencing; the objectives can be the time minimization to complete a number of picking or storage operations, the maximization of warehouse capacity. Decisions at this level strictly depend on the current state of the system, and so the availability of detailed and formal models is a primary need.
This hierarchical control architecture benefits from the separation of functionalities but limits the modularity and flexibility of the control system, being implemented in a centralized way. Recent advances in computation and communication capabilities have given rise to a new generation of high-performance, low-power electronic devices. In this context, nowadays each vehicle or conveyor in the warehouse, is equipped with motors, sensors and a controller making it able to communicate with other vehicles, to vary its speed, to compute the distance from its current location to another point along the guide-path, etc. Moreover, each vehicle is often able detect obstacles (e.g. other vehicles) on its path and can consequently modify the velocity to avoid collisions. These vehicles are also known as "smart vehicles".
The development of effective decentralized control architecture exploiting the functionalities of these smart vehicles is a challenge. The analysis and control of these systems are very complex because many factors (e.g., availability of resources, interaction between subsystems, variation of the number of the resources) must be taken into account. Moreover, to analyse a control strategy on the system must consider each component and smart device not in isolation from each other but rather as an integrated whole. It is evident that the use of a detailed formal model is necessary to support the design steps and it would be preferable to use a unique formalism to avoid translations between different modelling domains. This talk discusses the use of a Petri nets as promising formalism to achieve this goal [3].

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Using the singular value decomposition in inverse kinematics algorithms for robotic systems

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Motion planning and control of robotic systems require to deal with the relationship between the variables expressing the task to be accomplished and the variables related to the actuation of the system [1].
The mapping from the task position variables to the actuators position variables defines the so-called inverse kinematics mapping [2]. Remarkably, most inverse kinematics algorithms are based on the mapping between velocity variables, which is locally linear through a configuration-dependent Jacobian matrix that needs to be inverted [3]. A very important problem is then to properly handle the occurrence of singular configurations of the Jacobian matrix [4, 5].
This talk gives a survey on the use of the singular value decomposition as a key tool to analize the performance of inverse kinematic algorithms across the occurrence of singular configurations and to design effective motion control algorithms for robotic systems [6, 7].

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Convergence analysis of discrete-time closed-loop inverse kinematics solvers for time-varying task functions

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Extraordinary progress has been achieved in the control of multiple robots executing multiple tasks, including handling of redundant degrees of freedom and task priorities, as well as constraints related to the task itself or to the robot capabilities [1]. Many algorithms have been proposed, which demonstrated to exhibit amazing performance for complex tasks in real application scenarios. However, only a limited effort has been devoted to the investigation of the implementation difficulties of the various solutions, mainly related to the handling of kinematic singularities and to the discrete-time nature of the system at hand. Many methods for motion generation of robots executing multiple tasks rely on closed-loop inverse kinematics solvers. The convergence properties of such solvers are almost always studied for continuous-time algorithms [2]. However, it is obvious that such algorithms are always implemented in discrete time. Moreover, modern motion generation algorithms based on constraint-based programming offer time-varying task functions to execute complex tasks, which often involve multiple robots that need to be synchronized. The talk intends to present some recent results that extend early work on the stability of closed-loop inverse kinematics algorithms [3]. The investigations look for conditions which can guarantee that a specific module of closed-loop numerical solvers, at the kernel of some of the mentioned algorithms, converges to a feasible solution. The peculiarity of the investigation relies on the objective to prove the convergence in those cases when the task function is time-varying. This will yield conditions not only on the initial task error and the loop gain - as it happens for stationary task functions - but also on the minimum sampling time, depending on: the degree of nonlinearity and the maximum rate of variation of the task function as well as on the distance from the singularities of the task Jacobian. Numerical simulations of an illustrative example and the execution of an industrially relevant task involving time-varying task functions support the theoretical findings.

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Robotics Meets AI & 5G – The Future is Now!

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Robotics research has advanced in the last two decades through an intensive collaboration with other disciplines and research communities. Multi–disciplinary approaches are more successful in addressing the combined issues of cognition (perception, awareness and mental models), and physical attributes (safety, dependability and dexterity) in the world of robotics.
Previously separated from humans behind a fence, the new advanced robots (or cobots) are sharing our workspace and collaborating with us. Increasingly sophisticated built-in sensors enable them to see and feel the presence of humans and avoid accidental contact. The perception of robotics technology is improving, as we experience more ways it can positively affect our lives. In particular, the social and medical benefits of robots are starting to get more attention.
In this scenario, the terms artificial intelligence (AI) and robotics are liberally used, and frequently interchanged today. However, the physical nature of a robotic system distinguishes it from the pure abstraction of AI. We are experiencing a transition from Information and Communication Technology (ICT) to InterAction Technology (IAT).
The paradigm of convergence between physical entity and digital twin (phygital twin) will guide – with AI, augmented reality and new technologies such as 5G – the development of robotic applications in industrial environments, in the agri-food sectors and healthcare, as well as in hostile and unstructured environments, thus making a natural transition from the Internet-of-Things (IoT) to the Internet-of-Skills (IoS). Armed with these skills, robots can be controlled dynamically in real time and be connected to people and machines locally and globally.
In a future scenario in which humans and machines are called to coexist, the socialization process of robotics will conform to an anthropocentric approach, for the benefit of the community, towards a technological and digital humanism that can help us reaffirm the least artificial feature of our world: our humanity.

IS3 - How to integrate advanced artificial intelligence with industrial processes to achieve a high level of automation and personalization

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ABSTRACT

Industry 4.0 has paved the way for the evolution towards Industry 5.0, a concept that aims to integrate advanced artificial intelligence with industrial processes to achieve a high level of automation and personalization. Mathematics plays a crucial role in Industry 5.0, enabling the development and implementation of specialized artificial intelligence for the industrial sector. During the meeting, a group of companies operating in the Basilicata Region and affiliated with the Confindustria ecosystem will present concrete business cases in the field of artificial intelligence. These include predictive models for industrial maintenance and reengineering of production processes.

How to be good entrepreneurs

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To be good entrepreneurs of a company you have to be excellent entrepreneurs of yourself. Managing, guiding, following a work situation in the necessary times and dealing with unpredictable situations requires high mental strength, concentration and careful observation of the world around us. An indispensable attitude very similar to mathematical minds. But this is the starting point and it is not enough, the speech will highlight the need to create, manage and support a healthy system of relationships especially with young and enlightened people, aimed at digital innovation as fuel for the present.

On an alghoritm improving Customer Care for telecommunications companies

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Comunica.live is an innovative startup that has based its growth on innovative algorithms, in the field of customer service, aimed at improving customer care for telecommunications companies. The speech will detail the algorithm having led Comunica.live to be received the attention by Vianova spa, one of the major Italian companies in the field of TLC.

The ecosystem of Confindustria Basilicata

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During the speech, the ecosystem of Confindustria Basilicata, Innovative and Technological systems, will be described with expressive emphasis on services for businesses and how companies in Basilicata have an urgent need for STEM resources and new innovations to ride the imminent wave of Industry 5.0 .

The great challenge for ICT Companies and Modern Analysts

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In the Industry 5.0 Era we are in the critical moments of rethinking and redefining new and old concepts related to information and production flows. Companies are constantly evolving and creating digital systems that can follow them but also guide them. It is a great challenge for ICT companies and modern analysts, who have to link transversely logic, modeling and data management to innovative and enabling technologies of the Industry 5.0, where man and, therefore, infinite variability, is at the center of the processes.

The Business Process Redesign

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The Business Process Redesign takes into consideration all aspects of evolution of business processes: from their improvement and change, to the systems that support them up to the introduction of new processes to propose new products or services to the market. The operational action of Orchestra, an innovative startup, allows you to review business processes and redesign them with a view to improving the service towards the internal customer but above all in line with the needs of the business. Redesigning the own business processes means knowing them in detail in order to analyze them critically so as to bring out the opportunities for improvement that impact not only on activities but also on information systems. In fact, a process will be lean and agile only if managed by the right tool as well as implemented with the processor's goals in mind.

Processes of technology transfer and open innovation

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By facilitating the meeting between the technological needs of micro, small and medium-sized enterprises and the skills in Mathematical Science and Technologies available in the public research system, processes of technology transfer and open innovation are promoted. In a scenario of continuous change, digital transformation - linked to sustainability - represents a fundamental step not only at an organizational and corporate level, but also a strategic asset for corporate strategies. During the speech, best cases, startups and successful spinoffs will be described.

IS4 - Industrial Contributed Talks I

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Challenges for QTSPs in the Quantum Computers Era

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A Trust Service Provider is, according to the current eIDAS Regulation [1], a *natural or a legal person who provides one or more trust services;* here, by *trust services,* we mean services that, for instance, manage the identity of users connected to the Internet and the reliability of communications therein.
A subset of Trust Service Providers (often shortened as "TSPs") are the Qualified TSPs (or "QTSPs"), that must undergo an appropriate evaluation process operated by a regulatory body, and are listed in an ad-hoc list maintained by the European Commission [2].
Namirial is an Italian digital identity company and is one of the biggest QTSPs in Europe. Its services range from issuing of certificates for advanced or qualified signatures and seals to the supply of SPID (Digital Identity Public System, one of the two electronic identity means in Italy), in addition to the supply of timestamps and certified electronic mail (PEC). Today, Namirial is facing new challenges connected to recent progresses in technology and particularly in the field of Quantum Computing: according to Entrust's view, if a company owns any data that will retain any value in 2030, that company should start worrying. Namirial, acting as a QTSP, owns data that will have *legal* value at least 20 years starting from today. This is due to today's regulations that are more strict for QTSPs than for banks; as an example, if Namirial performs video-identification of a subject in order to provide them with a signature certificate, the process has by law to be recorded and stored, if possible encrypted, for at least 20 years. The technology used to encrypt data is, as usual in applications, the famous RSA encryption, or ECC with equivalent security level; it is well-known that both RSA and ECC can be broken in a reasonable amount of time by quantum computers; this raises several security issues, since also the almost entirety of master private keys for Certification Authorities are RSA 4096 bits. *What makes matters worse is that any encrypted communication intercepted today can be decrypted by the attacker as soon as he has access to a large quantum computer, whether in 5, 10 or 20 years from now; an attack known as retrospective decryption*, according to ENISA [2]. An alternative must be sought, but it can only be the result of a joint effort of researchers, national authorities, standardisation bodies, private companies and all the other stakeholders involved. We are ready to embrace this technological and standardisation effort, cooperating with anyone interested in the area.

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Betting Maths: Algorithms for modeling and odds calculating

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The term “bookmaking” means the activity of creating betting odds on sport events that derives from the practice of recording odds and payouts by bettors on a hardcover notebook, called book. The bookmaker who provides the odds and accepts bets on them.
Bookmakers make available the odds of the events on which to place bets both in pre-match mode, before the event, that in live during the event. The objective of the study is to determine algorithms that can calculate the probability that a betting event will occur. The aim is to develop a mathematical model that allows the development of the "fair" odds for derivative markets.
The main problem of the model is the creation of artificial intelligence tools that allows the development of learning methods with which the AI becomes able to interpret in-play mode, or according to the live performance of the match being wagered, the probability of an outcome and calculate fair odds in real time through the relevant calculation algorithms.

Numerical Model for Data Railway Fusion: diagnostic applications

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Several Data analysis techniques such as regression analysis, time series analysis, classification, and data visualization can be employed to gain insights and actionable recommendations from railway data. In the context of railway data, vertical displacement refers to the change in elevation or height of specific points along the railway infrastructure. It is a measure of the vertical movement or offset of railway tracks, bridges, tunnels, or other structures relative to a reference point or surface. By continuously monitoring vertical displacement, railway operators can identify early signs of track settlement or structural changes, allowing them to take appropriate maintenance and repair actions. As known, the measurements obtained from individual sensors are prone to inherent errors and uncertainties. Consequently, relying solely on these measurements for directly calculating vertical displacement may result in inaccuracies and limitations. To overcome this challenge, sensor fusion techniques have been developed, utilizing sophisticated mathematical algorithms that integrate and combine measurements from multiple sensors to estimate vertical displacement with improved accuracy and reliability. This fusion process considers the specific characteristics of each sensor, such as measurement accuracy and possible biases. By properly modeling these factors, fusion algorithms can compensate for the limitations of individual sensors and improve the overall accuracy of the estimation. In this talk, we explore some numerical methods to provide valuable insights into the dynamic behavior of a moving object and railways system. Experimental results obtained through extensive testing and analysis demonstrate the efficacy and potential of these fusion methodologies for predictive data analytics.

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Microbial soil community: how AI and mathematical modeling can predict agricultural soil health

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The interaction of organisms and microorganisms with soil, air, and water compounds is essential to the conservation and functioning of agricultural ecosystems. Management and cultural practices often fail to keep agriculture soils healthy. In particular, intensive farming, mono-cultivation, and limited crop rotations caused biodiversity loss, which is an indicator of soil health [1]. Soil supports a diverse microbial community, which is crucial to ecosystem processes. To accurately assess agricultural soil health, multiple measurements of each chemical, physical, and biological indicator are needed. This is especially important because microbiological communities change under different conditions (climate, pH, management practice) and give soil different properties. With the rise of "Agriculture 4.0", characterized by automated and robotic processes and sensors for crop biotic and abiotic parameters, the development of a forecasting model to guide farmers toward targeted and sustainable management is crucial [2]. We are developing a model that uses artificial intelligence and mathematical modeling to implement a Decision Support System (DSS). This model should be able to predict soil and crop health based on biotic and abiotic parameters and warn of environmental conditions that predispose to an adverse event, such as a pathogen attack. This talk will show our real-time data collection progress using Evja sensors. Field surveys and real-time agrometeorological data (humidity and temperature) have been collected. We use a field monitoring system and laboratory metagenomic analysis to assess microbial biomass quality and quantity. Analyzing and correlating preliminary data, an algorithm is used to build the mathematical model. The algorithm and mathematical model selection and development are critical due to the need for a lot of data to train the model. Because we need to understand microorganism activities to collect as much data as possible and fully understand the soil, we will show our work on such models and the enzymes that are produced by microorganisms to survive.

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Measurement for presentation-attack detection

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We examine a structured mathematical measurement for presentation-attack detection and proper execution, as a consistent measurement and analysis plan is critical for today's security systems. We will cover three aspects of such measures: the measure's development, the analysis of selecting a minimum sample size, and the usage of Neural Networks in the generation of samples for training and tests.

Presenting an artifact or human characteristics to a biometric capturing subsystem interferes with system policy. Common Criteria and other tools offer comparable security assessments. In particular ISO/IEC 30107 covers presentation attack detection (PAD) [1]. The ENISA report [2] covers international and EU remote identity proofing laws, regulations, and practices. It also provides a preliminary gap analysis of existing standards and regulations and emphasizes the need for remote identity-proofing harmonization and cross-recognition.

PAD subsystem evaluations report APCER (Attack Presentation Classification Error Rate) and BPCER (Bona Fide Presentation Classification Error Rate) for a PAI (presentation attack instrument). Most biometric security metrics are calculated by applying the same mathematical patterns to specific use case scenarios and synthesizing a pass or fail metric. The measurements are derived from statistical hypothesis testing in which a hypothesis is defined and then tested to determine whether it is true, with empirical data showing that the result is statistically significant. We synthesize those metrics and describe the generalization approach.

In addition to the sampling method, determining the minimum sample size might be difficult. Statistics faces the challenge of determining a minimal sample size that ensures consistency without requiring excessively expensive and/or inefficient sampling. Based on the information available about the subject population, this number can be calculated in a variety of methods. We will present a use case scenario as well as the findings and limitations of such results.

Finally, there are various methods for synthetically generating ID card images to train fraud-detection networks with more data [3]. We will provide an overview of the various options that are currently available and discuss our use case solution.

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Enhancement of Low-Light Retail Shelf Images

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Nowadays new technologies enable retailers to collect and process data directly from store environments (see, e.g., [1, 4]). In particular *realograms*, i.e. real-time shelf images, can be caught by in-store vision sensors and can be made available through applications performing either image processing or visualization.
However, the dynamism affecting the store management processes sometimes produces non-standard acquisition contexts over the time. For example, the reduction of illumination due to breakdowns, systems maintenance, or implementation of energy consumption reduction policies (this is actually a trending topic, because of the current energy crisis in Europe), has considerable effects on the realograms appearance. In fact, images caught from low-light environments often have insufficient brightness, low contrast, high noise levels, i.e. poor visual quality. As a consequence, this results in decreasing the performances in both computer vision and human tasks.
As far as image visualization tools are concerned (consider, for instance, a web application providing for the real-time remote view of in-store shelves together with the metadata encoding their relevant features and metrics), low-light images negatively affect the user experience. This issue leads us to deal with the problem of processing the enhancement of low-light images in the realograms domain.
The enhancement of low-light images is a quite challenging task (see, e.g., [3] and references therein). Deep learning-based approaches provide improved accuracy in image enhancement tasks. Indeed, by adapting the method presented in [2], we are able to obtain such a result on a dataset composed of images captured under different lighting conditions in a controlled environment simulating a store-like scenario.

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IS5 - Industrial Contributed Talks II

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Advancing Sleep Monitoring: Integrating OSAS Detection Algorithm in Wearable Devices for Improved Quality of Life

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Sufficient sleep and obtaining high-quality rest are essential for maintaining a healthy lifestyle. Low-quality sleep may cause daytime drowsiness, decreases study and work performance, or even worse, increases the probability of car crashes [1]. Not only a reduced total sleep time but also insomnia or Obstructive Sleep Apnea Syndrome (OSAS) may lead to reduced sleep quality, causing daytime sleepiness. The gold standard for sleep monitoring is polysomnography (PSG), a procedure that involves measuring multiple signals during sleep. These parameters include oxygen saturation (SpO2), brain activity, Electrocardiogram (ECG), and Electrooculogram (EOG). PSG is the most powerful and accurate way for sleep monitoring, but it is expensive, time-consuming, and requires a medical sleep expert. The previous work in [3], instead, was aimed to recognize OSAS by monitoring sleep using a reduced sleep parameter set. In recent years, multiple devices have been created for less invasive sleep monitoring. Some of them are wrist-worn devices with naso-cannulas, thermistors, and other sensors able to measure different human parameters [2]. Sleep monitoring has been made even less expensive and less invasive thanks to smartwatches, devices that can detect oxygen saturation (SpO2) and Heart Rate (HR) thanks to photoplethysmograph (PPG) sensors. The variety of signals collected with a smartwatch is reduced with respect to a PSG but allows an acceptable accuracy in estimating sleep stages and detecting apneas. This paper aims to demonstrate that it is possible to embed the algorithm presented in [3] in a wearable off-the-shelf device. To demonstrate this, an experimental activity was conducted, and the subjects were equipped with both PSG and a Garmin smartwatch, obtaining HR and SpO2. We then compared the HR and SpO2 acquired with the PSG and the Garmin smartwatch. Finally, we compared the performance of algorithm [3] when using PSG and smartwatch data.

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How Much to Simplify Prediction Models for the Model Predictive Control of Connected and Automated Vehicles?

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The control of Connected and Automated Vehicles (CAVs) requires both knowledge of the vehicle dynamics/kinematics and the constraints arising from the surrounding environment, characterized by other CAVs, human driven vehicles, and vulnerable road users, as well as time-varying road parameters (slope, friction), weather and traffic conditions. For this reason, the attention of Car Makers is focusing on Model Predictive Control (MPC) techniques to be performed at an intermediate layer between the Smart Road and the power-train. MPC techniques allow the use of simplified vehicle models and their interactions with the surrounding environment to predict the CAV's behavior over a certain time horizon, while minimizing a cost function that considers outputs tracking (e.g., speed, lane keeping), variations in the inputs (e.g., with respect to nominal values and/or the rate of change of torque request and steering angle), and possibly environment-related constraints (e.g., for energy management strategies). Then, MPC solves a constrained optimization problem considering constraints on predicted outputs and inputs. Netcom has been developing MPC strategies to be performed on an Intelligent On-Board Unit (I-OBU) [1] providing the vehicle with both connectivity and autonomous driving functionality, and a series of works have been published [2, 3], considering simplified vehicle dynamics, errors with respect to the road (lateral displacement, yaw angle error), a car-following model, and the vehicle kinematics, and then linearizing and discretizing at each time instant. However, even if linearization is performed cyclically (every 10 ms) and adaptively, and despite the real-time execution of the MPC, the considered simplifications may affect predictions and, consequently, the behavior of the CAV, as many nonlinearities are not considered. Therefore, how much to simplify prediction models for the control of CAVs? The need is to consider more complex models, nonlinear optimization methods, and mathematical methods compliant with the typical execution times in the automotive context.

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The Finwave's Financial Economic Plan

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The Finwave's Financial Economic Plan is mainly aimed at banks and trusts in order to guide the instructor analyst in the evaluation of loan/financing requests, bringing out the level of awareness of the entrepreneur and the real practical potential of the company. The level of awareness and the potential are measured through a series of specific criteria and technical indicators.

Math, Graph and Distributed Algorithms

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In this talk we will see how mathematics provides the theoretical foundations needed to understand and analyze distributed algorithms, while distributed algorithms apply mathematical concepts to solve complex problems involving the distribution of resources and computations on computer networks.

A novel Context Aware Paths Recommendation Approach applied in the Cultural Heritage field

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The will to travel leads humans to discover new places and enjoy new adventures. However, tourists usually need help knowing what to visit and, avoiding time issues, in which order to explore several Points of Interest (POIs).
In this field, new technologies can help tourists to improve their experiences and select the visiting path according to personal preferences. Therefore, the employment of Recommender Systems [1] allows the personalization of the experience through the appropriate POIs' selection. Moreover, RSs' analysis could take advantage of contextual information that suits the personalization in the specific environment where the elaboration happens, providing users with even more specific and tailored paths [2].
This paper aims to design personalized visiting paths combining a Context-Aware Recommender System (CARSs), based on Singular Value Decomposition [4] and Contextual Biases [3], and a linear integer programming model to maximize the number of visited POIs in the available time. The proposed approach is tested through a prototype, obtaining promising results.

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The sol-gel transition of a natural polymer by viscosity curves and nonlinear kinetics model

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The sol-gel transition of polymer materials is a topic of great scientific and technological interest [1, 2, 3]. The formation of hydrogels is important in the food, cosmetic, pharmaceutical and polymer industries, for example in the production of matrices in the biomedical field in drug delivery, tissue engineering and bioplastics. In this work, the sol-gel gelation kinetics of Agar-based polymer solutions was studied by means of viscosity versus time curves $\eta = \eta(t)$ obtained in a Couette viscometer with coaxial cylinders, parameterizing the flow rate, concentration, temperature and the mechanical history of the experiment. The viscosity of the dispersion is interpreted using the Einstein equation $\eta(c) = \eta_0(1 + k_E \cdot c)$which takes into account the concentration of the dispersed phase. An original theoretical model of the growth (coarsening) of sol clusters has been developed on the basis of the surface tension of the dispersed particles (Laplace's equation), of the shear-stress associated with the velocity gradient (Newton's equation), of the autocatalytic gelation kinetics (logistic equation) and diffusion processes (Fick's first law) in which the larger (more stable) particles grow at the expense of the smaller particles which dissolve and the solute molecules migrate under the action of the concentration gradient (Ostwald ripening). A nonlinear kinetic equation is obtained in which the constants are governed by the surface tension $k_1(\gamma)$ and the velocity gradient $k_{-1}(\nu)$

$$\frac{\partial c}{\partial t} = k_1 \cdot c - k_{-1} \cdot c^2$$

whose solutions correctly interpret the trend of the observed viscosity curves.

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Edu-SIMAI

Edu-SIMAI session

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Edu-SIMAI is the event that SIMAI devotes to the relationship with School, in continuity with previous editions (SIMAI 2016, SIMAI 2018 and SIMAI 2020+2021 conferences). The main objective of the initiative is to provide an opportunity for World of Education and World of Research to meet with a focus on the topics of applied mathematics, in order to promote a network of collaborations between universities, research centers, private companies and educational institutions.
The Edu-SIMAI event is held under the patronage of Ufficio Scolastico Regionale of Basilicata and of the italian projects "Liceo Matematico" and "Piano Lauree Scientifiche".

Matematica per scenari: oltre il problem-solving c'è la modellistica

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Le raccomandazione del Consiglio Europeo (2018) relativa alle competenze chiave per l'ap- prendimento permanente mette in evidenza la centralità della competenza matematica e della competenze di base in scienza, tecnologia e ingegneria[2]. Secondo Niss e Højgaard la *competenza matematica* è la prontezza intuitiva di qualcuno ad agire in modo appropriato in risposta a tutti i tipi di sfide matematiche relative a situazioni date. Inoltre, nelle indicazioni nazionali riguardanti gli obiettivi specifici di apprendimento (DPR 89/2010) si specifica che la competenza matematica è la capacità di sviluppare e applicare il pensiero e la comprensione matematica per risolvere una serie di problemi in situazioni quotidiane, e si aggiunge che la competenza matematica comporta a diversi livelli, la capacità di usare modelli matematici, mettendo l'accento sia sulla risoluzione dei problemi sia sul processo di modellizzazione.
Questo lavoro ha un duplice obiettivo. Da un lato si propone di condividere i costrutti teorici alla base del processo di modellistica [1] definendo i termini che li costituiscono, es. problema e modello matematico e la differenza problem-solving, matematizzazione e modellizzazione, ed estendendo il concetto di "reale" [4]. Dall'altro lato, ha l'obiettivo di presentare e di discutere esempi di problemi concreti da poter utilizzare in aula. A tal fine si presenterà il corso MOOC *Matematica per scenari* disponibile gratuitamente sulla piattaforma www.pok.polimi.it. Il corso propone esperienze didattiche basate su scenari realistici e fornisce agli insegnanti materiali ed approfondite indicazioni metodologiche per la loro attuazione in classe.
Durante l'intervento, si illustrerà un esempio di scenario, con particolare accento sugli aspetti didattici soffermandosi anche sugli effetti che essa ha avuto sui partecipanti, anche in termini emotivo-affettivi.

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Interdisciplinarità, competenze matematiche e modellizzazione: un incrocio possibile

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Oggi più che mai è importante promuovere l'utilità della matematica, non intesa come mero formalismo, ma come forma di cultura. OCSE PISA definisce la literacy matematica come la capacitá di un individuo di formulare, utilizzare e interpretare la matematica in una varietà di contesti. In quest'ottica, l'interdisciplinarità tra la matematica e le altre scienze, le attività di modellizzazione e il ricorso al laboratorio possono favorire la comprensione di concetti matematici, l'acquisizione di una maggiore fluidità procedurale, la capacità di formulare, rappresentare e risolvere problemi, lo sviluppo del ragionamento adattivo e migliorare la disposizione allo studio. Presenteremo qui una attività laboratoriale che parte dall'analisi del testo di un problema e si dipana per strade solo apparentemente opposte. La risoluzione del problema viene presentata attraverso la dimostrazione con strumenti propri della matematica e la sperimentazione laboratoriale più tipica di altre scienze. Faremo vedere come una educazione all'interdisciplinarità possa offrire una visione poliscopica di un problema ed attivi competenze trasversali per arrivare alla soluzione.

Dinamica di popolazioni, da Volterra alle epidemie (passando per Turing): spunti per un percorso didattico

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Il racconto di alcuni episodi storicamente rilevanti è il punto di partenza per affrontare queste domande:

- **Perché** abbiamo bisogno di modelli matematici
- **Cosa** intendiamo rappresentare: una o più popolazioni che interagiscono
- **Come**, ovvero le specifiche del nostro modello: deterministico o stocastico; discreto o continuo; spaziale o no; le funzioni di risposta
- **Dove** andremo a finire: le traiettorie, gli equilibri, il controllo

a cui tenterò di fornire delle risposte seguendo un approccio principalmente fenomenologico e qualitativo/simulativo. Tra gli strumenti utilizzati, testi didattici[3], scientifici[2] e di divulgazione[1].

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Laboratori interdisciplinari per modellizzare la realtà

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Il Liceo Scientifico Statale "*Pier Paolo Pasolini*" di Potenza è stato tra le prime scuole secondarie di secondo grado della Basilicata ad aver avviato il progetto Liceo Matematico nell'anno scolastico $2018-19$ in collaborazione con il Dipartimento di Matematica, Informatica ed Economia (DiMIE) dell'Università degli Studi della Basilicata[3].

Il progetto, arrivato al quinto anno di vita, si articola in laboratori didattici extracurriculari in cui la matematica è esplorata partendo dalla sua capacità di descrivere e modellizzare la realtà contaminandosi con discipline sia scientifiche che umanistiche. L'esperienza si articola in moduli: tre da 8 ore nel primo e nel secondo anno e due da 15 ore nei restanti tre anni: in ogni modulo sono proposti problemi di realtà riconducibili all'arte, alla logica, ai paradossi, all'informatica, alla letteratura e all'urbanistica.

Nell'ottica di contribuire alle celebrazioni del centesimo anniversario della nascita di Pier Paolo Pasolini, nel 2022 il laboratorio di "Matematica e urbanistica" si è ispirato al poeta, scrittore, autore e regista a cui è intitolato il Liceo. Partendo da Matera, set scelto per "Il Vangelo secondo Matteo", il laboratorio si è focalizzato sulla rappresentazione della città mediante nodi e connessioni. Il modello reticolare di Matera è stato confrontato con quello di Gerusalemme e di altri insediamenti urbani cari all'artista fino ad approdare alla periferia di Potenza, città di appartenenza del gruppo di lavoro. L'esperienza ha così consentito di apprezzare come città diverse obbediscono a leggi matematiche differenti e, contestualmente, di sperimentare l'efficacia della teoria dei grafi per schematizzare e semplificare situazioni reali complesse.

[3]La prima convenzione tra il Liceo Scientifico "*Pier Paolo Pasolini*" e il DiMIE-UNIBAS è stata sottoscritta a settembre 2018.

Dal Corso di Approfondimento a Scuole al DeMaCS: un'occasione irrinunciabile per formarsi e orientarsi al Dipartimento di Matematica e Informatica dell'UniCal

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Il Corso di Approfondimento in Matematica e Informatica ha come obiettivo principale quello di divulgare la Matematica e l'Informatica. Si compone di una serie di lezioni gratuite e aperte alla partecipazione di alunni e insegnanti delle scuole secondarie di secondo grado. Il corso si colloca nell'ambito delle attività di promozione della Matematica e dell'Informatica, e dell'orientamento alla scelta del corso di Laurea organizzate dal Dipartimento di Matematica e Informatica dell'Università della Calabria [1]. Il corso è parte importante delle attività dei Progetti del Piano Lauree Scientifiche in Matematica e Informatica e dell'UniCal. In questo talk ripercorriamo i dieci anni di storia del Corso di Approfondimento, raccontando le emozioni vissute, discutendo delle metodologie e degli strumenti adottati, e fornendo alcuni dati di interesse statistico.

References

[1] https://scuolealdemacs.unical.it/home

Un laboratorio *permanente* di ricerca-azione: esperienze didattiche attraverso le discipline STEAM al Liceo Matematico

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Il Liceo Artistico-Liceo Musicale e Coreutico "W. Gropius" di Potenza ha stipulato una convenzione con il Dipartimento di Matematica Informatica ed Economia dell'Università della Basilicata (DiMIE-UniBas) e ha inserito la sperimentazione del Liceo Matematico come ampliamento dell'Offerta Formativa a partire dall'anno scolastico 2021-2022.
Il presente contributo intende sottolineare alcuni aspetti relativi al biennio di sperimentazione 2021-2023 del modulo di "Matematica e Arte" tra i quali le esperienze didattiche e i laboratori di ricerca-azione relativi alle discipline STEAM, i risultati ottenuti, le prospettive di sviluppo e la pianificazione delle prossime attività.
L'aspetto fondante del Progetto di ampliamento dell'Offerta Formativa è stato sia la formazione dei docenti promossa dal DiMIE-UniBas sia la collaborazione con l'USR-Basilicata, attento al contesto istituzionale della scuola. Punti di forza sono stati la condivisione con il mondo accademico di obiettivi disciplinari e la ricerca delle metodologie più idonee per favorire l'apprendimento attivo e cooperativo.
L'aspetto comune alla base di ciascuna sperimentazione didattica è stata la visione interdisciplinare del Sapere e la ricerca di punti di raccordo tra la cultura scientifica e quella umanistica al fine di apprezzare non solo la valenza strumentale della Matematica, ma anche e soprattutto quella culturale.
I laboratori di ricerca-azione sono risultati, quindi, uno strumento fondamentale per favorire lo sviluppo di competenze trasversali di tipo esplorativo, argomentativo e di indagine e per facilitare l'orientamento delle studentesse e degli studenti in una società sempre più dinamica e complessa.
La ricerca si è incentrata, pertanto, sulla visione della Matematica come capacità di osservazione, immaginazione e creatività, fonte di soluzioni tecnologiche per problemi a scala globale, punto di raccordo tra il mondo scientifico e il mondo umanistico.
Gli alunni del Liceo Matematico del Liceo "W. Gropius" hanno partecipato nell'a.s. 2021-2022 al Concorso promosso dall'UMI "Ti racconto il Liceo Matematico" ricevendo la "Menzione Speciale Arte"[4] e nell'a.s. 2022-2023 al Concorso "Mathematics for everyone comic challenge" promosso da Maddmaths! nell'ambito delle celebrazioni della Giornata Internazionale della Matematica 2023. Il fumetto, candidato dai discenti, dal titolo *Soap Bubbles in Maths* è stato selezionato dalla Giuria[5].

[4] https://www.liceomatematico.it/concorso-ti-racconto-il-liceo-matematico/
[5] https://www.idm314.org/2023-comic-challenge-gallery#d/1/2023-cc-photo-2071

Il Liceo Matematico: un percorso interdisciplinare dall'astrazione alle applicazioni

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Il progetto Liceo Matematico è implementato da alcuni anni nell'ambito delle attività del gruppo di ricerca in Didattica della Matematica del Dipartimento di Matematica di UNISA. La metodologia sviluppata in tale contesto sperimentale ha consentito di far emergere, nel corso di una strutturata attività laboratoriale presso le istituzioni scolastiche coinvolte, i profondi legami interdisciplinari che sussistono nei diversi contesti teorici e di stimolare sia i docenti sia i discenti in direzione di un percorso di formazione sempre più lontano da un semplice nozionismo e in grado di favorire la crescita personale. In particolare, il progetto intende porre rimedio a quella tendenza (pericolosa e improduttiva) che conduce troppo spesso alla parcellizzazione e frantumazione dei saperi disciplinari che, laddove non posti in relazione tra di loro, restano - per usare una espressione di Edgar Morin - dei *segmenti morti*, incapaci di formare un pensiero complesso e di rispondere alle domande di conoscenza radicali che provengono da ambiti interconessi e intesi sempre come parti del più ampio sistema globale. Ciò si è rivelato quanto mai necessario per i giovani nell'ottica del consolidamento di competenze e abilità indispensabili in contesti diversi, giacché il mercato del lavoro attuale sembra richiedere non tanto delle figure preparate dal punto di vista meramente tecnico quanto dei giovani che, in virtù di uno spirito critico adeguatamente formato, siano in grado di adattarsi a situazioni sempre diverse e di svolgere, nel corso del tempo, mansioni e ruoli mutevoli cercando di lavorare in team ad assetto variabile, oltre che di passare con sufficiente disinvoltura in molteplici ambiti tematici.

Le azioni di monitoraggio poste in essere dal gruppo di lavoro del progetto, finalizzate anche alla verifica dei risultati nella fase ex post, hanno rivelato che, in un'ottica di medio periodo, l'acquisizione delle competenze da parte dei discenti durante la loro partecipazione alle attività laboratoriali - soprattutto laddove essa è stata continuativa per tutti gli anni di studi superiori - ha indubbiamente favorito il loro inserimento nel mondo del lavoro, non solo collaborando con aziende ma anche attraverso la progettazione di iniziative autonome valide, adeguate e soprattutto innovative. Infine è opportuno ricordare che, nelle molteplici occasioni di confronto e di dibattito pubblico a cui hanno partecipato anche autorevoli rappresentati delle diverse realtà produttive, si è avuto modo di constatare come i livelli di preparazione raggiunti dagli allievi del Liceo Matematico vengano considerati ottimali per incontrarsi fruttuosamente con le mutate esigenze del mondo imprenditoriale.

Index of speakers