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High order cell-centered schemes for the solution of nonlinear hyperbolic systems on moving unstructured meshes

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In this talk we present a new class of high order accurate one-step schemes for the solution of nonlinear systems of conservative and non-conservative hyperbolic partial differential equations [1, 2]. The numerical algorithms are designed for two and three space dimensions, considering moving unstructured triangular and tetrahedral meshes, respectively. WENO reconstruction techniques are used to achieve high order of accuracy in space, while an element-local space–time Discontinuous Galerkin finite element predictor on moving curved meshes is devised to obtain a high order accurate one-step time discretization. Within the space–time predictor the physical element is mapped onto a reference element using a high order isoparametric approach, where the space–time basis and test functions are given by the Lagrange interpolation polynomials passing through a predefined set of space–time nodes. Since the schemes are cell-centered, the final mesh motion is computed by using a suitable nodal solver algorithm. The connection of the old mesh configuration at time t^n with the new one at time t^{n+1} provides the space-time control volumes on which the governing equations have to be integrated in order to obtain the time evolution of the discrete solution. The first class of methods presented in this talk belong to the category of so-called direct Arbitrary-Lagrangian-Eulerian (ALE) schemes, where a space-time conservation formulation of the governing PDE system is considered and which already takes into account the new grid geometry directly during the computation of the numerical fluxes. We emphasize that our methods are moving mesh methods, as opposed to total Lagrangian formulations that are based on a fixed computational grid and which instead evolve the mapping of the reference configuration to the current one. We will address both high order finite volume (FV) as well as discontinuous Galerkin (DG) methods.

An algorithm working on moving meshes with topology changes will also be briefly introduced [3]. General polygonal grids are regenerated at each time step, and the closed space-time control volumes which arise from the discretization might exhibit polygons with a different number of sides as bottom and top faces.

The last part of the talk is devoted to the description of cell-centered updated Lagrangian schemes *sensu stricto*, where zero mass flux across element boundaries is rigorously ensured. This class of methods will be presented for hydrodynamics [4] and nearly incompressible solid mechanics [5] applications. Finally, a recent development involving a unified model for continuum mechanics will be shown, where pure Lagrangian finite volume schemes have been designed which accounts for asymptotic preserving properties and implicit-explicit time stepping. Here, applications range from ideal and viscous heat conducting fluids to elastic and elasto-plastic solids within the same set of equations.

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Mathematical Prospects and Challenges for Machine Learning in the Physical World

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The last decade has witnessed an experimental revolution in data science, led by the huge empirical success of Deep Learning (DL) methods across many areas of science and engineering. In order to capitalise on these successes, it has become increasingly important to provide a mathematical foundation that gives guiding design principles and mitigates the current data 'hunger' of these DL architectures, to enable further applications within computational science.

A distinctive trait of this challenge is the high-dimensional nature of the problem. As a result, such mathematical foundations must simultaneously cover approximation aspects, i.e. how to design architectures that approximate the target function faithfully in high-dimensions, statistical aspects, i.e. how to certify that population error is close to the empirical training error, and computational aspects, i.e. provide an efficient optimization algorithm in the high-dimensional regime. In all of these aspects, one is generally exposed to the so-called *curse of dimensionality*, capturing an exponential dependency between learning resources and input dimension. In order to provide valid mathematical foundations, this curse must be avoided simultaneously in all fronts.

In this talk, we will describe the crucial role that physics and data structure plays in constructing such foundations. First, we will discuss how physical principles of symmetry and scale separation allow us to define function approximation spaces where the curse of dimensionality is mitigated, via a geometrical perspective that unifies all successful DL architectures (CNNs, RNNs, Transformers, GNNs). Next, we will focus on learning and optimization aspects, by focusing on the class of shallow neural networks. Such class provides a rich computational landscape, that we will use to illustrate the thin transition between computational hardness results and positive learning guarantees, again relying on distributional assumptions. Finally, we will discuss open mathematical problems as well as applications of these models to computational science, emphasizing the incipient area of 'Scientific Machine Learning'.

This talk will cover joint work with Eric Vanden-Eijnden, Alberto Bietti, Luca Ventui, Marylou Gabrie, Carles Domingo-Enrich, Min Jae Song, Zhengdao Chen, Lei Chen, Jon Niles-Weed and Ilias Zadik.

Multi-scale modelling for traffic management by autonomous vehicles

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Macroscopic traffic flow models have become popular in transportation engineering and applied mathematics during the last decades. These models give a description of collective dynamics in terms of spatial density and average velocity, which evolve according to partial differential equations derived from fluid dynamics, coupled with suitable closure relations. In fact, even if the continuum hypothesis is clearly not physically satisfied, macroscopic quantities can be regarded as measures of traffic conditions and allow depicting the spatio-temporal evolution of traffic waves. Moreover, they are suitable for analytical investigations and very efficient from the numerical point of view. Therefore, they provide the right framework to state and solve control and optimization problems for real time applications.

At present, the expected deployment of Connected Autonomous Vehicles (CAVs) opens new perspectives for traffic management. Indeed, CAVs can potentially be used as endogenous actuators to improve traffic flow on road networks. Yet, the accurate description of the these interactions requires the development of specific models, taking into account CAV dynamics within bulk traffic flow.

In this talk, I will present a family of strongly coupled PDE-ODE systems designed to model the influence of controlled single vehicles or platoons on the surrounding road traffic [2, 3, 5]. The models consist of conservation laws with discontinuous flux describing the main traffic evolution and ODEs accounting for CAV trajectories, which depend on the downstream traffic conditions. The moving constraints are operated by inequalities on the flux funtion, which account for the bottlenecks created on the road by the presence of the controlled vehicles. Finite volume schemes are specifically developed to capture exactly the non-classical discontinuities that may arise at the constraint positions [1, 5], and they are then used to address numerically optimal control problems for traffic management [4, 6].

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Large stochastic systems of interacting particles

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I will present some recent results, obtained with D. Bresch and Z. Wang, on large stochastic many-particle or multi-agent systems. Because such systems are conceptually simple but exhibit a wide range of emerging macroscopic behaviors, they are now employed in a large variety of applications from Physics (plasmas, galaxy formation...) to the Biosciences, Economy, Social Sciences.

The number of agents or particles is typically quite large, with $10^{20} - 10^{25}$ particles in many Physics settings for example and just as many equations. Analytical or numerical studies of such systems are potentially very complex leading to the key question as to whether it is possible to reduce this complexity, notably thanks to the notion of propagation of chaos (agents remaining almost uncorrelated).

To derive this propagation of chaos, we have introduced a novel analytical method based on relative entropy method, which led to the resolution of two long-standing conjectures:

- The quantitative derivation of the 2-dimensional incompressible Navier-Stokes system from the point vortices dynamics, performed in [3];
- The derivation of the mean-field limit for attractive singular interactions such as in the Keller-Segel model for chemotaxis and some Coulomb gases, announced in [1] and fully proved in [2]. This setting introduces a weighted relative entropy which combines the basic entropy used in [3] together with the modulated energy of [4].

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Robust Statistics for (big) data analytics

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Data rarely follow the simple models of mathematical statistics. Often, there will be distinct subsets of observations so that more than one model may be appropriate. Further, parameters may gradually change over time. In addition, there are often dispersed or grouped outliers which, in the context of international trade data, may correspond to fraudulent behavior. All these issues are present in the datasets that are analyzed on a daily basis by the Joint Research Centre of the European Commission and can only tackled by using methods which are robust to deviations to model assumptions (see for example [6]).

This distance between mathematical theory and data reality has led, over the last sixty years, to the development of a large body of work on robust statistics. In the seventies of last century it was expected that in the near future "any author of an applied article who did not use the robust alterative would be asked by the referee for an explanation" [9].Now, a further forty years on, there does not seem to have been the foreseen breakthrough into the wider scientific universe. In this talk, we initially sketch what we see as some of the reasons for this failure, suggest a system of interrogating robust analyses, which we call "monitoring" [5]and describe a series of robust and efficient methods to detect model deviations, groups of homogeneous observations [10], multiple outliers and/or sudden level shifts in time series ([8]).

Particular attention will be given to robust and efficient methods (known as forward search) which enables to use a flexible level of trimming and understand the effect that each unit (outlier or not) exerts on the model (see for example [1], [2], [7]).

Finally we discuss the extension of the above methods to transformations and to the big data context. The Box-Cox power transformation family for non-negative responses in linear models has a long and interesting history in both statistical practice and theory. The Yeo-Johnson transformation extends the family to observations that can be positive or negative. In this talk we describe an extended Yeo-Johnson transformation that allows positive and negative responses to have different power transformations ([4] or [3]).

As an illustration of the suggested procedure we analyse data on the performance of investment funds, 99 out of 309 of which report a loss. The problem is to use regression to predict medium term performance from two short term indicators. It is clear from scatterplots of the data that the negative responses have a lower variance than the positive ones and a different relationship with the explanatory variables. Tests and graphical methods from our robust analysis allow the detection of outliers, the testing of the values of transformation parameters and the building of a simple regression model. All the methods described in the talk have been included in the FSDA Matlab toolbox freely donwloadable as a toolbox from Mathworks file exchange or from github at the web address https://uniprjrc.github.io/FSDA/

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Density Functional Kinetic Theory for Soft Matter

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1 Introduction

In the last decades kinetic theory has developed into a very elegant and effective framework to handle a broad spectrum of problems involving complex states of flowing matter, far beyond the original realm of rarefied gas dynamics.

The kinetic theory of gases in its original form as devised by Ludwig Boltzmann was restricted to binary collisions to pointlike particles hence formally limiting its application to dilute gases. Subsequent attempts to extend it to dense gases and liquids were notoriously plagued by several problems, mostly connected with infinities in the treatment of higher order collisions. Several strategies have been developed over the years to cope with such problems, but the kinetic theory of dense, heterogeneous fluids remains a difficult subject to this day. A similar statement applies to complex flows with interfaces often encountered in science, engineering, soft matter and biology. A particularly interesting framework to deal with such complex flows is provided by density functional theory (DFT). Essentially the idea is that much of the physics of the complex many-body problem associated with dense fluids can be explored by investigating the dynamics of the fluid density, namely a single one-body scalar field. Of course, such dynamics is subject to self-consistent closures, typically in the form of well-educated guesses on the generating functional from which the effective one-body equation for the density can be derived via standard functional minimization of the suitable free-energy-functional (FEF). Density functional theory has met with spectacular success for the case of quantum many body problem, leading to the development of powerful theorems and attending computational methods that still form the basis for modern Nobel-prize winning computational quantum chemistry. [7]. The classical version, albeit less spectacular than its classical counterpart, also provides a

milestone framework to describe an simulate complex flows with interfaces, which we now proceed to illustrate in some more detail [6].

2 Density Functional Kinetic Theory

In the framework of kinetic theory, the main ingredient is the non-ideal force associated with the forced-streaming term $\hat{S} = F_a[\rho]\partial_{v_a} f.$, where F_a is a density-dependent mean field force and latin indices run over spatial dimensions.

The natural question is: why would the kinetic formulation be computationally advantageous over the hydrodynamic one?

The main point is that in the kinetic framework the term S can be brought to the right hand side and treated as a soft-collision term. Note that the partial derivative in velocity space is handled by integrated by parts, This permits to move the distribution function along unperturbed, force-free (straight) characteristics $dx_v = vdt$ and include the effect of soft forces as a local correction/perturbation to this free-streaming motion.

In equations:

$$f(x + vdt, v, t + dt) - f(x, v, t) = (C - S)dt \tag{1}$$

where $\hat{C}$ stands for standard short-range collisions, and vector indices have been omitted for simplicity. A very popular choice is the single-time relaxation Bhatnagar-Gross-Krook model

$$C = (f^{eq} - f)/\tau$$

where f^{eq} is the local equilibrium and τ the relaxation time. The soft-collision term is conveniently turned into an algebraic source term

$$S = F[\rho] \sum_k s_k H_k(v),$$

by integrating by parts in velocity space and exploiting recurrence relations of tensor Hermite polynomials [2, 3].

The advantage of the above formulation is that the streaming step at the left hand side proceeds along constant characteristics, hence it is *exact*, i.e. zero round-off error in the numerical treatment. This stands in contrast with the hydrodynamic formulation in which information moves along spacetime dependent material lines defined by the fluid velocity itself, $dx_u = u(x, t)dt$.

This simple but key advantage lies at the heart of the success of lattice kinetic techniques and most notably Lattice Boltzmann method, in which the characteristics are restricted to a suitable set of discrete velocities $\{v_i\}, i = 0, N_v$, showing sufficient symmetry to recover the correct large scale hydrodynamic limit.

Differently restated, the highly complex physics of moving interfaces is entirely absorbed within the local source S.

Clearly, such perturbative treatment is limited to sufficiently weak forces, as gauged by the so-called cell-Froude number

$$Fr = \frac{adt}{v}$$

where a is the acceleration due to the non-ideal forces. In order to preserve the stability of the numerical scheme, the time-step must be chosen such that $Fr \ll 10^{-3}$, a condition which may eventually go broken in the presence of strong density gradients. This problem

can be mitigated by improving the time-marching scheme, typically via locally implicit formulations, but it must be watched carefully case by case.

Lattice DFKT as discussed above is currently being used over an amazingly broad spectrum of soft-fluid problems, definitely beyond the original realm of rarefied gas dynamics.

3 Lattice Formulations

The first lattice transcription of the free-energy functional has been proposed back in the mid 90's [1]. The main idea is to write the collision operator in single-relaxation form, i.e. $C = -(f - f^{eq})/\tau$, where f^{eq} is the Maxwell-Boltzmann equilibrium, and incorporate the effect of the soft term S within a generalized non-local equilibrium, reflecting teh non-locality of the Korteweg tensor. Ever since its inception, it has generated a wide body of interesting results, especially in multiphase microfluidics.

An alternative and possibly more straightforward route is to connect with is to write the non-ideal pressor directly in the form of a two-body convolution:

$$P_{ab}(x) = \int r_a \psi(x - \frac{r}{2}) G(x, r) \psi(x + \frac{r}{2}) r_b dr \tag{2}$$

where $G(x, r)$ is the two-body density correlator and $\psi(\rho)$ is a local functional of the density.

At variance with the free-energy approach, the correlator is designed top-down, i.e. by reverse-engineering the expression of $G(x, r)$ so as to obtain the desired physical phenomena, namely i) Non-ideal EoS, ii) Tunable surface tension, iii) Positive disjoining pressure.

The earliest and still very popular such top-down formulation is due to Shan-Chen [5] and makes use of just a single parameter correlator, taking the value G_0 within the first Brillouin lattice cell and zero elsewhere.

The Shan-Chen model has been subsequently extended in many directions, including the formulation of multi-range models designed to simulate dry foams and moderatley dense emulsions.

When it comes to dense emulsions, spurious effects have been reported on the disjoining pressure, due to lack of sufficient lattice symmetry.

To this regard, a very fruitful avenue turned out to be offered by a entirely rule-driven approach, based on the so called *Color Gradient* technique ("color" is just a mnemonics for different chemical species or different phases of the same species, in analogy with quantum chromodynamics). Essentially the idea is to add an explicit anti-diffusive flux sending particles of each species uphill along their density gradient instead of against it. By construction, such anti-diffusive flux helps interface formation against the coalescing effect of surface tension. here too, the parameters can be adjusted to recover the properies i)-iii) above independently.

In the lattice chromodynamics models for multicomponent flows, two sets of distributions functions(let's say red and blue) are introduced to code for two different fluids.

$$f_i^k(\mathbf{x} + \mathbf{c}_i, t + 1) = f_i^k(\mathbf{x}, t) + \Omega_i^k(\mathbf{x}, t) \tag{3}$$

In the above equation, $k = R, B$ denotes the fluid and Ω_i^k is a collision operator which can be written as the combination of three sub-collisional.

$$\Omega_i^k = (\Omega_i^k)^3[(\Omega_i^k)^1 + (\Omega_i^k)^2] \tag{4}$$

where $(\Omega_i^k)^1$ is the BGK collisional, $(\Omega_i^k)^2$ is a two-phase collision operator, generating an interfacial tension between the two immiscible components and $(\Omega_i^k)^3$ is an anti-diffusive operator which favours phase segregation and keeps interfaces sharp.

To note that, the stress-jump condition across the fluid interface, induced by the perturbation operator, can be augmented with a suitable repulsive term aiming at modelling the effect of short-range, repulsive near-contact forces induced by the presence of surfactants and colloids adsorbed at the fluid-fluid interface. The additional repulsive term can be added efficiently in the LB framework via a forcing term localized at the interface:

$$\mathbf{F}_{rep} = A_h[h(\mathbf{x})]\mathbf{n}\delta_\Sigma \tag{5}$$

the interested reader is referred to [4] and related literature.

4 Soft matter applications

As a an application, we show the capability of the multicomponent model with near-contact interactions to reproduce the formation of ordered droplets clusters in microfluidic channels. In figure 4(a) we reported the formation of multilayer hexagonal droplet

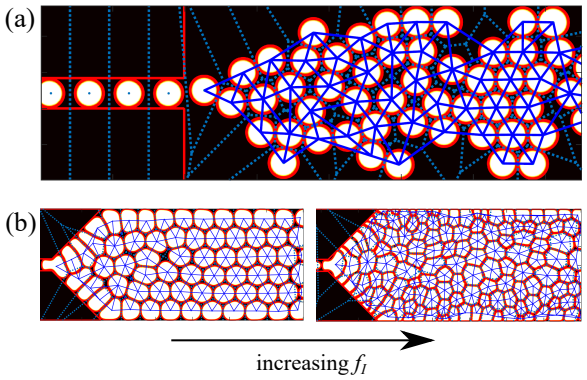

Figure 1: (a) Multi layer hexagonal droplets clusters in a microfluidic channel. Dashed lines represents Voronoi tessellation while solid lines Delaunay triangulation (b) Droplet self-assemblies within a microfluidic channel with a divergent opening angle $\alpha = 45°$ for two different inlet channel Capillary numbers ($Ca = 0.04$ left, $Ca = 0.16$ right).

clusters in a channel formed by a thin inlet and an outlet chamber. The droplets are continuously injected within the main channel by employing a recently developed internal periodic boundary condition. To note that the sponstaneous ordering of the droplets into hexagonal clusters is drive by a non trivial competition between local, short-range, repulsive interactions (i.e., the near-contact forces) and the surface tension.

In particular, small disturbances introduced by the short-range repulsive action of the near-contact interaction forces trigger the rupture of the initial, single-file crystal symmetry, driving the droplets towards a new spatial arrangement.

It is interesting to note that the process described above is somehow similar to the instability observed in densely packed granular materials subjected to force unbalances.

In panel (b) of figure 4 we reported the formation of dense emulsions in microfluidic devices formed by a divergent inlet channel connected to a downstream channel. Even in

this case the droplets are continuously injected within the system and let free to assemble within the outlet channel. By simply tuning the inlet capillary number it is possible to observe a spontaneous transition from a high-ordered emulsion, formed by hexagonal clusters flowing within the system (i.e. a wet emulsion) to a foam-like, dry-state, structure which results in a neat distortion of the Delauney triangulation (blue solid lines connecting thecenters of neighboring droplets).

In the simulations, both the dispersed and continuous phases' discharges are kept constant and the Ca is changed via the surface tension. The observed transition is likely to by due to (i) the breakup processes downstream the injection channel, promoting the formation of liquid films and (ii) the increased deformability of the droplets interface, due to the lower values of surface tension employed.

5 Conclusions

Summarising, lattice formulations of density functional kinetic theory provide a powerful theoretical and computational framework great for the numerical studies of complex flowing soft matter systems.

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Minisymposia

MS-1
New trends in Numerical Analysis: Theory and Applications - Part I

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The first part of this minisymposium, dedicated to Professor Mauro Diligenti in the occasion of his retirement, will be focused on recent theoretical and applicative aspects of Numerical Analysis, outlined by some of his friends, who gladly accepted to give their contribution.

Time-spectral solution of differential equations

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In this talk, the main aspects on the use of spectral methods for the efficient numerical solution of evolutionary problems will be briefly outlined. Their main feature is the ability of obtaining full machine accuracy approximations to the solution, despite the use of (relatively) large time-steps. This approach, at first devised for solving highly-oscillatory problems [1], has then been extended to deal with the numerical solution of Hamiltonan PDEs [2], general ODE-IVPs [3], and fractional ODEs [4]. A theoretical error analysis for the methods has been given in [5]. It must be stressed that the effective use of the methods has been made possible by the availability of the very efficient nonlinear iteration introduced in [6, 7].

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Virtual element analysis of the equilibrium of an immersed rigid body

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The Virtual Element Method (VEM) is a recent numerical technology introduced in [1, 2] for the discretization of problems governed by partial differential equations. It can be regarded as a generalization of the Finite Element Method (FEM) to meshes of general polytopes. Since its inception, the VEM enjoyed a wide success in the mathematics and engineering communities, because of its flexibility and robustness with respect to mesh design and handling.

The class of fluid-structure and immersed boundary problems is practically relevant and offers attractive possibilities and challenges to VEM and general polytopal meshes due to the interaction of different, perhaps deforming, domains. One could think, for instance, of using a fixed background grid for the fluid domain (Eulerian description), which is cut by a deforming solid at each time instant or iterative procedure step (Lagrangian description). Clearly, arbitrary mesh cuttings may generate polygonal elements of very bad quality (in terms of element anisotropy, possible non convexity, neighbor size ratio, etc.) and thus the numerical scheme must be reliable also in the presence of such hazards.

In order to explore the capabilities of a VEM for an immersed boundary problem and study its robustness and accuracy, we propose a simple 2D model problem inspired from the FEM analysis in [3]. The problem is that of a hinged rigid structure (a leaflet) of thickness ϵ with a rotational spring attached, immersed in a stationary incompressible fluid within a rigid channel (see Figure 1); all data are constant in time. We consider two extreme cases: the *fat leaflet* ($\epsilon > 0$), which is the most physically realistic case, and the *thin leaflet* ($\epsilon = 0$), which is the asymptotic limit of the former.

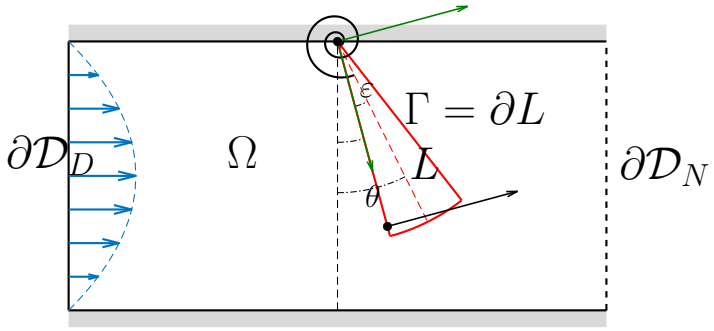

Figure 1: Leaflet immersed in a fluid

The equilibrium position of the leaflet corresponds to a balance between the angular momentum exerted by the rotational spring on the leaflet and the torque exerted by the fluid on the leaflet as a function of its angular position θ relative to the vertical axis. This problem is nonlinear because the torque depends on θ in an intricate nonlinear fashion. Its numerical approximation requires nonlinear iterations and thus entails solving the fluido-dynamics problem for several arbitrary leaflet positions. This leads to various fundamental issues, both theoretical and computational, that have to be resolved to get a reliable and accurate numerical method.

Firstly, we investigate the well-posedness of the exact problem, using shape differential calculus to analyze the torque functional. Next, we discretize the problem using the divergence-free VEM of degree $k = 1, 2$ for the Stokes fluid proposed in [4]. The background uniform grid of quadrilaterals is cut be the leaflet, generating polygons with extremely degenerate shapes; they can be handled without problems by the VEM approach. We investigate the approximation properties of the ensuing discrete torque functional and prove a quasi-optimal first-order error estimate, uniform in θ. Finally, we illustrate the performance of the method by several numerical experiments.

We refer to [5] for further details.

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A saddle point formulation for linear viscoelastic analysis by Boundary Integral Equations

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The first true variational formulation for initial value problems dates back to Gurtin's work [6], [7], [8], and [10]. It is based on the use of time-convolutive integrals and it is valid for a large class of linear time-dependent problems, including viscoelasticity, elastodynamics and the heat conduction problem.
It should be emphasized that Gurtin's variational principles and relevant generalizations are not saddle point principles or extremum principles. The convolutive bilinear form was also used to obtain variational formulations in space and time for the viscoelastic, elastodynamic and heat conduction problem, written in terms of boundary integral equations [2], [3], [4] and [9].
We present a symmetric, double-integration-based boundary integral equation approach to linear viscoelastic analysis in the time domain. In particular, we develop a formulation of BIE viscoelastic analysis based on time-dependent Green's functions [1] for both static and kinematic discontinuities, Stieltjes time-convolutions, and two consequent variational characterizations (of Gurtin's type) of the boundary solutions. The former concerns the history of the boundary unknowns over an arbitrary time interval; the latter is a saddle point theorem and it holds only when the time interval is large enough or, at the limit, goes to infinity. Following the approach used in [5], the new variational formulations are gathered from the decomposition of the time interval of interest into two subintervals of equal length. Separating the variables defined over the first subinterval from those related to the second one, we obtain a formal doubling of the unknowns. It is shown that the part of functional concerning the unknowns on the first time subinterval has the meaning of the Helmholtz free energy. It is also shown that the first functional is minimum with respect to the kinematic variables on the first time subinterval, maximum to the static variables on the first time subinterval and only stationary with respect to both static and kinematic variables on the second time subinterval. This functional turns into the second one of the saddle point type when the creep rate under step stress loading tends to zero in the second time subinterval.

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Fourier and Lagrange operators. Some remarks

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The Fourier operator and its discrete version are important tools in Approximation Theory and Numerical Analysis.

In this short talk I will show some related problems in different contexts.

On the Discrete Time Convolution - Space Collocation BEM for the Numerical Solution of Wave Propagation Problems in Unbounded Domains

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After recalling the (Time) Discrete Convolution Quadrature (TDCQ) obtained by Ch. Lubich in 1988 [7], we briefly describe recent coupling of it with a classical space collocation Boundary Element Method (BEM), that have been proposed and examined by S. Falletta, G.M. and L. Scuderi, to solve some 2D wave propagation problems in unbounded domains. These include problems defined by the classical wave equation [2][3], as well as linear elastodynamics problems [5]. For the latter, after performing the classical Helmholtz decomposition, the above TDCQ-BEM discretization was also applied to an alternative formulation of the elastodynamics equation, obtained by decomposing the latter into an equivalent couple of wave equations. This decomposition was proposed in [1] for the solution of an interior problem by means of a finite element method.

The above approach has also been used to define a non reflecting boundary condition [4], which then allows to solve, in the bounded region of interest, the original PDE problem by means of a finite element method.

However, while in the above cases, stability and convergence have been proved for the discrete convolution - Galerkin BEM numerical scheme [8] (see also [6]), for the collocation case we only have numerical evidences that these properties hold. We will however show that, both in the 2D and in the 3D case, the collocation approach is equivalent to a discretization of the corresponding Galerkin one, obtained by approximating the inner product integral by a proper quadrature rule. In the 2D case, some results are then derived for the collocation linear system.

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A Nyström method for second kind Fredholm integral equations based on anti-Gauss quadrature rules

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Anti-Gauss quadrature rules (QRs) were proposed by D. P. Laurie in [2]. They provide an approximation of an integral whose error has the same magnitude as the error of the Gauss QRs and opposite sign, under suitable assumptions on the integrand function. We introduce a Nyström type method based on Anti-Gauss QRs for the solution of Fredholm integral equations of the second-kind, which is both stable and convergent [1]. We show that the Nyström interpolants based on the Gauss and the anti-Gauss QRs bracket the solution of the equation under weak assumptions, for a particular weight function. Numerical results are presented.

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MS-2
New trends in Numerical Analysis: Theory and Applications - Part II

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The second part of the minisymposium, dedicated to Professor Mauro Diligenti in the occasion of his retirement, will involve new contributions in the field of Numerical Analysis and its applications, presented by some of his alumni who then embarked on academic career or reached a leading position in industrial companies.

FEM uncommon applications in steel structures design

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The research of new and amazing shapes in the architectural design or new technological applications forces the structural engineering to find and carry out new ways, new materials and new numerical calculations to create them, since the physical problem hides non linear and unusual issues that the FEM technique helps to solve.
In this respect, we show three interesting case studies: a dry dock's roller roof, a complex 3D steel connection in between timber beams and concrete columns, and a large tent covering a square.
In each one, the use of commercial FEM software, leaded by a deep analysis, lets us solve several difficult and detailing problems such as: wind distribution loads around curvilinear surface, monolateral constraint, contact surfaces, buckling load factor.

ACA based acceleration of the Energetic Galerkin BEM for 2D wave propagation problems

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We consider scalar and vector wave propagation problems in 2D unbounded domains, reformulated in terms of space-time Boundary Integral Equations (BIEs). For their solution, we employ a weak formulation related to the energy of the system and we solve them by a Galerkin-type Boundary Element Method (BEM): this energetic approach allows to overcome the instabilities rising from the discretization of the standard weak formulation applied to this kind of integral problems [1, 2]. However it results that, when standard Lagrangian basis functions are considered, the BEM matrices have Toeplitz lower triangular block structure, where blocks are in general fully populated, and the overall memory cost of the energetic BEM is $O(M^2N)$, M and N being the number of the space degrees of freedom and the total number of time steps performed, respectively. This drawback prevents the application of such method to large scale realistic problems. As a possible remedy, we propose a fast technique based on the Adaptive Cross Approximation (ACA) [3]. The core of this procedure is the approximation of sufficiently large time blocks of the energetic BEM matrix through the ACA algorithm, which allows to compute only few of the original entries. This leads to reduced assembly time, which for the energetic BEM is generally relevant, coupled with reduced memory storage requirements. Additionally, the consequent acceleration of the matrix/vector multiplication together with a marching in time procedure, leads to remarkable reduction of the computational solution time. The effectiveness of the proposed method is theoretically demonstrated and several numerical results are presented and discussed.

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Energetic Galerkin BEM for 2D elastodynamic exterior problems with Neumann conditions: comparison between direct and indirect formulations

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The purpose of this work is to study by Boundary Element Method (BEM) the propagation of elastic waves throughout a 2D unbounded domain Ω_e, which could be external to an open arc Γ, namely $\Omega_e = \mathbb{R}^2 \setminus \Gamma$, or complementary to a set Ω_i with Lipschitz closed boundary $\Gamma = \partial\Omega_i$, namely $\Omega_e = \mathbb{R}^2 \setminus \overline{\Omega_i}$. The mathematical problem is governed by Navier equation, having as unknown the vectorial displacement $\mathbf{u}(\mathbf{x}, t) = (u_1, u_2)^\top(\mathbf{x}, t)$. Implementation of BEM requires to express the unknown $\mathbf{u}$, assuming vanishing initial conditions and null external body forces, by means of the following integral representation formula

$$\mathbf{u}(\mathbf{x}, t) = \int_\Gamma \mathbf{G}^{uu}(\mathbf{x}, \boldsymbol{\xi}, \cdot) *^{(t)} \mathbf{p}(\boldsymbol{\xi}, \cdot) d\Gamma_{\boldsymbol{\xi}} - \int_\Gamma \mathbf{G}^{up}(\mathbf{x}, \boldsymbol{\xi}, \cdot) *^{(t)} \mathbf{u}(\boldsymbol{\xi}, \cdot) d\Gamma_{\boldsymbol{\xi}}, \quad (\mathbf{x}, t) \in \Omega_e \times (0, T], \tag{1}$$

where $*^{(t)}$ indicates a convolution product in time. We observe that in formula (1) the 2D fundamental elastodynamic solution $\mathbf{G}^{uu}$, defined by components as follows

$$G^{uu}_{ij}(\mathbf{x}, \boldsymbol{\xi}; t, \tau) = \frac{1}{\rho c_{\mathrm{P}}} \frac{1}{2\pi} H[c_{\mathrm{P}}(t-\tau) - r] \left[\frac{2c_{\mathrm{P}}^2(t-\tau)^2 - r^2}{\sqrt{c_{\mathrm{P}}^2(t-\tau)^2 - r^2}} \cdot \frac{r_i r_j}{r^4} - \frac{\delta_{ij}}{r^2} \cdot \sqrt{c_{\mathrm{P}}^2(t-\tau)^2 - r^2} \right]$$
$$- \frac{1}{\rho c_{\mathrm{S}}} \frac{1}{2\pi} H[c_{\mathrm{S}}(t-\tau) - r] \left[\frac{2c_{\mathrm{S}}^2(t-\tau)^2 - r^2}{\sqrt{c_{\mathrm{S}}^2(t-\tau)^2 - r^2}} \cdot \frac{r_i r_j}{r^4} - \frac{\delta_{ij}}{r^2} \cdot \frac{c_{\mathrm{S}}^2(t-\tau)^2}{\sqrt{c_{\mathrm{S}}^2(t-\tau)^2 - r^2}} \right], i, j = 1, 2,$$

and the fundamental traction $\mathbf{G}^{up}$ are involved. For both functions, the dependence on the space variables is given only by the differences $r_i = x_i - \xi_i$, $i = 1, 2$, and the distance between the source and the field points $r = \|\mathbf{x} - \boldsymbol{\xi}\|_2$. The constants c_P and c_S are the phase speeds of the pressure and the shear waves, typical of elastodynamic problems, ρ is a mass density and $H[\cdot]$ is the Heaviside function.
Our goal is to solve hard scattering problems and, to do that, we apply the Hooke tensor

to formula (1) and we execute a limit in space from $\mathbf{x} \in \Omega_e$ to $\mathbf{x} \in \Gamma$, in order to obtain the following *Boundary Integral Equation* (BIE)

$$\frac{1}{2}\mathbf{p}(\mathbf{x},t) = \int_\Gamma \mathbf{G}^{pu}(\mathbf{x},\boldsymbol{\xi},\cdot) *^{(t)} \mathbf{p}(\boldsymbol{\xi},\cdot) d\Gamma_{\boldsymbol{\xi}} - \int_\Gamma \mathbf{G}^{pp}(\mathbf{x},\boldsymbol{\xi},\cdot) *^{(t)} \mathbf{u}(\boldsymbol{\xi},\cdot) d\Gamma_{\boldsymbol{\xi}}, \quad (\mathbf{x},t) \in \Sigma = \Gamma \times (0,T], \tag{2}$$

where the traction $\mathbf{p}$ corresponds to the Neumann datum assigned on Σ. The operators depending on the 2D tensors $\mathbf{G}^{pu}$ and $\mathbf{G}^{pp}$ are identified in literature as *double layer* and *hypersingular* integral operators, respectively. BIE (2) is reformulated in a weak form linked to the energy $\mathcal{E}(\mathbf{u},T)$ of the elastodynamic system and we solve it by a Galerkin-type technique, in order to reconstruct $\mathbf{u}$ at the boundary and, subsequently, to replace it in the representation formula (1). This kind of energetic approach has been already theoretically analyzed for the scalar wave problem in [1] and also proposed for soft scattering elastodinamic problem in [2], providing, in both contexts, excellent long time stability results. Note that, in order to solve hard scattering problems, we can use also the indirect BIE

$$\mathbf{p}(\mathbf{x},t) = -\int_\Gamma \mathbf{G}^{pp}(\mathbf{x},\boldsymbol{\xi},\cdot) *^{(t)} \boldsymbol{\psi}(\boldsymbol{\xi},\cdot) d\Gamma_{\boldsymbol{\xi}}, \quad (\mathbf{x},t) \in \Sigma = \Gamma \times (0,T], \tag{3}$$

in the unknown vector density $\boldsymbol{\psi}$, involving only the hypersingular integral operator. Also the equation (3) can be set in energetic weak form.

Discretization in time-domain of the energetic weak formulation, applied to either direct or indirect strategy, leads to the resolution of a linear system with a block lower triangular Toeplitz matrix. The core of the entire method is the computation of the matrix entries: after an analytical time integration, these are expressed as the sum of double space integrals over Γ, with a kernel, deriving by the discretization of the hypersingular operator, characterized by a space singularity of order $\mathcal{O}(1/r^2)$. The use of specific product quadrature formulas is therefore necessary to guarantee a correct approximation of these integrals (see [3]).

Moreover, the integration domains, in local variables, have a geometry strictly connected to the values of the velocities c_P, c_S and other spatial and temporal discretization parameters: the study of the shape of the integration domains is fundamental in order not to treat directly the discontinuous Heaviside functions, deriving from the definition of the fundamental solution $\mathbf{G}^{uu}$.

In case of direct formulation, similar integration methodologies can be used to construct the right-hand side of the system, which can be computed as a matrix-vector product of the discretized double layer operator by a column vector depending on the Neumann datum. The matrix entries, in this case, are characterized by a space singularity of order $\mathcal{O}(1/r)$.

The proposed quadrature strategies allow to improve the efficiency and the effectiveness of the entire method, that can be further speeded up by the parallel computing technique. Application of the energetic BEM to elastodynamics benchmark problems will be presented and discussed.

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Chemo-mechanical degradation of monumental stones

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The aim of this work is to study the degradation of monumental stones under the combination and the mutual interaction between mechanical actions and environment/pollution conditions. In particular the stone degradation has been estimated as a function of the environmental conditions and the prediction of damaging phenomena, which can compromise permanently the fruition and/or the stability of the monuments.

A macroscopic phenomenological model has been developed that couples the main aspects of the problem: the chemical reaction and the mechanical behavior of stones. In particular, the sulphation reaction and the diffusion of the pollutant agents will be described by suitable mathematical equations that will be coupled to a variational formulation of the fracture mechanics. The proposed model permits to evaluate how much aggressive atmospheric agents contribute to the decay of the mechanical properties of the stones as well as to establish the impact of the synergic chemical aggression and stress state. This latter will also be influenced by the chemical reaction and by the evolving mechanical properties of the material. The capability of the approach will be illustrated by specific numerical simulations.

Advances in inverse problem solvers, and optimally inverting waves

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Inverse problems arise whenever one is trying to recover a quantity of interest given some indirect and noisy measurements thereof. In the linear and discrete case, inverse problems involve the solution of linear systems of equations, whose coefficient matrices are ill-conditioned and whose right-hand-side vectors are perturbed: in these situations, 'naive' solution(s) cannot be trusted (Prof Diligenti lectured me about this is my first Numerical Analysis course about 15 years ago) and some form of regularization should be employed; see, e.g., [3].

In this talk I will describe some of the issues encountered when solving large-scale inverse problems, mainly arising in imaging applications such as computed tomography in medicine. I will then describe some regularizing projection methods based on Krylov subspace methods, focusing in particular on regularization parameter choice rules that exploit the links between the symmetric Lanczos algorithm and Gauss quadrature (a topic that Prof Diligenti lectured me in my second Numerical Analysis course); see, e.g., [1]. I will conclude by formulating an optimal sensor placement problem for the full-waveform inversion method, which is used in geophysics to infer physical parameters of the underground given wavefront measurements; see, e.g., [2].

These are the results of joint collaborations with Shaunagh Downing, Ivan Graham, Malena Sabaté Landman, and Euan Spence, all from the University of Bath.

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High-order discontinuous Galerkin methods on polyhedral grids for wave propagation problems

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The study of direct and inverse wave propagation phenomena is an area of intensive research and find important applications in different engineering areas including acoustics, aeroacoustics, electromagnetics and computational seismology.
From the mathematical perspective, the physics governing these phenomena can be modeled by means of the wave equation. From the numerical viewpoint, a number of distinguished challenges arise when tackling such kind of problems, and reflect onto the following features required to the numerical schemes: accuracy, geometric flexibility and scalability.
In recent years, high order discontinuous Galerkin (dG) methods have became one of the most promising tool for the solution of wave propagation problems. Indeed, thanks to their local nature, dG methods are particularly apt to treat highly heterogeneous media, complex geometries and sharp variation of the wave field by allowing for space and time adaptivity within the approximation.
In this work we present a high-order dG finite element method for the approximate solution of wave propagation problems on computational meshes made by polyhedral elements. We analyze the well posedness of the resulting formulation, prove a-priori error estimates, and present a dispersion analysis, showing that polyhedral meshes behave as classical simplicial/quadrilateral grids in terms of dispersion properties. Finally, we present applications of the method to cases of geophysical interest.

Integral formulation for fracture propagation as a standard dissipative process: application to hydraulic fractures.

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Recent publications framed the problem of three-dimensional quasi-static crack propagation in brittle materials into the theory of standard dissipative processes [1]. Variational formulations, stated therein, characterize the three dimensional crack front quasi-static velocity 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 [2].

Although the theoretical setting is sound, the derived crack tracking procedures suffered from a major drawback that limited the interest in the method to its theoretical content. Specifically, the need of still currently unavailable accurate approximations for weight functions made the approach of minor interest from the numerical standpoint. Such a drawback was overcome in [3], where a viscous regularization of the fracture propagation in brittle materials was formulated. Rate-dependency provided a simple and accurate approximation of the crack front velocity, thus allowing to formulate effective crack tracking algorithms.

That idea is further developed here to model hydraulic fracture processes [4]. The problem is governed by a differential equation for the fluid response (the so-called lubrication equation) and by a hypersingular integral equation for the (unbounded) domain elastic response. Considering a symmetrically loaded penny shaped crack to exploit the axis symmetry of the problem, hypersingular integrals simplify and can be evaluated in polar coordinates along the radius of the circular crack. The singularity analysis has been carried out, with Hadamard finite parts evaluated analytically.

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. The formulation can be easily extended to elastodynamics following [5], and further to account for fractures pressurized by gas or other substances.

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MS-3
Soft tissue biomechanics: From experiments to mathematical modelling

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The last two decades have witnessed an explosion of scientific, medical and industrial activity in the area of "living tissues modelling", with a particular focus on biological soft tissues. Understanding the mechanics of soft tissues is an intriguing and, at the same time, a difficult task. The difficulty primarily arises from the strong multidisciplinary approach which is necessary to encompass multiscale, experimental and theoretical aspects at the same time.

On the one hand, rapid advances of experimental techniques have significantly improved the availability and accuracy of data on the behaviour of living tissues; on the other hand, this deeper insight seems to generate more questions than providing answers. What is becoming clear is the prominent role of mechanics at all scales, from the sub-cellular to the tissue level. However, foundational questions on the behaviour of living tissues remain largely unanswered to date. Their complex hierarchical behaviour, their mechanisms of growth and remodelling, the existence of preferred "homeostatic" states, the origin and role of residual stresses, altogether with their mathematical description, are only some of the open problems.

The aim of the proposed mini-symposium is to gather specialists in the field of soft tissues biomechanics, ranging from bio-physicists and applied mathematicians to mechanical

engineers to share their views on this vibrant research field. Due to the significant breadth of this matter, the community of researchers involved on these problems is rather sparse and heterogeneous: for this reason, we believe that a SIMAI minisymposium on this topic is a timely opportunity to help the circulation and discussion of very different ideas, which is a necessary step to advance this fundamental branch of applied mathematics.

C-looping of the Heart Tube

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Before septation processes shape its four chambers, the embryonic heart is a straight tube that spontaneously bends and twists breaking the left-right symmetry [1]. In particular, the heart tube is subjected to a cell remodelling inducing ventral bending and dextral torsion during the c-looping phase. We propose a morphomechanical model for the torsion of the heart tube, that behaves as a nonlinear elastic body. We hypothesize that this spontaneous looping can be modeled as a mechanical instability due to accumulation of residual stresses induced by the geometrical frustration of tissue remodelling, which mimics the cellular rearrangement within the heart tube. Thus, we perform a linear stability analysis of the resulting nonlinear elastic boundary value problem to determine the onset of c-looping as a function of the geometry of the tube and of the internal remodelling rate. We perform numerical simulations to study the fully nonlinear morphological transition, showing that the soft tube develops a realistic self-contacting looped shape in the physiological range of geometrical parameters.

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Extra-cellular matrix in multicellular aggregates acts as a pressure sensor controlling cell proliferation and motility

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A gentle compression (500 Pa) drastically reduces the growth rate of multicellular aggregates [1, 2, 3], whereas it has no impact on the same cells, when grown individually. A major difference between individual cells and multicellular aggregates is the presence of Extracellular Matrix (ECM), which is permeated by interstitial fluid and 1000-folds more compressible than cells. Thus, a gentle compression of multicellular aggregates mainly affects the ECM. Therefore, the ECM properties mainly determine the mechanical response of aggregates. Interestingly, the ECM compression has also a large impact on cell proliferation, migration and morphology[4]. We conclude that the ECM play the role of a pressure sensor in a multicellular context.

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Can the size of a growing object be determined through local controls alone?

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How does a cell in an organ know the overall size of the organ? It is thought that the *Drosophila* wing disc grows to the right size because its cells respond to both signalling proteins (morphogens) and mechanical stress. We investigate if size regulation can be achieved if cells respond exclusively to stress with an anisotropic growth response. To test this, we develop a continuum model which assumes the spatial uniformity of cell proliferation in the wing disc and predicts compression in the disc center, tension in its periphery, and a sigmoidal evolution of the disc size, all of which have been observed in experiments. However, while the purely local response to stress alone can lead to a smooth growth arrest, it does not allow to reliably fix the size of the final tissue. We introduce a mechanism that amends the currently most popular model of mechanical feedback, enabling to set the final size through purely local controls. Finally, we speculate on the nature of this mechanism and on its microscopic physical origin.

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A Mechanical Model for Glioblastoma Multiforme Growth including Brain Hyperelasticity and Patient-Specific Data

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Among the existing types of brain tumour, Glioblastoma Multiforme (GBM) is one of the most aggressive and malignant, as well as the most common. The origin of the suffix *multiforme* is eloquent: it was meant to describe the appearance and morphology of this cancer, which is characterized by necrosis, hemorrhages and cysts. Moreover, GBM frequently grows along the fibres of the white matter or along vessels, following the physical structures in the neighbouring healthy tissue. Depending on the amount of such features, GBM can take various shapes and may appear very different from an individual to another. In addition, this type of tumour exhibits a dramatic invasive potential and is very resistant to common therapies, due to its deeply infiltrating nature and its multi-scale heterogeneity.

For all these reasons, it is critical to understand and reproduce the biological complexity of brain tissue, in order to predict GBM progression and arrange therapeutic strategies efficiently. To this end, mathematical and computational models can provide powerful instruments for investigating cancer progression, especially in those cases which are particularly difficult to be treated with current therapeutic protocols. In the last decades, several models that describe brain cancer growth have been proposed, using different frameworks and accounting for different characteristics. However, the majority of these models does not include a proper mechanical and constitutive description of brain tissue. Instead, the presence of a growing solid mass may be critical and should be described as realistically as possible: an accurate prediction of stresses and deformations may be

helpful to predict the progression of GBM and to analyse the reorganization of healthy tissues occurring after surgical resection.

Concerning the mechanical characterization of brain tissue, which is very soft, fundamental advances have been made towards a constitutive description, despite the difficulties in performing experimental tests. Most of the works agree upon the highly nonlinear and viscoelastic or hyperelastic nature of the brain, and experiments by Budday et al. [2] established that despite the intrinsic microstructural anisotropy due to the presence of nerve fibers, the human brain tissue is nearly isotropic from a mechanical viewpoint.

Motivated by these observations and by the need to elaborate a richer description of GBM growth in patients, we present a mathematical multiphase model that explicitly includes brain hyperelasticity. This allows to evaluate the effects of structural alterations and nonlinear elastic deformations of the healthy tissue caused by the growing tumour mass. In particular, we consider the brain as a biphasic mixture composed by an ideal fluid phase and by a hyperelastic isotropic Mooney-Rivlin solid, whose parameters are derived from the experimental literature. Moreover, the tumour is represented by a steep mollification of an indicator function, and growth is described using the multiplicative decomposition of the deformation gradient to account for inelastic distorsions occurring in the process.

Then, following [1, 3], simulations of the mechanical model are performed on a realistic three-dimensional brain geometry, reconstructed from patient-specific Magnetic Resonance Imaging (MRI) and Diffusion Tensor Imaging (DTI) data. At the same time, thanks to the medical images, we are able to explicitly introduce the functional anisotropy of brain tissue in the equations, by building spatially dependent diffusion and fluid permeability tensors. Finally, the inclusion of a mechanical description of the tissue allows to employ the deformation to modify MRI and DTI data in time, accounting for variations due to GBM growth and to the impact on the surrounding tissue.

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A diffuse-interface model for epidermal wound healing

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The epidermal wound healing process is one of the most frequent phenomena occurring during the lifetime of an organism. To have a deeper understanding of the biological phenomenon, several mathematical models on the wound healing have been proposed in literature. In this talk, we present a new model for the wound closure which accounts for the interplay between two mechanisms: the crawling with lamellipodia protusions and the purse-string tension, as suggested from in vitro assays [3]. The proposed model consists of a Cahn-Hilliard-Brinkman system subject to the incompressibility constraint. The Cahn-Hilliard and the Brinkman equations are bidirectionally coupled and describe how the healthy and injured tissue evolve during the wound healing process. A perturbative analysis [2] of the model has been performed in order to show how the two mechanisms mentioned above act as external forces leading the wound edge movements. Finally, to validate the proposed model, numerical simulations based on finite element methods [1] were performed and the obtained results were compared with the ones from biological experiments.

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MS-4
New Trends and Applications in Approximation Theory - Part 1

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Approximation theory is a fundamental branch of mathematics studying approximation processes of general functions by simple building blocks as, for instance, polynomials, wavelets, finite elements or Fourier expansions. New developments in approximation

theory therefore have a deep impact on various other scientific fields as the numerical solution of partial differential equations, image processing, inverse problems, statistical computing or data analysis. For example, interpolation with splines and radial basis functions is an important technological tool in the geometric design of automotive and aerospatial vessels, while wavelets and their generalizations as curvelets and shearlets are fundamental tools in the compression of large digital images and videos. Recently, approximation methods have also been developed to obtain compressed sensing methods for the sparse representation of signals or to understand deep learning algorithms.

This minisimposium aims to provide a platform for senior and young researchers in the field of approximation in order to exchange ideas of their current research and to discuss new trends in this area. It is also intendend to be a meeting point for italian and foreign experts to provide new solutions for real-world and industrial approximation problems.

Data-driven extrapolation via feature augmentation for multi-exponential decay curves

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Data driven extrapolation requires the definition of a functional model depending on the available data and has the application scope of providing reliable predictions on the unknown dynamics. Since data might be scattered, we drive our attention towards kernel models that have the advantage of being meshfree. Precisely, the proposed numerical method makes use of the so-called Variably Scaled Kernels (VSKs) [1], which are introduced to implement a feature augmentation-like strategy based on discrete data [3]. Due to the possible uncertainty on the data and since we are interested in modelling the behaviour of the target functions, we seek for a regularized solution by ridge regression [4]. Focusing on polyharmonic splines, we investigate their implementation in the VSK setting and we provide error bounds in Beppo-Levi spaces. The performances of the method are then tested on functions showing exponential or rational decay and investigated on real data sets from nuclear magnetic resonance acquisitions in the context of food science [2].

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Solving Poisson Equation with Dirichlet Conditions Through Multinode Shepard's Operators

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The multinode Shepard operator is a linear combination of local polynomial interpolants with inverse distance weighting basis functions. This operator can be rewritten as a blend of function values with cardinal basis functions, which are a combination of the inverse distance weighting basis functions with multivariate Lagrange fundamental polynomials. The key for simply computing the latter, on a unisolvent set of points, is to use a translation of the canonical polynomial basis and the PA=LU factorization of the associated Vandermonde matrix. In this talk, we propose a method to numerically solve a Poisson equation with Dirichlet conditions through multinode Shepard interpolants by collocation. This collocation method gives rise to a collocation matrix with many zero entrances and a smaller condition number with respect to the one of the well known Kansa method. Numerical experiments show the accuracy and the performance of the proposed collocation method.

Rational Hermite interpolation on six-tuples and scattered data

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The main objective of this talk is to construct an approximant, with cubic precision and quartic approximation order, which interpolates functional values and first order derivatives on a set of scattered data. This approximant is a combination of six-point Shepard basis functions with rational interpolants based on six-tuples of nodes. An explicit expression of the remainder term and its bound are given depending on the shape of the hexagons. The numerical results show the efficiency and the accuracy of the proposed method, which is implemented by a fast algorithm that makes it useful in several domains of application.

Spherical data interpolation with positive preservation using radial kernels

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Recently, the spherical approximation of positive data by spherical spline was considered in [1]. Here we investigate the problem of constructing radial basis functions (RBFs) interpolants on the sphere preserving the data positivity. Such problem was already analyzed in the bidimensional setting and a solution was proposed using global [3] and local RBFs [2]. The motivation is given by the several natural phenomena that are range restricted, for example amount of rain, humidity or pollution.

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Multi-dimensional Dirac delta Approximations for Uncertainty Quantification in Singular Source term Flows

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In this work, we analyze the steady flow generated by a line-source within a geological formation, modelled as a random space function; and as a consequence, flow variable becomes random fields [3]. Fluid flow in heterogeneous porous media is modeled by treating hydraulic conductivity as a stationary random space function. The flow variables, the pressure head, and the velocity field are also random functions, and we are primarily concerned in finding their mean values, by quantifying their uncertainty with Monte-Carlo simulations. Singular terms in differential equations present significant difficulties for numerical approximations on regular grids [1]. Steady flow take place in a d-dimensional unbounded domain Ω^d. The velocity field and the hydraulic head h obey a mass conservation equation

$$\nabla \boldsymbol{v} = -\delta(\boldsymbol{x}),$$

where $\delta(\boldsymbol{x})$ represent a source or a sink; and a Darcy's law

$$\boldsymbol{v} = -K\nabla h.$$

This gives rise to

$$\nabla \cdot [K(\boldsymbol{x})\nabla h(\boldsymbol{x})] = \delta(\boldsymbol{x});$$

and when K is constant, $K\nabla^2 h(\boldsymbol{x}) = \delta(\boldsymbol{x})$, the fundamental solution for this heat equation is known [2]. However, convection terms, time dependence and random based fields need numerical simulations, and a major concern is to select the appropriate approximation for the Dirac delta function $\delta(\boldsymbol{x})$ [1, 4].
More in detail, we replace the Dirac delta function δ by a more regular function δ_ϵ, that may be employed on ordinary computational grids to solve differential equations with singular source terms; we are, in particular, interested in multi-dimensional delta functions. Finally, we presented a survey and examined how effectively different Dirac approximations, when combined with PDE numerical solvers, can reliably match a known solution, as well as how they perform in the uncertainty scenario.

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The use of Approximation Theory in an ongoing industrial application

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In this talk we relate the experience gained during a stage activity in the Finder SpA company, aimed at the redaction of a Master thesis. The industrial application consists essentially of a heating system control problem. As a first step, we try to model the simulation of the temperature changes in an apartment. In this phase, the fitting of functional data coming from actual temperature measurements is required. The difficulty lies in the accommodation within the mathematical framework of "sudden" unexpected events, that abruptly change the measured values, such as openings of doors and windows. These phenomena are therefore difficult to interpolate, as both their timings, duration and intensities are unknown. The clever use of the approximation schemes devised in the algorithm allows however to successfully capture the properties of the data during these phenomena. A suitable combination of the values of the function and its derivative constitute the basic approximation tool in this context. Some examples will be presented. Future perspectives will also been broadly discussed.

MS-5
New Trends and Applications in Approximation Theory - Part 2

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Approximation theory is a fundamental branch of mathematics studying approximation processes of general functions by simple building blocks as, for instance, polynomials, wavelets, finite elements or Fourier expansions. New developments in approximation theory therefore have a deep impact on various other scientific fields as the numerical

solution of partial differential equations, image processing, inverse problems, statistical computing or data analysis. For example, interpolation with splines and radial basis functions is an important technological tool in the geometric design of automotive and aerospatial vessels, while wavelets and their generalizations as curvelets and shearlets are fundamental tools in the compression of large digital images and videos. Recently, approximation methods have also been developed to obtain compressed sensing methods for the sparse representation of signals or to understand deep learning algorithms.

This minisimposium aims to provide a platform for senior and young researchers in the field of approximation in order to exchange ideas of their current research and to discuss new trends in this area. It is also intendend to be a meeting point for italian and foreign experts to provide new solutions for real-world and industrial approximation problems.

Second kind Volterra integral equations: a Nyström method in weighted spaces of continuous functions

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This talk aims at describing a Nyström method for the following second kind Volterra integral equation

$$f(y) + \int_{-1}^{y} k(x,y) f(x)(y-x)^{\alpha}(1+x)^{\beta} dx = g(y), \quad y \in (-1,1),$$

where $\alpha, \beta > -1$, f is the unknown solution and k and g are given functions defined on $(-1,1) \times (-1,1)$ and $(-1,1)$, respectively.

The pathology of this equation is due to the kernel which can be singular along the boundary $y = x$, as $y \to x$, and along the side $y = -1$, as $y \to -1$. Consequently, the solution f inherits a weak singularity at $y = -1$, even if the right-hand side function g is smooth.

Because of this singularity, in order to obtain accurate results, many numerical methods available in the literature are based on regularization techniques which transform the initial equation into another one, having smoother solution.

Here, in order to skip the use of smoothing transformations, we consider the equation in spaces of weighted continuous functions endowed with the uniform norm.

Specifically, we develop a Nyström method based on a stable and convergent product integration rule. The method leads to a well-conditioned linear system whose solution allows us to construct the Nyström interpolant. Under suitable assumptions, we prove the stability and the convergence of the method. An error estimate is provided and several numerical tests are given to show the accuracy of the method and its performance compared with other methods.

A linear barycentric interpolant on two-dimensional starlike domains

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Consider the trigonometric barycentric interpolant of an arbitrary 2π-periodic function between equidistant points in $[0, 2\pi)$, it converges exponentially when the nodes are images of equidistant points under a periodic conformal map.

We present a bound for the Lebesgue constant of the trigonometric barycentric interpolant for a class of nodes, called *periodic well-space nodes*, derived from the non periodic family introduced by Bos et al. in [2]. These nodes guarantee a logarithmic growth of the constant and they also includes periodic conformal mapped nodes as the ones constructed with the map introduced in [1].

After that, we introduce a method for interpolating a function via a tensor product of barycentric rational interpolants in starlike domains inside a Jordan curve, and we propose a method for approximating a function also inside a non-smooth curve.

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Identification of different meditation sessions by LDA analysis of reconstructed brain activity maps

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The MEG inverse problem aims at localizing the neural sources responsible for the neuroelectric activity inside the brain. The primary unknown is the current density flowing inside the head. The neural current is modeled as a sum of current dipoles located on the source spaces, i.e., the vertices of the triangulation of the brain obtained by segmentation of the MRI. The data is the magnetic field measured by sensors located on a helmet put on the head.

The inverse problem can be reformulated in the Bayesian setting assuming that both moment and variance of each dipole are not fixed a priori, but are modeled as random variables. In particular, the dipole variances are assumed to follow a non-conjugate gamma distribution with variable scaling and shape parameters that allow us to control the shape of the neural sources. Thus, the MEG inverse problem can be solved by an iterative alternating sequential (IAS) algorithm that uses a Krylov subspace iterative method at each iteration step.

We use the IAS algorithm to reconstruct the neural activity maps of Buddhist monks practicing focused attention (Samatha) and open monitoring (Vipassana) meditation. Then, we use the linear discriminant analysis (LDA) to separate the different states and to identify the brain regions that contribute to the separation. Our findings are supported by meditation studies available in the literature.

This is a joint work with D. Calvetti, A. Pascarella, E. Somersalo, B. Vantaggi.

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Filtered integration rules for the finite Hilbert Transform

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Let $u(x) = v^{\gamma,\delta}(x) := (1-x)^\gamma(1+x)^\delta$, $\gamma, \delta > -1$, be a Jacobi weight and let

$$\mathcal{H}^u f(t) = \int_{-1}^{1} \frac{f(x)}{x-t} u(x)dx = \lim_{\epsilon \to 0} \int_{|x-t|\geq \epsilon} \frac{f(x)}{x-t} u(x)dx, \qquad -1 < t < 1,$$

be the finite Hilbert transform in $[-1, 1]$.

Fixed another Jacobi weight $w(x) = v^{\alpha,\beta}(x)$, and the corresponding orthonormal sequence $\{p_j(w)\}_j$, we propose a new quadrature rule for $\mathcal{H}^u f$, by approximating f with the filtered de la Vallée Poussin (VP) polynomial defined as:

$$V_n^m(w, f, x) = \sum_{k=1}^{n} f(x_k)\Phi_{n,k}^m(x), \qquad 0 < m < n,$$

where $\{\Phi_{n,k}^m\}_{k=1:n}$ are the fundamental VP polynomials

$$\Phi_{n,k}^m(x) = \lambda_{n,k}(w) \sum_{j=0}^{n+m-1} \mu_{n,j}^m p_j(w, x)p_j(w, x_k),$$

$\lambda_{n,k}(w)$ and x_k being the Cristhoffel numbers and the zeros of $p_n(w)$ respectively and $\mu_{n,j}^m$ are the following filters

$$\mu_{n,j}^m := \begin{cases} 1 & \text{if} \quad j = 0, \ldots, n-m, \\ \dfrac{n+m-j}{2m} & \text{if} \quad n-m < j < n+m. \end{cases}.$$

We study the convergence and stability of this quadrature rule in suitable Besov type spaces. A comparison with other quadrature rules proposed in the literature is done.

Nyström method for the numerical resolution of linear Volterra integral equations on infinite intervals

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This talk deals with the numerical solution of linear Volterra integral equations of the second kind on the half line

$$f(t) - \int_0^t k(s,t) f(s)\, ds = g(t), \quad t \geq 0,$$

where the kernel $k(s,t)$ is a given function defined on $\Delta = \{(s,t) \,|\, 0 \leq s \leq t\}$, $g(t)$ is a known function on $\mathbb{R}^+$ and $f(t)$ is the unknown solution.

Such kind of integral equations are of interest since they are involved in many applications which include elasticity, semi-conductors, scattering theory, seismology, heat conduction, metallurgy, fluid flow, chemical reactions, population dynamics, etc.

The case when $t \in I$, for a bounded interval $I \subset \mathbb{R}$, has been extensively studied and a large variety of numerical methods have been developed for an accurate approximation of the solution $f(t)$. Here we are interested in the case $t \in [0, +\infty)$, which, according to our knowledge, has not been so widely treated from a numerical point of view in literature.

The proposed numerical method is of Nyström type and is based on a truncated Lagrange interpolation process and a truncated gaussian quadrature formula. The stability and the convergence of the method in suitable weighted spaces of functions are studied and some numerical examples showing its reliability are presented.

In particular, the proposed method has been tested for the numerical resolution of some Volterra integral equations arising from the reformulation of differential models describing metastatic tumor growth whose unknown solutions represent biological observables as the metastatic mass or the number of metastases [1, 2].

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A new stable numerical method for Mellin integral equations in weighted spaces with uniform norm

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In this talk a new modified Nyström method is proposed to solve linear integral equations with fixed singularities of Mellin convolution type of the following form

$$f(y) + \int_0^1 k(x,y)f(x)dx + \int_0^1 h(x,y)f(x)dx = g(y), \quad y \in (0,1], \tag{1}$$

where $k(x,y)$ is continuous for all $x, y \in [0,1]$ such that $x + y > 0$ and has a fixed singularity at the origin of Mellin-type, i.e.

$$k(x,y) = \frac{1}{x}\bar{k}\left(\frac{y}{x}\right) \tag{2}$$

for a given function $\bar{k}$ on $[0,+\infty)$ satisfying certain assumptions, while the kernel $h(x,y)$ and the right-hand side $g(y)$ are smoother known functions on $[0,1]\times[0,1]$ and $[0,1]$, respectively. The function $f(y)$ represents the unknown.

The method is based on the application of a suitable Gauss-Radau quadrature formula for the discretization of the integral operators involved in equation (1), properly modified close to the singularity $y = 0$.

The main difficulty in solving such type of equations is the proof of the stability of the numerical method, being the noncompactness of the Mellin integral operator the chief theoretical barrier. In this talk we address the concern over the stability of the numerical procedure in a weighted space of continuous functions. The convergence of the method is also proved, giving an error estimate for the numerical solution under certain assumptions on the Mellin kernel.

The efficiency of the method is shown through some numerical results which highlight that the error estimate is sharp.

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MS-6
New Trends and Applications in Approximation Theory - Part 3

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Approximation theory is a fundamental branch of mathematics studying approximation processes of general functions by simple building blocks as, for instance, polynomials, wavelets, finite elements or Fourier expansions. New developments in approximation theory therefore have a deep impact on various other scientific fields as the numerical

solution of partial differential equations, image processing, inverse problems, statistical computing or data analysis. For example, interpolation with splines and radial basis functions is an important technological tool in the geometric design of automotive and aerospatial vessels, while wavelets and their generalizations as curvelets and shearlets are fundamental tools in the compression of large digital images and videos. Recently, approximation methods have also been developed to obtain compressed sensing methods for the sparse representation of signals or to understand deep learning algorithms.

This minisimposium aims to provide a platform for senior and young researchers in the field of approximation in order to exchange ideas of their current research and to discuss new trends in this area. It is also intendend to be a meeting point for italian and foreign experts to provide new solutions for real-world and industrial approximation problems.

Dynamic concentration reconstruction for magnetic particle imaging using splines

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In many technical and physical applications, the quantity of interest is not directly measurable such that it has to be computed by measurements related to the sought quantity via a physical model. So-called inverse problems are classically solved methods in a static setup. However, in recent years dynamic inverse problems, where a spatio-temporal quantity from temporal distributed data points has to be determined, have attracted notice. Such problems appear in particular in imaging applications, for instance dynamic computer tomography or new tomographic applications such as magnetic particle imaging (MPI).

MPI is capable of capturing fast dynamic processes in 3D volumes, based on the non-linear response of the magnetic nanoparticles to an applied magnetic field [1]. It can be used for the visualization of dynamic tracer concentration in blood vessels and organs with high spatio-temporal resolution. Possible medical applications are therefore blood flow monitoring, stroke detection or live tracking of instruments [3]. The image reconstruction is ill-posed and computationally demanding due to a non-sparse system matrix. To increase the field of view in MPI, multi-patch measurements are taken. However, during the scan of one patch no data is acquired for the remaining patches. Therefore, we propose a spatio-temporal regularization method allowing discontinuities in space but assuming smoothness in time. The approach adapted from [2] is based on an approximation of the particle concentration in time by cubic B-splines in every voxel. We will present numerical results from a phantom study.

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Univariate Dual Interpolating Subdivision via Bezout-like Equations

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Subdivision schemes are well-established tools for the construction of curves and surfaces. Given an initial set of data attached to an initial grid, a subdivision scheme repeats the process of refining the current grid and computing new data attached to the new grid in order to obtain a smooth limit. This talk concerns univariate interpolating subdivision schemes, i.e., schemes working on one-dimensional grids and whose limit curves interpolate the initial data. Usually, interpolation is achieved keeping, at each refinement step, the data already computed at the previous steps (step-wise interpolation). As shown in [3], it is however possible to create *dual interpolating schemes* that do not have the step-wise interpolation property. The family of all dual interpolating schemes has been then characterized algebraically in [2]. This characterization involves Laurent polynomials associated to a subdivision scheme, called symbols. However, while simple from a theoretical point of view, it is not so practical when it comes to the design of a dual interpolating scheme. This talk is based on [1], where the construction of such a scheme is reduced to the solution of a certain polynomial Bezout-like equation. In this context, under reasonable assumptions, it is possible to study a priori the existence of a dual interpolating scheme with a given degree of polynomial reproduction.

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(β, γ)-Chebyshev functions and points

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Chebyshev polynomials have been long-studied in scientific literature, and they have been considered in many fields of research. For example, the related zeros are particularly suitable for polynomial interpolation on the interval $[-1, 1]$ due to their well conditioning. Moreover, the extrema of Chebyshev polynomials, along with the set $\{-1, 1\}$, form the set of *Chebyshev-Lobatto* (CL) points, which are *quasi-optimal* interpolation nodes as well.

In this talk, we introduce the new class of (β, γ)-Chebyshev functions and points, which can be seen as a generalization of classical Chebyshev polynomials ad points. After providing some motivations supporting this study, we present some theoretical findings concerning (β, γ)-Chebyshev functions, proving that they are orthogonal in certain subintervals of $[-1, 1]$ with respect to a weighted arc-cosine measure. Then, we investigate on the behavior of the Lebesgue constant related to the polynomial interpolant at (β, γ)-CL nodes.

Reduced models for smoothing splines

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Surrogate models for kernel based schemes are a state-of-the-art technique for learning data [1, 2]. In this work we extend the idea to smoothing splines [3]. Their main drawback consists in possible *overfitting* and consequent boundary oscillations. To partially overcome this, starting by a few data, we *optimize* the fitting points by an incremental selection based on the minimization either of the residual (f-greedy) or of an upper bound for the approximation error based on the Lebesgue functions (λ-greedy). This allows us to construct an adaptive selection of the quasi-optimal points (independent of the function values) and give an upper bound for the pointwise error.

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Sampling strategies for approximation in kernel spaces

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Kernel methods provide powerful and flexible techniques to approximate functions defined on general domains, with possible high-dimensional input and output dimension, and using samples at scattered locations.

In this context, the problem of choosing the location of the sampling points is of great interest, both from a practical and a theoretical viewpoint. On one hand, it is of theoretical interest to know the limit and benefits of the choice of optimal point location, and to design feasible algorithms to select them. On the other hand, several applications are described by large datasets, and it may be interesting to select a possibly small portion of the data that allows an accurate reconstruction of the full problem.

In this talk we will discuss some greedy methods and show that they are effective techniques in both scenarios [1, 2, 3, 4].

In particular, we will first introduce some results on the general structure and theory of kernel-based greedy methods, and describe their efficient implementation. We will then show that, in certain circumstances, they may be proven to be worst-case optimal.

We will focus mainly on interpolation, and mention some application to quadrature. Moreover, we will discuss the use of these techniques on some real world applications.

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Faithful interpolation of non-regular functions from scattered data

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Accurate interpolation of non-regular two-variate functions $f : \Omega \subset \mathbb{R}^2 \mapsto \mathbb{R}$ 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 Ω.

The choice of the interpolation model plays a crucial role for 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.

For instance if the function has edges, and a straight direct interpolation is attempted, the Gibbs phenomenon is likely to arise producing highly oscillatory behaviours in regions close to the discontinuities. In the case of gradient faults, over-smoothing of creases will occur.

A key tool in this context are the so called variably scaled kernels that are truly performing when information on discontinuities are known, but in general these information are not available and must be obtained from the data.

In this talk we discuss an effective adaptive strategy to extract from the data the information needed by variably scaled kernels. This is done by using a smoothness indicator based on the norm of local interpolants and support vector machine techniques.

MS-7
In memory of Alberto Gandolfi: following Alberto in his excursions through biology

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We propose a symposium dedicated to the memory of our friend and colleague Alberto Gandolfi who passed away in August 2019 while, as usual, he was actively involved in several scientific activities. Since 1975, the research activity of Alberto encompassed different application fields of system engineering, applied physics, and mathematics, focusing in particular on mathematical modeling in biology and medicine, also providing valuable contributions to SIMAI activities.
The symposium contributions aim at commemorating Alberto and his work illustrating three subjects on which he worked until very recently: mathematical models for tumor growth and treatments, epidemic dynamics and epidermis growth. Each subject will be illustrated by coauthors of Alberto, who collaborated with him closely and for a long time. A list of proposed contributions follows here below:
"Everything began with a Floppy Disk" (Alberto d'Onofrio)
"A mathematical model for tumor angiogenesis" (Antonio Fasano)
"A model to predict the evolution of the HIV epidemic in Italy from clinical and demographic data" (Federico Papa)
"An epidemic model with within-host pathogen-immune dynamics" (Andrea Pugliese)

"The dynamics of the epidermis" (Mimmo Iannelli)

Everything started with a Floppy Disk

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I will summarize 22 years of Science and Friendship with Alberto Gandolfi.

A mathematical model for tumor angiogenesis

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Alberto Gandolfi

This work was almost finished when Alberto Gandolfi passed away unexpectedly. It was a sad experience to complete it without his support. The paper considers the propagation of a tumor from the stage of a small avascular sphere in a host tissue with the progressive onset of a vasculature stimulated by an angiogenic factor secreted by hypoxic cells. The way new vessels are formed involves cells sprouting from existing vessels and following a trail via a chemotactic mechanism which is biased by the angiogenic factor gradient, but which includes also a random change in direction giving rise to a diffusive component. The tumor progression is favored by its acidic aggression towards the healthy cells. The model describes the evolution of many biological and chemical species. Numerical simulations show the onset of a traveling wave eventually replacing the host tissue with a fully vascularized tumor. The results fit experimental data quite reasonably.

A model to predict the evolution of the HIV epidemic in Italy from clinical and demographic data

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The present talk deals with Alberto's recent activities in epidemiology, which resulted in the formulation of an ODE model of the HIV epidemic in Italy. The study was part of a PRIN project (2013) and shows the great scientific versatility of Alberto and how confident he was not only with mathematical modelling but also with data analysis.

Nowadays the HIV antiretroviral therapies have the potential of achieving the viral suppression, i.e. the reduction of plasma viral load below the threshold of detectability. Such a condition makes the virus untransmittable and guarantees both an increase of the number of CD4+ cells and a drastic reduction of viral replication, so minimizing the probability of emergence of drug resistant virus strains. Nevertheless, a non-negligible fraction of treated patients can still show a partial control of viraemia (also in high developed countries), mainly due to poor adherence to therapy or temporary therapy interruptions.

The present study aims at highlighting the impact of the fraction of treated patients achieving viral suppression, as well as of the role played by different ART-initiation strategies, on the HIV epidemic in Italy. To this end, we extended our previous model formulation given in [1] and we developed a time-varying ODE model with immigration and treatment, where the naive and non-naive populations of infected are distinguished, and

different compartments account for treated subjects virally suppressed and not suppressed [2]. Moreover, naive and non-naive individuals with AIDS are considered separately. A single susceptible population, without distinction of high-risk subgroups, is considered in the model formulation, while the naive infected population is distributed over four compartments in cascade according to the CD4 counts, reproducing the intra-host disease progression.

Clinical data from the nationwide database ARCA have been used to reconstruct the history of the fraction of virally suppressed patients since HAART introduction, as well as to assess some model parameters. The other parameters have been set according to the literature or determined by a fitting procedure exploiting epidemic data over the years 2003-2015. Predictions on the HIV epidemic evolution up to the end of 2035 were made assuming different future trends of the fraction of virally suppressed patients and different eligibility criteria for treatment. Increasing the viral suppression fraction is found to reduce the HIV incidence rate, the new AIDS cases and the AIDS deaths per year, especially in combination with early ART initiation.

The asymptotic properties of a time-invariant formulation of the model are studied, and the existence and global asymptotic stability of the unique positive equilibrium are proved.

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Within-host and between-hosts epidemic dynamics: a journey with Alberto

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In the past 20 years several authors have analysed models in which within-host infection dynamics is coupled to between-host transmission. Frequently in such models within-host dynamics was used to build appropriate functions appearing in epidemic models in order to study evolutionary problems [2], or to better describe the dynamics of immune boosting and waning [1]. Alberto, Carmela and I worked at a model [3] in which epidemic dynamics could affect within-host dynamics because the initial viral inoculum depended on the state of the infectant, and thus on the overall state of the epidemics; this two-way interaction yields new dynamical patterns, with subsequent epidemic waves in absence of external perturbations.
A shortcoming of that model is the fact that once a host is infected, s/he cannot be reinfected at any stage; Alberto was aware of the problem, and had prepared a manuscript draft in which reinfections were allowed at the beginning of an infection, where they can be relevant for the dynamics. Unfortunately, we were not able to complete the work before Alberto's premature death. In the current COVID epidemic it has been shown that infected individuals may vary widely in viral load, and this has been thought to be important for epidemic dynamics. A model has been proposed that takes account of this phenomenon through a system of ODEs in which mildly and severely infected individuals are distinguished, and an important role is played by the initial exposure, thus showing the potential relevance of the theoretical models analysed with Alberto.

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The dynamics of the epidermis

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When Alberto passed away, we had just submitted our last manuscript, coauthored with Gabriela Marinoschi, on the dynamics of cell growth within the basal layer of epidermis. The paper finally appeared on line in February 2020 and I regret so much Alberto could not see it published. We all know how everyday work stays hidden behind the lines of a manuscript and, indeed, this manuscript hides long discussions with Alberto and his great contribution to the effort of making our model substantial and based on experimental evidence.

The model for the basal layer followed our previous papers focused on the supra-basal multi-layer structure of the skin. Actually, the model we had proposed for the supra-basal region, initially included the contribution from the basal layer as an assigned boundary condition, but we realised that, to capture the whole dynamics of the epidermis, we had to implement the supra-basal model by the inclusion of the dynamics in the basal layer. Namely, we had to couple two different models, one of them focused on the basal layer dynamics to provide a dynamical input as a boundary condition to the supra-basal model. In this talk I will sketch the basic features of our description of the epidermis showing how the two models are connected and presenting a few simulations of the dynamics.

MS-8
Effective solvers for innovative discretizations of partial differential equations and applications - Part I

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Complex multiphysics phenomena arising in different fields of applied sciences are governed mathematically by systems of partial differential equations (PDEs). The numerical approximation of these PDEs is highly challenging, because of the multiscale properties of the physical phenomena involved. In recent years, a huge effort of the scientific computing community has been devoted to the development of innovative numerical technologies

for the spatial discretization of PDEs. In particular, we mention isogeometric analysis and polytopal element methods, such as mimetic finite difference, polygonal/polyhedral discontinuous Galerkin and virtual element methods. At the end of the discretization process, all these methods yield the solution of large scale and ill conditioned linear systems, for whose solution the development of effective solvers is mandatory. The aim of this minisymposium is to bring together researchers working on the construction, analysis and implementation of effective parallel and multilevel solvers for the solution of the linear systems arising from innovative discretizations of PDEs in different areas of engineering, earth and life sciences.

Agglomeration-based solvers for high-order Discontinuous Galerkin methods on polygonal/polyhedral grids.

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In this talk I will present agglomeration-based fast solution algorithms for high-order discontinuous Galerkin finite element methods which employ general polygonal/polyhedral elements. In particular, I will discuss and analyse a family of multigrid schemes on nested and non-nested agglomerated meshes [1] as well as Schwarz-type domain decomposition preconditioners [2]. The performance of the proposed solvers will be tested on both two- and three-dimensional test cases.

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Space-time shape uncertainty quantification of the inverse problem in electrocardiography with a boundary integral formulation

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In electrocardiography, the "classic" inverse problem consists of finding electric potentials on a surface enclosing the heart from remote recordings on the body surface and an accurate description of the anatomy. The latter being affected by noise and obtained with limited resolution due to clinical constraints, a possibly large uncertainty may be perpetuated in the inverse reconstruction.

In this talk we will study the effect of shape uncertainty on the forward and the inverse problem of electrocardiography. To this aim, the problem is first recast into a boundary integral formulation and then discretised with a collocation method to achieve high convergence rates and a fast time to solution. The shape uncertainty of the domain is represented by a random deformation field defined on a reference configuration. We propose a periodic-in-time covariance kernel for the random field and approximate the Karhunen-Loève expansion using low-rank techniques for fast sampling. The space-time uncertainty in the expected potential and its variance is evaluated with an anisotropic sparse quadrature approach and validated by a quasi-Monte Carlo method.

We present a numerical example to illustrate the validity of the approach with parametric dimension up to 600. For the forward problem the sparse quadrature is very effective. In particular, we prove the parametric regularity of the solution with respect to shape perturbations. In the inverse problem, the sparse quadrature and the quasi-Monte Carlo methods perform as expected except with total variation regularisation, in which convergence is limited by lack of regularity. We finally investigate an $H^{1/2}$ regularisation,

which naturally stems from the boundary integral formulation, and compare it to more classical approaches.

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Efficient loosely-coupled segregated solvers for fluid-structure interaction

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We consider two loosely-coupled schemes for the solution of the fluid-structure interaction problem in presence of large added mass effect, in particular, the Robin-Robin and Robin-Neumann (RN) explicit schemes where suitable interface conditions of Robin type are introduced. We study analytically on a model problem the dependence of the stability of the RN method on the interface stabilization parameter in the Robin condition [1]. Moreover, for an effective selection of the interface parameters which guarantee stability of the numerical solution for general FSI problems, we propose a strategy based on the optimization of the reduction factor of the corresponding strongly-coupled (implicit) scheme, obtained by means of the Optimized Schwarz method [2]. To check the suitability of our proposals, we present some numerical results both in an ideal cylindrical domain and in a real human aortic aneurysm. Our results confirm the theoretical findings and show the validity of our proposal for the calibration of the interface parameters, which leads to stable and accurate results and highlight the effectiveness in term of CPU time of the proposed schemes.

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Newton-Krylov-BDDC Solvers for Implicit Discretizations of Cardiac Reaction-Diffusion Systems

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The development of efficient and scalable solvers for cardiac electro-mechanical models has increasingly grown in the last decade. In particular, the need to handle the multiscale systems arising from the numerical discretization of such models has required the development of specific techniques to both accurately represent physiological data and reduce the computational costs of the resulting large-scale simulations.

In this work, we focus on the numerical simulation of the cardiac electrical activity, by solving a system constituted by two nonlinear parabolic reaction-diffusion equations describing the propagation of the electric impulse in the cardiac tissue (known as Bidomain model), coupled with the Roger-McCulloch ionic membrane model.
Applying a finite element discretization in space and the Backward Euler method in time, we need to solve at each time step a nonlinear system. Instead of facing this monolithic nonlinear system, we decouple the implicit discretization by solving the ionic equation first: thus, each time step is divided into two sub-steps where we need to subsequently solve a linear and a nonlinear system.

Therefore, for the solution of the nonlinear system, we propose here Newton-Krylov type methods, where the decomposition of the problem is performed after the Newton linearization. Fast convergence is ensured by preconditioning with non-overlapping domain decomposition techniques. In particular, we focus our attention on the classes of dual-primal substructuring iterative methods.

We prove a theoretical estimate for the condition number bound of the preconditioned operator, based on the recent deluxe-scaling considered by [1]. We investigate numerically the quasi-optimality and scalability of these preconditioners, thus confirming the convergence rate, by implementing a three-dimensional parallel code based on the PETSc library from the Argonne National Laboratory. The results obtained provide a basis for an extension of this study to the inclusion of more complex realistic membrane models and to monolithic discretizations of cardiac electro-mechanical models.

This is a joint work with Simone Scacchi (Univ. of Milan) and Luca F. Pavarino (Univ. of Pavia).

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A Nonsymmetric Variational Setting and a Quasi-optimal and Robust Discretization for Biot's Consolidation Model

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In the theory of poroelasticity, the Biot's consolidation model describes the flow of a fluid inside an elastic porous medium. In the simplest two-fields formulation, the unknowns are the displacement of the medium and the fluid pressure. We consider the problem resulting from the time discretization of the model with the backward Euler scheme. A typical difficulty encountered in the discretization of this problem is the robustness with respect to various physical parameters. Indeed, for extreme values of the parameters, undesired numerical artifacts, such as volumetric locking, spurious pressure oscillations and loss of mass, are often observed. We deal with these issues by observing that the problem is uniformly stable, irrespective of all parameters, in a suitable nonsymmetric variational setting. Guided by this result, we design a novel nonconforming discretization. We prove that the proposed discretization is quasi-optimal and robust in a parameter-dependent norm and discuss the consequences of this result. Finally, following [1], we propose a robust block-diagonal preconditioner for a symmetric three-fields formulation of the problem obtained by introducing an auxiliary variable.

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Isogeometric FETI-DP/BDDC preconditioners for almost incompressible elasticity and $\mathbf{H}(curl)$ problems.

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FETI-DP (Finite Element Tearing and Interconnecting Dual-Primal) and BDDC (Balancing Domain Decomposition by Constraints) are two very successful domain decomposition algorithms for a variety of elliptic problems. We introduce parallel deluxe FETI–DP/BDDC preconditioners for almost incompressible elasticity and Stokes problems discretized by mixed isogeometric analysis with continuous pressures. The convergence rate depends on the model inf-sup constant and the condition number of a closely related BDDC algorithm for compressible elasticity. This bound is scalable in the number of subdomains, polylogarithmic in the ratio of subdomain and element sizes, and robust with respect to material incompressibility and parameters discontinuities across subdomain interfaces. We will conclude by reviewing ongoing work extending FETI-DP/BDDC preconditioners to $\mathbf{H}(curl)$ problems in the plane.

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MS-9
Effective solvers for innovative discretizations of partial differential equations and applications - Part II

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Complex multiphysics phenomena arising in different fields of applied sciences are governed mathematically by systems of partial differential equations (PDEs). The numerical approximation of these PDEs is highly challenging, because of the multiscale properties of the physical phenomena involved. In recent years, a huge effort of the scientific computing community has been devoted to the development of innovative numerical technologies for the spatial discretization of PDEs. In particular, we mention isogeometric analysis and polytopal element methods, such as mimetic finite difference, polygonal/polyhedral

discontinuous Galerkin and virtual element methods. At the end of the discretization process, all these methods yield the solution of large scale and ill conditioned linear systems, for whose solution the development of effective solvers is mandatory. The aim of this minisymposium is to bring together researchers working on the construction, analysis and implementation of effective parallel and multilevel solvers for the solution of the linear systems arising from innovative discretizations of PDEs in different areas of engineering, earth and life sciences.

The INTERNODES method for the solution of PDEs in multidomain settings featuring non-conforming interfaces

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INTERNODES is an interpolation-based approach for dealing with the solution of PDEs in domains partitioned into non-overlapping subregions featuring non-conforming interfaces. The non-conformity could be of geometric type (non-watertight interfaces) and/or of discretization type (when the mesh sizes and/or the local polynomial degrees inside the subdomains differ). The discretization inside each subdomain can be achieved by a Galerkin-based method like, e.g., Finite Elements, Spectral Elements, or Isogeometric Analysis.

INTERNODES was introduced in [1] and its convergence was analyzed in [3] for $hp-$fem. In particular, when the mesh sizes in the two adjacent subdomains decrease uniformly, then INTERNODES achieves optimal convergence in the broken-energy norm with respect to the maximum mesh size, exactly as the well celebrated Mortar method does.

INTERNODES has been applied with success to multiphysics problems, Fluid-Structure Interaction problem was discussed in [2] while Stokes-Darcy equations in [4].

In this talk, I'm going to present recent results about the INTERNODES method with an emphasis on conservativity, a crucial property that a multidomain approach has to observe. By conservativity of a multidomain method we mean the ability of the method itself to preserve some quantities (typical of the continuous solution of the PDE) at the interface of the decomposition. For example, for the linear elasticity problem, these quantities are the balance of the forces and the null total work at the interface.

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FETI-DP for the three-dimensional Virtual Element Method

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We deal with the Finite Element Tearing and Interconnecting Dual Primal (FETI-DP) preconditioner [3] for elliptic problems discretized by the Virtual Element Method (VEM) [1]. We extend the result of [2] to the three-dimensional case. We prove polylogarithmic condition number bounds, independent of the number of subdomains, the mesh size, and jumps in the diffusion coefficients. Numerical experiments validate the theory.

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Three-field optimization formulation for flow simulations in fracture networks

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Effective simulations of fractured porous media are still challenging from a computational standpoint. One of the key issues concerns the complexity of the computational domain. In some circumstances the porous matrix can be neglected, such that the problem is reduced to the resolution of a system of PDEs in a network of fracture. Nonetheless, such networks can be extremely intricate, with a large number of intersections, and consisting of geometrical features with sizes that can span several orders of magnitude. Discrete fracture network models (DFNs) reproduce such networks modeling fractures as planar polygons and fracture intersections as one-dimensional segments. Such dimensional reduction, however, can only partially alleviate the geometrical complexity, as fractures can still form networks with a multi-scale nature. A large variety of numerical tools has been recently suggested for this kind of problems. Among them, one method is based on the reformulation of the problem as a PDE-constrained optimization problem. A cost functional is introduced to measure the error in the fulfillment of the coupling conditions at fracture intersections and it is minimized constrained by the PDE equations expressing the physics on the fractures. The structure of the functional allows to decouple the problem into fracture-local problems [1, 2]. Starting from such optimization based framework, a new approach is devised, based on a three-field formulation of the constraint equations [3]. The resulting scheme is still robust in handling complex geometries and ready for parallel implementation . Further, it allows for a simplified minimization process as the functional is mono-objective and gives local mass-conservation properties to the solution across fracture intersections [4].

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An isogeometric solver for tensor-product multi-patch geometries

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In this talk we present a solver for elliptic problems discretized with the isogeometric approch [2] on a multi-patch geometry, obtained by combining a domain decomposition approach with an efficient inexact solver for the local problems.

Our starting point is the All-Floating-FETI method (AF-FETI), a variant of the classical FETI method where both the continuity of the solution through the patches and Dirichlet boundary conditions are weakly imposed by introducing a set of Lagrange multipliers [4]. The interface is defined as the union of all local boundaries, thus endowing all local problems with a full tensor product structure.

In our approach, which in the spirit of [3], is named All Floating-IsogEometric Tearing and Interconnecting (AF-IETI) method, we introduce a saddle point formulation that allows to employ inexact solvers for the local problems [1]. These problems are possibly large, but they can be efficiently tackled with an inexact solver based on the Fast Diagonalization (FD) method. FD method has already been employed in a efficient preconditioner for the local problems of an overlapping Schwarz method in [5]. In AF-IETI the local problems always have the required tensor structure, even if a face of the patch is not wholly associated with a single kind of boundary condition, or it does not wholly touch the boundary of other patches. To show the potential of our approach, we compare numerically the performance of AF-IETI coupled with the inexact FD-based preconditioner with the exact preconditioner. Our results indicate that the inexact approach requires orders of magnitude less time than the exact one. Moreover, its performance does not deteriorate as the degree p is increased.

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Matrix-Free Methods for High-Order Discretization in Cardiac Electrophysiology

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In recent years mathematical and numerical modeling of cardiac electrophysiology have assumed a key role to investigate and better understand the whole cardiac function and to provide answers to clinical problems [3]. In this work we tackle the monodomain equation endowed with suitable ionic models [2], which describe the space and time evolution of the trans-membrane potential and of chemical species in myocardial cells. The solution to this problem exhibits sharp propagating wave fronts, thus selecting accurate and efficient numerical methods for its resolution is a challenging issue.

We present different benchmark problems of increasing complexity for cardiac electrophysiology, from a simple toy model with an exact solution to a realistic ventricular simulation. Different numerical schemes and techniques are assessed and compared on such problems: first, we focus on high-order discretization by comparing spectral elements with numerical integration (SEM-NI [1]) to a classical *hp*-FEM approach, showing that the former method is more efficient due to a better conditioning number when fine time-discretizations are employed; then we propose a matrix-free solver implementation, whose computational costs and memory footprint are proved to be overall more convenient than a standard *assemble-and-solve* finite element code; finally, we compare the effectiveness of the two naivest approaches of increasing the accuracy of the simulation results, *i.e.* by choosing a higher polynomial degree p or a smaller mesh size h, deducing that the former choice leads to a more beneficial ratio between accuracy and computational costs.

The aforementioned methods have been implemented in `life`$^{\texttt{x}}$ (`https://lifex.gitlab.io/lifex/`), a new `C++` high-performance parallel library for cardiac applications, based on the `deal.II` (`https://www.dealii.org/`) finite element core.

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Efficient domain decomposition solvers for cardiac mechanics

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The development of realistic cardiac models is an active area of research, with the numerical approximation of these models being a great computational challenge. The main bottleneck is the repeated solution of large-scale and ill conditioned linear systems of algebraic equations, which require scalable preconditioners to obtain efficient iterative solvers [1]. The most well-established iterative method for this aim is the preconditioned GMRES algorithm, the preconditioner being commonly the Algebraic Multigrid (AMG) method. It has become widely popular as it provides a black-box solution for preconditioning that works most of the time, but there are certain aspects that do not perform optimally: (i) it requires the tuning of many parameters, which is a highly non-trivial task, (ii) it does not scale in real applications and (iii) it does not handle higher order finite elements approximations.

Balancing Domain Decomposition by Constraints (BDDC) [2] methods provide an alternative to AMG methods, which in classic linear problems have been shown to provide quasi-optimal conditioning, and as they work through substructuring, the complexity of the problem is equally distributed. This finally results in more robust preconditioners that have been shown to scale up to hundreds of thousands of parallel processors. In this talk, we present the performance of this type of preconditioners for cardiac mechanics for both first and second order conforming finite elements, together with low-level optimizations that allow for peak performance. Our results suggest that BDDC preconditioners outperform AMG for large scale simulations, as well as for higher order finite elements approximations.

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MS-10
Mathematical models and methods for economics and finance

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In recent years the research for mathematical tools to be applied in financial contexts has gained additional importance. In fact the latest financial crisis has highlighted the need for a more scientific approach to the problem of pricing and risk control. Moreover, we can now take advantage of more advanced statistical and mathematical skills and of the availability of numerical techniques and faster computer systems.

In this minisymposium, a variety of advanced mathematical modelling tools, numerical methods and scientific computation techniques for different current problems will be presented. More precisely, this minisymposium is devoted to the use of mathematical models in economics and finance: quantitative finance, mathematical economics, decision theory, stochastic models, mathematical finance, and optimization models.

Model-free Computation of Risk Contributions in Credit Portfolios

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Portfolio credit risk represents one of the most important sources of risk that any financial institution has to face with. As an important part of the credit risk management process, some common risk measures are usually employed like the well-known Value-at-Risk (VaR) and Expected Shortfall (ES). Besides the calculation of these measures, the decomposition of the total risk of a given portfolio into the individual risk contribution of each obligor is a classical problem of paramount importance in practice. Identification of risk concentrations, portfolio optimization or capital allocation are, among others, relevant examples of application.

The problem of obtaining the risk contributions to VaR (VaRC) and ES (ESC) represents a great challenge from the computational standpoint. Within the credit risk literature, many authors rely on Monte Carlo simulation, since it is straightforward to implement and can be easily extended to multi-factor models. This fact makes Monte Carlo methods very attractive for practitioners. By following this approach, the problem of computing the risk contributions is reduced to the computation of a certain expectation conditioned on a rare event, which makes the direct application of Monte Carlo method rather inefficient. To overcome this issue, most of the methodologies proposed in the last few years usually include more advanced simulation tools. By far, the so-called *Importance Sampling* technique (originally applied as a variance reduction technique) appears to be the most promising development, providing a significant performance gain with respect to the plain Monte Carlo. However, this approach still requires a relatively big computational cost to control the variance.

The computation of risk contributions by means of Monte Carlo simulation is a two-stage procedure. Within the first stage, VaR (or ES) is obtained from the simulated losses, while the second stage consists of estimating the expected value of individual losses conditioned on the event that the total loss equals the VaR value. In this work, we propose a non-parametric density estimation based on wavelets. The starting point is the sample of the total loss variable generated within the first stage of Monte Carlo simulation. Then, the density is estimated either with Haar or Shannon wavelets and the VaR and ES are obtained. Finally, according to the Euler's capital allocation principle, we take derivatives of the risk measures (VaR or ES) with respect to the exposures and we obtain the VaRC and ESC. While the Haar family has desirable properties like compact support and gives us positive densities by construction, we finally prefer the Shannon family due to its

robustness and easy handling. We test our method with one- and multi-factor Gaussian and t-copula models. These models belong to the class of structural models and they are currently used in practice, since they are the models in force given by the regulators. The computation of VaRC by means of Monte Carlo simulation is particularly difficult. In contrast, the wavelets based method gives impressive results, both in accuracy and speed. For obtaining comparable results in accuracy, Monte Carlo needs between 25 (for the one-factor model) and 1000 times (for multi-factor models) the CPU time required by our method. While the wavelet machinery is not affected by increasing the number of factors in the model, Monte Carlo needs three times more seconds of CPU time when moving from 5 to 25 factors. Moreover, our methodology is model-free in the sense that it stays the same and it applies in the same manner, regardless of the model employed for driving the defaults. To the best of our knowledge, this is the first time that this technique is used for solving the capital allocation problem by means of Euler's capital allocation principle. Multiple tests carried out along this work make us think that this novel method can be used within the risk management toolkit of financial firms.

Do financial markets affect real economy? Influences of professional and non-professional beliefs

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Economics and finance research deals with the interdependence between stock returns and macroeconomic events. Connecting asset returns to real economy allow to understand how assets volatility influences economic fluctuations and vice-versa. To this aim, a general equilibrium (GE) approach has been defined by [2] as a "largely unexplored new land", indispensable to understand how macroeconomic variables interact with financial market. In order to separate the influence of professional and non professional beliefs as in [3], we study an economy in which individuals have risk propensity but no direct access to financial market and the financial mediator is boundedly rational. As in [1], the evolution of real economy depends on the saving rate of workers as well as on the dividend policy. Empirical literature found that the dividend payout ration is correlated to stock's price volatility. We analyse influences within real economy and financial market assuming that managers adopt a stable dividend policy.

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Machine Learning model in the Insurance sector

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In this talk we use the Random Forest methodology to predict the lapse decision of life insurance contracts by policyholders.

The decision to lapse an insurance contract has been analyzed in a large literature, both from a theoretical and an empirical point of view. A "rational" lapse decision refers to a low interest rate, that renders more convenient to switch to another life contract, or to weak economic conditions of the policyholder. Testing these hypotheses on microdata, the evidence is limited: the fraction of the variability of the lapse decision captured by proxies of these motivations is not high. Behavioral and commercial reasons seem to play a significant role. To investigate them in an agnostic way, i.e., starting from a large set of variables, it is useful to use Machine Learning tools that allow data to speak for themselves.

We show that Machine Learning techniques can be easily used to forecast the lapse decision, with good performances, and that Random Forest performs better than the classical logistic model to predict the lapse decision, even if the interactions between features are taken into account.

Exploiting local and global interpretability, the Machine Learning methodology also allowed us to discern the relevance of a wide set of exogenous variables to explain the lapse decision.

The main result of our analysis is that the important drivers of the lapse decision are the time passed from the incipit of the contract and the time to expiry, as well as the insurance company, the contract size, and premium. Other features of the policyholder (gender, age of the policyholder, region) or of the contracts (product type) as well as macroeconomic variables (with the exception of the disposable income growth rate with a nonlinear effect) play a limited role. This is in contrast with results obtained using linear models and confirms that traditional hypotheses that associate the lapse decision to economic convenience or to the economic condition of the policyholder have a weak capability to explain the phenomenon. These results also confirm that linear models are not able to fully capture the heterogeneity of financial decisions.

From option values to additive processes

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In option pricing one typically starts from a "realistic" underlying (martingale) stochastic processes and hopes it produces easy-to-use equations for describing market values. But it is also possible to proceed the other way around: start from option values which admit no-arbitrage ("increasing in convex order" functionals) and then devise a process which admits marginals fitting those equations. A prime example is Dupire [3] equation, but more sophisticated techniques, not necessarily involving continuous processes, are by now known (as expounded by e.g. Madan and Yor [5]). However, the processes obtained are typically very general and do not make use of the properties of any specific distribution implicit in option prices. We have recently discovered in [1] that certain "natural" (i.e. arising from functions popular in applied sciences) expressions for vanilla option values yield to distributions of logistic type for the underlying (or its logarithm), which are known to be infinitely-divisible. When an appropriate term function (i.e. not allowing calendar arbitrage) is supplied to the valuation equation the corresponding family of time-dependent infinitely-divisible distributions determines an additive process for the underlying security price which turns out to be a martingale. Therefore parsimonious and simple underlying processes exist which support elementary option valuation equation capturing returns skewness, kurtosis, self-similarity and other stylized facts. The additive structure additionally allows for path-dependent derivative valuation along the lines of well-established methodologies.

In the further developments of [2], in an effort to increase the amount of implied volatility skew and convexity picked up by the models, we modified the underlying distributions of the additive processes involved with an additional parameter, without perturbing the martingale property. This can be seen as equivalent to use logistic beta-generated skew distributions, as introduced by Jones [4], to model options implied distributions. Equivalent descriptions of these models are given in term of put digital option prices which essentially coincide with the underlying security CDF. Vanilla option formulae can be seen to overlap with those studied by McDonald and Bookstaber in [6], but with the added dimension entailed by a consistent no-arbitrage term structure leading to a proper stochastic process and martingale dynamics. Empirical tests of this latter modelling approach are ongoing.

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Identifying financial instability using high frequency data

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Financial crises prediction is an essential topic in finance. We propose an Early Warning Indicator (EWI) for predicting possible financial crises or, more generally, market instability conditions. Our system is based on the so called price-volatility feedback rate, which is supposed to describe the ease of the market in absorbing small price perturbations.

We present an indicator of financial instability based on the computation of the decay rate for the propagation of a given market shock. The rate of variation through time of an initial perturbation of a given high frequency financial time series enables us to understand if such a shock will be rapidly absorbed or, on the contrary, it will be amplified by the market. The indicator combines non-linearly volatility, leverage and covariance between leverage and price and is model-free. Consistency results and other properties of the indicator under the CEV model have been investigated in [2].

A logit regression Early Warning System is employed to predict future financial crises and EWIs based on the realized variance (RV) and on the price-volatility feedback rate are considered. Our study conducted in [1] on the S&P 500 index futures reveals that, while the RV may sometimes fail in predicting crises, the EWI employing the price-volatility feedback rate is always an important predictor of financial instability.

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MS-11
Advances in Data Analysis: Mathematical Models, Numerical Methods and Learning Approaches

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In the Internet of Things and the Big Data era, the analysis of data plays a really important role in terms of new knowledges and services for several application fields: from the civil engineering to biomedical world, up to the astronomical one. Moreover, the limited resources represents a problem for some applications (e.g. topics like eco-sustainability, energy saving, environmental improvement, and energy efficiency, all related to the thermal insulation), and there is an increasing need for more accurate forecast models, oriented to solve especially issues related to the climate changes. This data analysis can be face through three different levels: the use of appropriate mathematical

models, solved via novel, accurate and efficient numerical methods, supported by promising learning approaches.
The aim of this Minysimposium is to summarize different skills, theoretical and numerical ones, bringing together pure and applied mathematicians into a lively environment for discussing methodologies and challenges around the data analysis applied to different areas which are of great interest from several point of views, some more theoretical, others more practical for real applications thanks to learning methodologies.

Machine learning for flare forecasting

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The Sun is an enigmatic star that produces some of the most powerful explosive events in our solar system, such as solar flares and coronal mass ejections (CMEs). Studying these eruptions can provide a unique opportunity to better understand fundamental processes on the Sun, and to understand their space weather impacts at Earth and throughout the solar system. Machine learning offers great potential to learn the characteristics of the Sun-Earth system and to use them to both predict space weather impacts on timescales ranging from hours to days and improve the accuracy of the propagation models.

Space weather forecasting relies on the availability of two ingredients: data and computational methods for data analysis. It is well-established that solar Active Regions (ARs) host major flares and therefore flare prediction needs experimental data on AR properties. Since February 2010, the *Helioseismic and Magnetic Imager* on board the *Solar Dynamics Observatory* (SDO/HMI [1]) is providing both line-of-sight and vector magnetograms of the full solar disk at a cadence of 12 minutes. By means of pattern recognition techniques, SDO/HMI magnetograms can be used to infer a variety of AR properties for prediction purposes. From a deep learning perspective, HMI images/movies can feed Convolutional Neural Networks (CNNs) that automatically extract peculiar features and perform probabilistic forecasting.

In this talk I will discuss both approaches. First, by using data sets of almost 200 features determined from properties extracted from SDO/HMI vector magnetograms I will address the problem of flare forecasting so as the identification of the image properties that mostly impact the event prediction [2]. Second, I will show first results obtained following an innovative approach based on deep learning, whereby HMI images are used as input of trained Convolutional Neural Networks that will automatically provide us with the forecasting indicators.

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Radial Basis Function Partition of Unity Methods: Solution of Problems in Applications

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The Radial Basis Function Partition of Unity Method (RBF-PUM) is a powerful numerical tool, which is commonly used in scattered data approximation or in solution of differential problems [1, 5, 6]. In practice, when data are regular or quite uniform, a standard RBF-PUM scheme can successfully be applied. However, in case of non uniform data or steep function variations, the use of modified or adaptive schemes is essential for the construction of effective RBF-PUMs. In this study we present some computational techniques to numerically solve large interpolation problems [2, 4] and elliptic partial differential equations [3]. Numerical experiments support our analysis.

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An optimization problem in thermal insulation with Robin boundary conditions

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We study thermal insulating of a bounded body $\Omega \subset \mathbb{R}^n$. Under a prescribed heat source $f \geq 0$, we consider a model of heat transfer between Ω and the environment determined by convection; this corresponds, before insulation, to Robin boundary conditions. The body is then surrounded by a layer of insulating material of thickness of size $\varepsilon > 0$, and whose conductivity is also proportional to ε. This corresponds to the case of a small amount of insulating material, with excellent insulating properties. We then compute the Γ-limit of the energy functional F_ε and prove that this is a functional F whose minimizers still satisfy an elliptic PDEs system with a non uniform Robin boundary condition depending on the distribution of insulating layer around Ω. In a second step we study the maximization of heat content (which measures the goodness of the insulation) among all the possible distributions of insulating material with fixed mass, and prove an optimal upper bound in terms of geometric properties. Eventually we prove a conjecture in [1] which states that the ball surrounded by a uniform distribution of insulating material maximizes the heat content. The results we describe are contained in the paper [2].

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Kernel-based approximation methods on graphs

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We study how concepts from harmonic analysis as positive definite functions can be transferred from a classical group setting to a more general graph setup. In order to approximate signals on graphs with generalized shifts of a positive definite graph basis function (GBF) we merge kernel-based approximation with spectral theory on graphs [3]. In this way, we obtain graph analogs of radial basis function methods or spherical basis functions. We provide several descriptions of positive definite functions on graphs, the most relevant one is a Bochner-type characterization in terms of positive Fourier coefficients. These descriptions allow us to design GBF's and to study GBF approximation in more detail: we are able to characterize the native spaces of the interpolants, we give explicit estimates for the approximation error and provide ways on how to calculate the approximants in an efficient manner. Moreover, we investigate how GBF approximation can be combined with partition of unity methods on graphs [1] and how kernel-based models can be applied for classification tasks and influence maximization on graphs [2].

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Score-Oriented Loss functions (SOL)

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In the deep learning context, a model is trained by minimizing a certain target function, which includes the so-called *loss function*. However, the assessment of the classification performances is achieved by considering different *skill scores*, which are usually chosen according to the specific application. These scores are built upon the entries of the so-called *confusion matrix* and they can not be directly maximized in the training process, since they are discontinuous functions with respect to the predictions given by the model. Therefore, they are usually maximized after the training of the network by varying the value of the threshold.

In this talk, a new class of score-oriented loss functions is presented. The core idea consists in treating the threshold that influences the entries of the confusion matrix not as a fixed value, but as a random variable. We theoretically show that the so-constructed loss functions are indeed derivable with respect to the weights of the network, and they provide an automatic optimization of the target score in the training phase. Then, we present some classification experiments that support the theoretical findings.

MS-12
Applied Mathematics in STEM Education

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The second decade of 21st Century has begun with the a well documented crisis in K-12 STEM (Science, Technology, Engineering, and Mathematics) education [1]. In this context, many countries recognized the importance of addressing STEM fields in K-12 education and reliable guides have been proposed for an effective STEM education reform [2],[3].
An effective K-12 education, grounded on making sense of STEM-related topics in daily lives, deeply rely on sound mathematical knowledge and skills, including computational skills since "the act of writing or modifying programs and thinking about computer algorithms can frequently deepen our understanding of the underlying science" [4]. Thus the ability to do computational tasks in science and technology-related learning paths is a useful skill for high school and undergraduate students.
The proposed mini-symposium is framed within this scenario and presents creative and experiential activities aimed to foster STEM education in high school student.

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An educational approach to the problem of crowd behaviour

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Crowds are common occurrences and can be seen in sporting events, music concerts, shopping sales, and amusement parks. Can we consider the sudden and messy exit of a crowd from a subway or from a stadium as a chaotic or predictable behavior? In the presentation, we start from the study of an exercise called "North Curve"(published in Italy in 2015 to improve students'preparation for scientific high school diploma) in order to analyze the problem of the crowd behaviour from an educational point of view according to: a) a microscopic approach, crowd is made up of individual pedestrians who take up a position and speed in a range of time, both can change suddenly. The complete pedestrian's walking is a geometrical object characterized by fractal dimension [3]; b) a macroscopic approach, the pedestrians all together become similar to a fluid distributed in the space [1], hence crowd follows the hydrodynamics' properties [2] for example the continuity equation. The educational project was achieved in BPL (Based Project Learning) modality during extra-time lessons. The main goal of this project is to demonstrate how some laws and principles of Mathematics and Physics can find applications in real-life problems and they can contribute to give a solution. In the project Mathematics, Physics and Technology,according to an educational STEM approach, are not separate subjects but they are integrated into a cohesive learning paradigm based on real-world applications.

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A computational toy-model for viscosity

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The development of computational skills is very useful to improve STEM education. Its educational relevance is clearly evidenced by one of the most authoritative journals in the area of science education (notably of physics education), i.e. the American Journal of Physics, which hosts a section of the Journal specifically dedicated to computational aspects [6] and [1]. In fact, it has been argued that "the act of writing or modifying programs and thinking about computer algorithms can frequently deepen our understanding of the underlying science" [6]. Thus, the ability to do computational tasks in science and technology-related learning paths is a useful skill for high school and undergraduate students [2] and [3]. In this context, we propose a computational approach to a physical quantity (i.e. viscosity) which is frequently obscured by misconceptions [4]. In particular, we present a toy-model for a fluid in laminar flow, in which viscosity emerges as a transport property determined by the transverse diffusion of momentum. The computational model is implemented by using Python, a programming language increasingly popular for computational applications in educational contexts [5].

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Multidimensional Scaling in Cluster Analysis: examples in Science and Mathematics Education

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Several researches in STEM education research highlight the advantages of an integrated approach to these disciplines that relates knowledge and know-how, design and implementation, theoretical and practical problems [5, 4, 6]. In some researches, the effectiveness of these approaches on students conceptual understanding and motivation and has been studied through the use of quantitative analysis tools such as cluster analysis (CLA) [1, 7]. Through CLA it is possible to characterize students analyzing the strategies they deploy to tackle, for example, questionnaires built so as to investigate the lines of reasoning implemented by them when they are proposed with problematic situations. In particular, it is possible to characterize the students in terms of a limited number, m, of typical ways of answering the questionnaire questions [2]. Each student is therefore identified by a binary vector (each component can be 1 or 0) with m dimensions. Cluster Analysis techniques allow students to be grouped into homogeneous groups based on common characteristics and the representation of these groups is ideally referred to an m-sized space. However, for reasons of simplicity and clarity, it is often preferred to perform the representation of groups in three or two dimensional spaces. One of the techniques used for this purpose is Multidimensional Scaling [3] (MDS). It allows the researcher to move from the m-sized space to a space with a smaller number of dimensions that is a function of the initial m-dimensional representation, preserving the global distances between the group elements. However, the application of the MDS methodologies depends strongly on the typology of the initial data and a non-thorough knowledge of the mathematical details at their base can lead to obtaining results that are not reliable and / or of little significance. In this paper we will study a MDS methodology based on Principal Component Analysis, with particular reference to a set of binary data, highlighting how the results obtained through this methodology can be reliable and significant for the researcher in education.

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Reconstructing a computational paradigm: some school experiments

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Our goal in this work is to illustrate and study the reconstructive function that can be played by some well-known paradoxes of infinity, notably Hilbert's Hotel and Thomson's Lamp, in the context of several workshops held in secondary schools across Italy and the UK (see [2] for an analysis of some among these activities). Our starting point is the idea that paradoxes may be viewed as methodological signposts. They point to the construction of means to fix the terms of a problem that their formulation offers in elusive terms, i.e. ones not integrable into any explicitly codified inferential process. For instance, Hilbert's Hotel is about a hotel that is full but whose number of rooms cannot be given. It also calls for arithmetical evaluations that cannot be carried out by handling the needed numerical specification. Many other paradoxes exhibit analogous numerical lacunae, which it is possible to reinterpret as so many demands for an extended computational methodology, capable of supplementing current resources. By making use of the extended computational paradigm introduced in [4] and amenable to a logical treatment within the axiomatic theory from [4], we confronted students from the later years of secondary school with a range of activities revolving around the paradoxes of infinity designed to arouse, on the basis of personal reflection, a need for computational reconstruction. Students were made responsible for such reconstruction, which it is was possible for them to articulate by engaging in preparatory exercises that enabled them to master the central ideas of [4]. It was then up to them to find a way of applying these ideas to the paradoxes, regaining for them an originally lacking numerical dimension. The results generated by school workshops (a partial discussion is in [2]) showed that structured work on paradoxes can effectively organise an experience of the initial phases of enquiry (especially the dynamics of suggestions and ideas, in the sense of [1]), which enables a more direct appreciation of the creative element typical of mathematical thinking on the part of students.

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Computational skills in STEM Education: a critical overview

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Computation plays a central role in STEM disciplines and, in particular, it is so pervasive in physics [1] to justify such statements as "…a curriculum in which computation is absent or plays a minor role is inauthentic to the contemporary discipline" [2]. Scientific and engineering disciplines (and then their teaching and learning processes) traditionally are based on two pillars: theory and experiment. This landscape has profoundly changed in the last decades, since a real paradigm shift has occurred due to the ubiquity of computers and computational tools [3]. The theory/experiment dichotomy has been significantly altered by the irruption of a real third pillar, i.e. computation, that "… has blurred the distinction between theory and experiment" [3]. This state of affairs claims for a major role of computation and programming in the preparation of high school and university undergraduate students [4] and, even earlier, in primary education [5].
Moreover, algorithmic thinking is a powerful intellectual tool [4] which can be fostered by problem solving activities making use of computation and programming. In turns, programming (intended as a way of thinking) has a profound impact on reasoning skills in all scientific areas, and, consequently, assumes a major importance for the teaching and learning processes of the STEM disciplines [6], [7].
In this contribution, a critical overview of the role of computation and programming in STEM education will be presented and some suggestion will be drawn on curricula design, with special emphasis on physics education and teacher preparation.

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Applied mathematical problem-solving to improve the interdisciplinary curriculum in higher education

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Interdisciplinary Mathematics Education (IdME) - a relatively new field of research in mathematics education - is becoming increasingly prominent internationally because of the political agenda around Science Technology, Engineering and Mathematics (STEM) [4],[7].
In fact, STEM education has become a central goal of educational policy in many countries worldwide in an attempt to prepare students for a scientific and technological society.
The advantages of STEM education has become evident through many cross-discipline teaching experiments, and recently research studies have begun to produce empirical evidence that promotes these ways of teaching and learning [1],[2] and [3].
Applied mathematical problem-solving, as a practice and key competence within mathematics education standards, could be interpreted as an excellent example not only to promote 21st century skills and to encourage students' interests in STEM fields, but also interdisciplinary mathematics education in school [4],[5] and [6].
The talk is part of the debate surrounding the integrated approach to STEM in the curriculum of Italian higher education, with special focus on Applied Mathematical problem-solving as a vehicle to help students not only to develop conceptual understanding, reasoning skills, but also to construct their awareness of science and engineering concepts through experiental learning methods.
The aim is to favour the simplification of real-world problems, while retaining important characteristics such that the solution to the problem is still of practical or theoretical interest, and that the problem should invoke non-trivial modelling and problem-solving activities. Moreovor, the talk focuses on the implementation of the STEM integrated approach by discussing the implication for the learning and teaching of mathematics, and the relationships between mathematics and STEM.

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MS-13
Innovative numerical methods for evolutionary partial differential equations. Part I: Kinetic models

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The purpose of the MS is to gather researcher interested in the development of innovative techniques for the numerical solution of evolutionary partial differential equations, concentrating in particular on the numerical treatment of mathematical models described by hyperbolic and kinetic equations. A broad range of physical systems is governed by hyperbolic systems of conservation or balance laws. Among these we recall the classical fields of gas dynamics and shallow water equations describing free surface waves, or more recent models describing traffic flow. Likewise, kinetic models, originally introduced to provide an accurate statistical description of a large collections of gas particles, can be effectively adopted to describe other behaviours, such as pedestrian flow, swarming, and other kinds

of social dynamics. In several models, control problems can be effectively described by Hamilton-Jacobi type equation, whose mathematical structure has strong analogies with the structure of hyperbolic systems of conservation laws. The mini-symposium will deal with several issues related to the numerical solution of such models, including, among others, multi-scale issues, asymptotic preserving schemes, high order discretisation in space and time, and stability analysis.

The MS is divided in three interconnected sessions, according to the main focus of the talks: I-Kinetic models, II-Hyperbolic models, III-Control and multiscale.

Mean-field particle swarm optimization

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In this talk we survey some recente results on the global minimization of a possibly non-smooth and non-convex high dimensional objective function by means of a multi-agent derivative-free method [1, 5, 6]. To this aim we introduce a continuous description based on stochastic differential equations of the particle swarm optimization (PSO) process and derive in the large particle limit the corresponding mean-field approximation based on Vlasov-Fokker-Planck-type equations. Subsequently, in the small inertia limit, we compute the related macroscopic hydrodynamic equations that clarify the link with the recently introduced consensus based optimization (CBO) methods [2, 3, 4]. Rigorous results concerning the mean-field limit and the convergence of the method towards the global minimum are provided.

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Moment-driven predictive control of mean-field collective dynamics

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Mathematical description of collective behavior has been studied in a wide spectrum of applications such as animal behavior, cellular aggregation, opinion dynamics, and human crowd motion. Our research addresses the design of external control actions able to influence a large system of interacting agents towards prescribed stable patterns. We address this challenge by means of optimal control techniques, thus minimizing an energy measure of both the control and the state of the system. In order to circumvent the solution of such large scale non-linear optimization problem we introduce mean-field optimal control problems, where the microscopic dynamics is approximated by the evolution of a nonlocal PDE model. For the numerical realization of these problems, a linearization-based approach is used for the computation of sub-optimal feedback laws obtained from the solution of differential matrix Riccati equations. Quantification of dynamic performance of such control laws leads to theoretical estimates on suitable linearization points of the nonlinear dynamics. Subsequently, the feedback laws are embedded into non-linear model predictive control framework where the control is updated adaptively in time according to dynamic information on moments of linear mean-field dynamics. The efficiency and robustness of these methods is validated with several numerical examples for the control of flocking and swarming behaviors.

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Multiscale control of generic second order traffic models by driver-assist vehicles

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We present the derivation of Generic Second Order macroscopic Models (GSOMs) of vehicular traffic out of a Follow-the-Leader particle description via a kinetic approach. In the vehicle interactions we introduce a binary control modelling the automatic feedback provided by driver-assist vehicles, then we upscale such a controlled particle dynamics by means of an Enskog-based hydrodynamic limit. The resulting macroscopic model contains in turn a control term inherited from the microscopic interactions. We show that such a control may be chosen so as to optimise global traffic trends, such as the vehicle flux or the road congestion, constrained by the GSOM dynamics. By means of numerical simulations, we investigate the effect of this control hierarchy in some specific case studies, which exemplify the multiscale path from the vehicle-wise implementation of a driver-assist control to its optimal hydrodynamic design.

This talk is based on [2], which is part of a more extended research line comprising also works [1, 3, 4, 5, 6, 7].

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High order finite volume schemes with IMEX time stepping for the Boltzmann model on unstructured meshes

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In this talk, we present a family of time and space high order finite volume schemes for the solution of the full Boltzmann equation. The velocity space is approximated by using a discrete ordinate approach while the collisional integral is approximated by spectral methods. The space reconstruction is implemented by integrating the distribution function, describing the state of the system, over arbitrarily shaped and closed control volumes using a Central Weighted ENO (CWENO) technique. The full discretization is then obtained by combining the previous phase-space approximation with high order Implicit-Explicit (IMEX) Runge Kutta schemes. Comparisons of the Boltzmann model with simpler relaxation type kinetic models (like BGK) are proposed showing the capability of the Boltzmann equation to capture different physical solutions. The methods are also tested on several standard two-dimensional benchmark problems in comparison with Direct Simulation Monte Carlo results.

High order pressure-based semi-implicit IMEX schemes for the 3D Navier-Stokes equations at all Mach numbers

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This work [1] aims at developing a high order pressure-based solver for the solution of the 3D compressible Navier-Stokes system at all Mach numbers. We propose a cell-centered discretization of the governing equations that splits the fluxes into a fast and a slow scale part, that are treated implicitly and explicitly, respectively. A novel semi-implicit discretization is proposed for the kinetic energy as well as the enthalpy fluxes in the energy equation, hence avoiding any need of iterative solvers. The implicit discretization yields an elliptic equation on the pressure that can be solved for both ideal gas and general equation of state (EOS). A nested Newton method is used to solve the mildly nonlinear system for the pressure in case of nonlinear EOS. High order in time is granted by implicit-explicit (IMEX) time stepping, whereas a novel CWENO technique efficiently implemented in a dimension-by-dimension manner is developed for achieving high order in space for the discretization of explicit convective and viscous fluxes. A quadrature-free finite volume solver is then derived for the high order approximation of numerical fluxes. Central schemes with no dissipation of suitable order of accuracy are finally employed for the numerical approximation of the implicit terms. Consequently, the CFL-type stability condition on the maximum admissible time step is based only on the fluid velocity and not on the sound speed, so that the novel schemes work uniformly for all Mach numbers. Convergence and robustness of the proposed method are assessed through a wide set of benchmark problems involving low and high Mach number regimes, as well as inviscid and viscous flows.

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Local velocity grid conservative semi-Lagrangian schemes for the BGK model

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Most numerical schemes proposed for solving kinetic equations for rarefied gas dynamics, such as Boltzmann equation and BGK model, are based on the discrete velocity approximation [5, 6, 7]. Recently developed conservative semi-Lagrangian schemes allow accurate solutions on a wide range of Knudsen numbers, with very mild restrictions on the time step [3]. In general, such approaches use fixed velocity grids, and one must secure a sufficient number of grid points in phase space to resolve the structure of the distribution function. When dealing with high Mach number problems, where large variation of mean velocity and temperature are present in the domain under consideration, the computational cost and memory allocation requirements become prohibitively large. Local velocity grid methods have been developed to overcome such difficulty in the context of Eulerian based schemes [1, 2]. In this talk, we introduce a velocity adaption technique for the semi-Lagrangian scheme applied to the BGK model. The velocity grids will be set locally in time and space. We apply a weighted minimization approach to impose global conservation, generalizing the L^2-minimization technique introduced in [4]. We demonstrate the efficiency of the proposed scheme in several numerical examples.

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MS-14
Innovative numerical methods for evolutionary partial differential equations. Part II: Hyperbolic models

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The purpose of the MS is to gather researcher interested in the development of innovative techniques for the numerical solution of evolutionary partial differential equations, concentrating in particular on the numerical treatment of mathematical models described by hyperbolic and kinetic equations. A broad range of physical systems is governed by hyperbolic systems of conservation or balance laws. Among these we recall the classical fields of gas dynamics and shallow water equations describing free surface waves, or more recent models describing traffic flow. Likewise, kinetic models, originally introduced to provide an accurate statistical description of a large collections of gas particles, can be effectively

adopted to describe other behaviours, such as pedestrian flow, swarming, and other kinds of social dynamics. In several models, control problems can be effectively described by Hamilton-Jacobi type equation, whose mathematical structure has strong analogies with the structure of hyperbolic systems of conservation laws. The mini-symposium will deal with several issues related to the numerical solution of such models, including, among others, multi-scale issues, asymptotic preserving schemes, high order discretisation in space and time, and stability analysis.

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A Structure-Preserving Staggered Semi-Implicit Scheme for Continuum Mechanics

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In this talk, we present a new class of structure-preserving semi-implicit schemes for the unified first order hyperbolic model of Newtonian continuum mechanics proposed by Godunov, Peshkov and Romenski (GPR). The GPR model is a geometric approach to continuum mechanics, which is able to describe the behavior of moving elasto-plastic solids as well as viscous and inviscid fluids within one and the same governing PDE system. This is achieved via appropriate relaxation source terms in the evolution equations for the distortion field and the thermal impulse. In previous work it has already been shown that the GPR model reduces to the compressible Navier-Stokes equations in the stiff relaxation limit when the relaxation times tend to zero. The governing PDE system belongs to the class of symmetric hyperbolic and thermodynamically compatible systems (SHTC), which have been studied for the first time by Godunov in 1961 and later in a series of papers by Godunov and Romenski. An important feature of the proposed model is that the propagation speeds of all physical processes, including dissipative processes, are finite.

In the absence of source terms, the homogeneous part of the GPR model is endowed with some natural involutions, namely the distortion field A and the thermal impulse J need to remain curl-free. In this talk we present a new structure-preserving scheme that is able to preserve the curl-free property of both fields exactly also on the discrete level. This is achieved via the definition of appropriate and compatible discrete gradient and curl operators on a judiciously chosen staggered grid. Furthermore, the pressure terms are discretized implicitly in order to capture the low Mach number limit of the equations properly, while all other terms are discretized explicitly. In this manner, the resulting pressure system is symmetric and positive definite and can be solved with

efficient iterative solvers like the conjugate gradient method. Last but not least, the new staggered semi-implicit scheme is also able to reproduce the stiff relaxation limit of the governing PDE system properly, recovering an appropriate discretization of the compressible Navier-Stokes equations. To the best of our knowledge, this is the first pressure-based semi-implicit scheme for nonlinear continuum mechanics that is able to preserve all involutions and asymptotic limits of the original governing PDE system also on the discrete level. Computational results for several test cases are presented in order to illustrate the performance of the new scheme.

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Adaptive High Order Well Balanced Compact Approximate Method for Systems of Conservation and Balance law

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A new family of well-balanced high-order shock-capturing finite difference numerical methods for systems of balance law is presented. These methods, called Well-Balanced Adaptive Compact Approximation Taylor (WBACAT) schemes, use centered (2p + 1)-point stencils, where p may take values in 1, 2, …, P according to a family of smoothness indicators in the stencils. The methods are an extension of the Adaptive Compact Approximate Taylor (ACAT) methods introduced in Carrillo, Macca, Parés, Russo and Zorío (2020) [1]-[2] to systems of balance law. The expression of ACAT methods for 1D and 2D systems of conservative law and its well-balance extension to systems of balance laws will be presented together with their applications several linear and nonlinear problems.

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One- and multi-dimensional CWENOZ reconstructions for implementing boundary conditions without ghost cells

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We address the issue of point value reconstructions from cell averages in the context of third order finite volume schemes, focusing in particular on the cells close to the boundaries of the domain. In fact, most techniques known in the literature (with the notable exception of [1] and related works) rely on the creation of ghost cells outside the boundary and on some form of extrapolation from the inside that, taking into account the boundary conditions, fills the ghost cells with appropriate values, so that a standard reconstruction can be applied also in boundary cells.

In [2], motivated by the difficulty of choosing appropriate boundary conditions at the internal nodes of a network, a different technique was explored that avoids the use of ghost cells, but instead employs for the boundary cells a different stencil, biased towards the interior of the domain.

Extending the approach of [2], which does not make use of ghost cells and relies on the adaptive-order CWENOZ reconstructions introduced in [3], we propose a more accurate reconstruction for the one-dimensional case and a two-dimensional one for Cartesian grids. In several numerical tests we compare the novel reconstruction with the standard approach using ghost cells.

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Efficient implementation of characteristic-based schemes on unstructured triangular grids

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Using characteristics to treat advection terms in time-dependent PDEs leads to a class of schemes, e.g., semi-Lagrangian and Lagrange–Galerkin schemes, which preserve stability under large Courant numbers, and may therefore be appealing in many practical situations. Unfortunately, the need of locating the feet of characteristics may cause a serious drop of efficiency in the case of unstructured space grids, and thus prevent the use of large time-step schemes on complex geometries.

In this work [1], we perform an in-depth analysis of the main recipes available for characteristic location, and propose a technique to improve the efficiency of this phase, using additional information related to the advecting vector field. This results in a clear improvement of execution times in the unstructured case, thus extending the range of applicability of large time-step schemes.

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Angle dependence in coupling conditions for shallow water equations at canal junctions

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In this talk we propose a numerical Riemann problem solver at the junction of one dimensional shallow-water canal networks. The junction conditions take into account the angles with which the channels intersect and include the possibility of canals with different sections. Away from the junction we assume the solution to be one dimensional, while we describe the junction as a two dimensional region where coupling occurs between the branches. We then consider the triangle formed by the intersection points of the walls of the three channels and, to this two dimensional domain, we apply conservation of mass and of the two components of momentum. We obtain three non linear equations which include a dependence on the angles, for the six unknowns at the junction to be coupled with the three equations of the characteristic curves.

The solver is illustrated with several numerical tests which underline the importance of the angle dependence to obtain reliable solutions.

High Order Semi-implicit WENO Schemes for All Mach Full Euler System of Gas Dynamics

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In this paper, we propose high order semi-implicit schemes for the all Mach full Euler equations of gas dynamics. Material waves are treated explicitly, while acoustic waves are treated implicitly, thus avoiding severe CFL restrictions for low Mach flows. High order accuracy in time is obtained by semi-implicit temporal integrator based on the IMEX Runge-Kutta (IMEX-RK) framework. High order in space is achieved by finite difference WENO schemes with characteristic-wise reconstructions adapted to the semi-implicit IMEX-RK time discretization. The schemes are proven to be asymptotic preserving and asymptotically accurate as the Mach number vanishes. Besides, they can well capture discontinuous solutions in the compressible regime, especially for two dimensional Riemann problems. Numerical tests in one and two space dimensions will illustrate the effectiveness of the proposed schemes.

MS-15
Innovative numerical methods for evolutionary partial differential equations. Part III: Control and Multiscale

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The purpose of the MS is to gather researcher interested in the development of innovative techniques for the numerical solution of evolutionary partial differential equations, concentrating in particular on the numerical treatment of mathematical models described by hyperbolic and kinetic equations. A broad range of physical systems is governed by hyperbolic systems of conservation or balance laws. Among these we recall the classical fields of gas dynamics and shallow water equations describing free surface waves, or more recent models describing traffic flow. Likewise, kinetic models, originally introduced to provide an accurate statistical description of a large collections of gas particles, can be effectively adopted to describe other behaviours, such as pedestrian flow, swarming, and other kinds of social dynamics. In several models, control problems can be effectively described by

Hamilton-Jacobi type equation, whose mathematical structure has strong analogies with the structure of hyperbolic systems of conservation laws. The mini-symposium will deal with several issues related to the numerical solution of such models, including, among others, multi-scale issues, asymptotic preserving schemes, high order discretisation in space and time, and stability analysis.

The MS is divided in three interconnected sessions, according to the main focus of the talks: I-Kinetic models, II-Hyperbolic models, III-Control and multiscale.

Dynamic Programming on a tree for the approximation of finite horizon optimal control problems

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The classical Dynamic Programming (DP) approach to the finite horizon optimal control problem is based on the characterization of the value function as the unique viscosity solution of an evolutive Hamilton-Jacobi-Bellman (HJB) equation. The DP scheme for the numerical approximation of viscosity solutions of those equations is typically based on a time discretization which is projected on a fixed space triangulation of the numerical domain. The time discretization is obtained by a one-step scheme for the dynamics and the projection on the grids typically based on a polynomial interpolation. This approach allows to compute optimal controls in feedback form and is very powerful for low dimensional optimal control problems although general convergence results have been proved in $\mathbb{R}^d$. Several methods have been proposed to mitigate the curse of dimensionality of DP schemes arising in real applications (e.g. for the control of PDEs).

We present a new approach for finite horizon optimal control problems [1, 2] where we compute the value function on a tree structure generated by the time discrete dynamics avoiding the construction of a space grid/triangulation to solve the HJB equation. This allows to drop the cost of the space interpolation, moreover the tree will guarantee a perfect matching with the discrete dynamics. We prove first order convergence to the value function for a first order discretization of the dynamics. We also discuss extensions to high-order schemes and to problems with state constraints showing also some numerical tests.

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Macroscopic and Multi-Scale Models for Multi-Class Vehicular Dynamics with Uneven Space Occupancy: A Case Study

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In this talk we propose two models describing the dynamics of heavy and light vehicles on a road network, taking into account the interactions between the two classes. The models are tailored for two-lane highways where heavy vehicles cannot overtake. This means that heavy vehicles cannot saturate the whole road space, while light vehicles can. In these conditions the creeping phenomenon can appear, i.e. one class of vehicles can proceed even if the other class has reached the maximal density.

The first model we propose couples two first-order macroscopic LWR models, while the second model couples a second-order microscopic Follow-the-Leader model with a first-order macroscopic LWR model.

Numerical results show that both models are able to catch some second-order (inertial) phenomena like stop & go waves.

Models are calibrated by means of real data measured by fixed sensors placed along the A4 Italian highway Trieste-Venice and its branches, provided by Autovie Venete S.p.A.

A Semi-Lagrangian Scheme for Hamilton-Jacobi-Bellman Equations with Oblique Boundary Conditions

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We propose a fully-discrete semi-Lagrangian approximation of second order possibly degenerate Hamilton-Jacobi-Bellman (HJB) equations on a bounded domain $\mathcal{O} \subset \mathbb{R}^N$ with oblique boundary conditions. These equations appear naturally in the study of optimal control of diffusion processes with oblique reflection at the boundary of the domain [2]. The scheme is shown to satisfy a consistency type property, it is monotone and stable. Our main result is the convergence of the numerical solution towards the unique viscosity solution of the HJB equation. The convergence result holds under the same asymptotic relation between the time and space discretization steps as in the classical setting for semi-Lagrangian schemes in $O = \mathbb{R}^N$ [1]. We show some numerical results that confirm the numerical convergence of the scheme.

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Time multiscale of sorption kinetics

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We consider numerical methods for solving a 2D transport-diffusion equation in the highly oscillatory regime. This work is part of a long project for the multiscale simulation of surfactant diffusion in presence of a moving trap. The domain of interest is typically a region inside a cylinder exterior to a bubble, which is an oscillatory spheroid. Bubble oscillations of the order of a few nanometers are selectively excited, and surfactant transport is accurately measured [4]. The oscillation frequency is of the order of hundreths Hz while the diffusing time is of the order of hours, thus the different scales in time introduce a multiscale challenge.

We start by the assumption that the motion of the bubble and the fluid are periodic in time, with a period proportional to a small parameter ε (so that it is much shorter than typical diffusion time). An approximate model is then derived, based on the asymptotic expansion of the solution in the small parameter ε.

The computational domain is defined with a 3D axisymmetric geometry, so it can be discretized on a 2D Cartesian mesh in cylindrical coordinates [3]. A detailed solution of the Stokes (or Navier-Stokes) governing the fluid motion is numerically pre-computed over a period, by a suitably developed second order scheme based on a ghost-point level-set method on a regular Cartesian grid [2]. The drift-diffusion equation on the moving fluid are then solved. The effect of the attractive-repulsive potential of the bubble is treated by a suitable boundary condition derived in [3].

We obtain an efficient and robust integrator for the detailed computation of the solution of the surfactant diffusion in presence of an oscillating trap, which is able to solve the problem without resolving the small oscillation time scale.

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Modeling and numerics of sorption kinetics

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The treatment of diffusion of surfactants (anions and cations) in presence of an oscillating bubble is an interesting interdisciplinary problem.

The system is described by drift-diffusion equations, in which the effect of the bubble is modelled through an attractive-repulsive potential acting on the anions [1, 2]. In spite of the apparent simplicity of the model, from the computational point of view the problem is a challenging one, for various reasons.

First, the problem is intrinsically multiscale in space, because the range of interaction between the bubble and the anions (nanometers) is orders of magnitude smaller than the size of the domain of interest (millimeters). Second, if the bubble oscillates then the diffusion of the ions is coupled with the motion of the fluid which has to be computed in a moving domain. Third, in typical experiments with an oscillating bubble, the period of oscillations (few milliseconds) is orders of magnitude smaller than the diffusion time (hours).

The aim of the talk is to describe a model that solves the challenge of the multiple scales in space. A multiscale single carrier model has been derived, which describes the interaction of the bubble on the anions by a suitable boundary condition of the diffusion equation for the ions, derived by mass conservation and asymptotic analysis in the region near the trap. The interaction potential is assumed to be of a small thickness δ, still with a non-negligible effect on the diffusant. The solution is formally expanded in terms of the small parameter δ. It is shown that to lowest order in δ the concentration is in local equilibrium, with a shape given by a Boltzmann distribution. From this one can derive an effective boundary condition relating the time dependence of the boundary concentration to the flux (and therefore to the normal gradient of the concentration).

The multiscale model is extended to take into account the effect of saturation (i.e. non negligible concentration), which may be relevant near the trap.

Numerical solutions are obtained by discretizing the equations on a regular Cartesian grid by a ghost-point level-set method. The resulting large sparse linear system is efficiently solved by a multigrid technique [3].

Both models are validated by comparison with accurate solutions of the drift-diffusion equation in one and two space dimensions. It is observed that as δ decreases, the discrepancy between the fully resolved model and the reduced multiscale one is approximately proportional to δ.

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An improved Rational EXponential Integrator for hyperbolic and oscillatory PDEs

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Rational exponential integrators (REXI) [2, 3] are a class of numerical methods that are well suited for the time integration of linear partial differential equations with imaginary eigenvalues. Since these methods can be parallelized in time they are well suited to exploit modern high performance computing systems. In this talk, we propose a novel REXI [1] scheme that drastically improves accuracy and efficiency. The chosen approach will also allow us to easily determine how many terms are required in the approximation in order to obtain accurate results. We provide comparative numerical simulations for a shallow water equation that highlight the efficiency of our approach and demonstrate that REXI schemes can be efficiently implemented on Graphic Processing Units.

This is a join work with Lukas Einkemmer, Alexander Moriggl, and Alexander Ostermann.

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MS-16
Recent Developments and Applications of Computer Aided Geometric Design

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The acronym CAGD (Computer Aided Geometric Design) denotes the set of mathematical and computational methods for shape analysis, reconstruction and modeling. Therefore CAGD can be seen as multidisciplinary research area where algebraic, geometric, analytical and numerical competencies are applied. CAGD reached the peak of popularity at the beginning of this millennium [2], when its basic research lines have been well established. Among them we recall Bézier and B-spline representations of free form curves and surfaces, Pythagorean Hodograph forms, subdivision algorithms, parameterization techniques and parametric interpolation and approximation also with shape constraints. Recently new advancements have been done in the area, for example, of splines on triangulations, local approximation schemes, generalized splines and adaptive multivariate spline spaces. These new developments have increased the connection of CAGD with different fields, e.g. image analysis and robotics [1, 3]. In addition, other research challenges come from the Isogeometric Analysis, which is a powerful approach

for the numerical treatment of PDEs, strictly connected to CAGD. This minisymposium aims to present some of the most recent developments and applications of CAGD.

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Chebyshevian splines, refinable B-spline bases and applications

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B-splines and their rational version (NURBS) are the mainstream technology on which CAD (Computer Aided Design) systems are based. They have also recently become crucial tools with a view to solving PDEs by means of Isogeometric Analysis methods. In both geometric design and engineering analysis it was shown that NURBS can sometimes be advantageously replaced by generalized B-splines (see, e.g., [3] and associated literature). Now, NURBS as well as generalized B-splines are few examples in the very large class of piecewise Chebyshevian splines. The splines in this more general class have proved to be useful in many domains including design, interpolation, approximation and multiresolution analysis and can as well be considered natural candidates to build isogeometric analysis methods. The main reason of the effectiveness of Chebyshevian splines is that the parameters attached to these spaces can be efficiently used to modify/improve the solutions to classical problems and that they permit the exact representation of a very large variety of geometric models.

The difficult and crucial question to answer upstream is to be able to say when spaces of such splines behave like their polynomial counterparts and in particular when they possess refinable B-spline-type bases, these bases being a prerequisite in several applications. In this talk, we will review the fundamental theoretical notions connected to the existence of refinable Chebyshevian B-spline bases (see [4] and references therein) and then introduce practical numerical procedures to check this existence, and, as the case may be, to construct the bases themselves [1, 2].

We will also illustrate how these results enable us to take full advantage of the great flexibility of Chebyshevian spline spaces by discussing a variety of application examples, which span from geometric design and interpolation up to isogeometric analysis.

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C^1 hierarchical splines on multi-patch geometries for Isogeometric Analysis

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Recent years saw a considerable development of locally refinable spline spaces, due to their application to create adaptive algorithms for modelling, approximation and analysis. In particular, in Isogeometric Analysis (IgA), it was proved that using hierarchical splines leads to efficient methods for the solution of PDEs with optimal convergence rates (see, e.g., [1] for a recent overview). Since the combination of IgA with multi-patch geometries and C^1 spline spaces defined on them is a natural way to handle high-order problems, there is the need for spaces providing such continuity. This issue was recently addressed in the case of tensor-product spaces with two or more patches (see, e.g., [3, 4]). We combine these techniques with the hierarchical framework: starting from the approach employed for the two-patch case [2], we show that we can obtain the desired locally refinable C^1 continuous spline spaces defined on multipatch geometries.

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Surfaces (Re)Construction and Approximation via Hermite spline Quasi-Interpolation

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In the present talk, the quasi-interpolant (QI) operator presented in [1] is adopted, in a tensor-product fashion, to deal with complex multipatch structures.

Primitive shapes, like spheres, cylinders, cones, and free form surfaces are combined with C^0 joints to form complex geometries. The Hermite QI easily allows us to approximate the whole considered object with a global spline representation of the desired smoothness, according to the chosen degree. The obtained QI-spline has continuous derivatives but, due to the different original parameterization of the combined shapes, some unwanted oscillations could arise, hence, reducing the quality of the final representation. In order to tackle this issue, the QI-spline global approximant is derived by using an integral-splines representation.

Moreover, thanks to the optimal approximation power properties of this Hermite QI, downsampling can be applied to reduce the required memory storage and to improve efficiency when any further simulation is needed. Typical examples include the application to real and satellite data acquired for digital elevation models: the surface reconstruction can be firstly done patch-wise, using C^0 joints and secondly, a global spline representation can be obtained.

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Geometric interpolation of ER frames with G^2 Pythagorean-hodograph curves of degree 7

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Polynomial Pythagorean–hodograph (PH) curves in space ([1]), characterized by the property that the unit tangent is rational, have many important features for practical applications. One of them is that these curves can be equipped with rational orthonormal (ON) adapted frames, among which the most straightforward one is the Euler-Rodrigues (ER) frame. This makes PH curves very useful for motion design applications. More precisely, to construct a motion of a rigid body, one needs to know how each point on this body translates and rotates. Positioning the rigid body into a local coordinate system determined by ON frame vectors prescribes the rotational part of the motion, while the origin of the coordinate system moves along the PH curve.

In this talk we first reveal the connection between geometric continuity of PH curves and their associated ER frames ([2]). We show how to construct G^k continuous ER frames that imply G^{k+1} continuous PH curves for any $k \geq 0$. General results are then applied to derive the G^2 continuous PH (spline) curves of degree 7 with G^1 continuous ER frames that interpolate on each segment the given boundary points as well as given frame and frame velocity quaternions. The problem is nonlinear and reduces to three algebraic equations with one extra free parameter that affects the ratio between lengths of both boundary tangents and can be considered as a shape parameter. A detailed asymptotic analysis of solutions in the case of interpolation data sampled from a smooth parametric curve, equipped with a general adapted frame, reveals very interesting results. Sampling the data from the Frenet frame provides us with PH interpolants that approximate the given curve with the approximation order at most 4, while sampling the boundary frames from other adapted frames (including the rotation-minimizing frame) we obtain PH interpolants of optimal approximation order 6. This confirms the known fact that the Frenet frame does not behave well for motion design applications. Several numerical examples are presented, which confirm the theoretical results.

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Spectral Signal Processing for CAGD Applications

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In geometry processing and shape analysis, several applications have been addressed through the properties of the spectral kernels and distances, such as commute-time, biharmonic, diffusion, and wave kernel distances. Spectral distances are easily defined through a filtering of the Laplacian eigenpairs and have been applied to shape segmentation and comparison with multi-scale and isometry-invariant signatures. In fact, they are intrinsic to the input shape, invariant to isometries, multi-scale, and robust to noise and tessellation.

In the context of CAGD, we will discuss the properties, discretization, computation, and main applications of the Laplace-Beltrami operator, the associated differential equations (e.g., harmonic equation, Laplacian eigenproblem, diffusion and wave equations), the Laplacian spectral kernels and distances (e.g., commute-time, biharmonic, wave, diffusion distances) [1, 2, 7]. While previous work has been focused mainly on specific applications of the aforementioned topics on surface meshes, we propose a general approach that allows us to review the Laplacian kernels and distances on graphs [3], surfaces and volumes [5, 6, 8], for signal and vector fields [4], and for any choice of the Laplacian weights [9, 10].

All the reviewed numerical schemes for the computation of the Laplacian spectral kernels and distances are discussed in terms of robustness, approximation accuracy, and computational cost, thus supporting the audience in the selection of the most appropriate method with respect to shape representation, computational resources, and target applications.

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Spline surfaces with C^1 PH isoparametric curves

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Although the isoparametric curves have no intrinsic geometrical significance, they are nevertheless useful in practical applications, such as path planning for the machining or inspection of surfaces. On the other hand, Pythagorean-hodograph (PH) curves have a distinct advantage over ordinary polynomial curves in this respect, since their arc lengths are simply polynomial functions of the curve parameter. In the present work we aim to investigate the feasibility of constructing tensor–product spline surfaces incorporating a single family of isoparametric C^1 PH spline curves. Such a construction is carried over in two steps. In the first step a bi–patch is determined in a 'Coons–like' way having as boundaries two PH curves forming a single section of the given spline curves, and two polynomial curves, see [1] for preliminary studies. In the second step the bi–patches are put together to form a globally C^1 continuous surface. In order to determine the final shape of the resulting surface, some free parameters are set by minimizing suitable shape functionals. The method can be extended to general boundary curves by preliminary approximating them with PH splines.

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MS-17
Trending topics in Uncertainty Quantification - Part I

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In many engineering applications the parameters of the underlying PDE model (e.g., coefficients, forcing terms, boundary and initial conditions, domain shape) are hampered by uncertainty. A very convenient framework is offered by probability theory: the unknown parameters can be effectively described as random variables or random fields with known probability laws. The goal of Uncertainty Quantification (UQ) is to estimate how the randomness in the input parameters affects the outputs of the PDE - typically its solution or related quantities of interest. Other related tasks are (i) to infer the probability density function of the input parameters exploiting measurements of the PDE output (inverse problems); (ii) to achieve some target by controlling the PDE system subject to uncertainty (optimization problems).

UQ techniques often rely on sampling approaches, i.e. the repeated solution of the PDE at hand for various combinations of the input parameters, thus entailing a significant computational effort. Nowadays, the most promising strategies to reduce the computational complexity are: (i) Reduced Order Modeling, which aims at replacing the original high-dimensional PDE problem with a surrogate model for the sake of UQ analyses; this approach often requires some dimensionality reduction, where the parameters with limited impact on the quantity of interest are identified and neglected; (ii) Multi-fidelity paradigms, where most of the variability is explored by querying cheap computational models, still relying on a moderate use of the computationally intensive models to correct the predictions based on the cheap models. Last, but not least, artificial intelligence and machine learning techniques are also more and more employed in this context.

The aim of this minisymposium is to bring together researchers working at the methodological level to make UQ methods more effective, as well as scientists concerned with the applications of these models to large-scale problems.

Unbiased Estimation of Log-Likelihood Gradient for a Class of Continuous-Time State-Space Models

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We consider static parameter estimation for a class of continuous-time state-space models. Our goal is to obtain an unbiased estimate of the log-likelihood gradient, which is an estimate that is unbiased even if the stochastic processes involved in the model must be discretized in time. To achieve this goal, we apply a doubly randomized scheme, that involves a novel coupled conditional particle filter (CCPF) on the second level of randomization. Our novel estimate helps facilitate the application of gradient-based estimation algorithms, such as stochastic gradient descent (SGD). We illustrate our methodology in the context of SGD in several numerical examples and compare with the Rhee & Glynn estimator. Results show consistency of the method.

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Graph Informed Deep Learning for Uncertainty Quantification in Discrete Fracture Networks

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Flow and transport characterization through fractured media in the subsurface is a crucial issue in many engineering and industrial applications, e.g. in oil and gas extraction or water resources preservation and analysis. In these applications Discrete Fracture Network (DFN) models are required, since they can accurately simulate flow through networks of subsurface fractures; unfortunately, exact position, size, orientation and hydrogeological properties of all fractures are not available, as only a statistical distribution of these data is, in general, given.

Due to the probabilistic nature of DFNs, uncertainty quantification (UQ) is a key issue in the framework of flow and transport characterization in a real fractured medium; UQ analysis usually requires thousands of DFN generations and simulations. Therefore, in order to speed up simulation processes and reduce the computational complexity of the problem, it is worth considering the application of Neural Networks (NNs) [1, 2] to perform flux regression tasks. In [1], given a set of DFNs with fixed geometry and random fracture transmissivities characterized by a log-normal distribution, for each DFN a fixed number of multitask Feed-Forward NNs have been trained with the purpose of predicting the fluxes exiting from the main boundary fractures of the network, varying the fracture transmissivities. The results obtained for the Neural Networks (NNs) show

good regression performances and a good approximation of the flux distributions of the outflowing fractures.

In this work, we describe a new NN layer to build alternative NN architectures different from the multitask ones used in [1] and [2]. We introduce extra knowledge about the DFN geometry and relationships between fractures. Specifically, we take advantage of the graph that represents the DFN and characterizes the fracture intersections; then we build a Graph Informed NN (GINN), with layers characterized by the adjacency matrix of the graph. The graph-based layers created for the GINNs of this work are inspired both by Graph and Convolutional NNs but, de-facto, the GINNs can be considered a novel typology of Spatial-Based Graph Convolutional Neural Network. The flux regression performances of GINNs are analyzed, showing the advantages of using such a kind of NN in the UQ context.

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Discontinuity Learning with Discontinuous Neural Networks

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In several practical situations related to uncertainty quantification frameworks, the Quantity of Interest (QoI) can exhibit jumps or gradient discontinuities, whose location cannot be predicted or easily detected. This situation can occur, e.g., when a problem is characterized by a complex geometry, affected by uncertainty: a small variation of the stochastic parameters may induce an abrupt change in the topological structure of the domain, which is then reflected by a jump in the values of an associated QoI.

Non-smoothness of the QoI prevents an effective use of standard stochastic collocation approaches on sparse grids, as the error decay in the numerical integrations would be exceedingly slow. To avoid this drawback, one could resort to multi-element techniques [1]; this approach however requires to properly identify a suitable partition of the parameter space; the problem of localizing discontinuity interfaces is by far non-trivial, especially in realistic problems, possibly with high stochastic dimensions. In general, the topological structure of the singularity set may be rather complicated, with non-predictable shape.

Aiming at approximating discontinuous function, and simultaneously detecting discontinuity interfaces, we consider an approach involving Neural Networks. In particular, we define a novel typology of Neural Network layers endowed with new learnable parameters and discontinuities in the space of the activation functions. These layers allow to create a completely new kind of Neural Networks, not only able to approximate discontinuous functions but also to learn and detect the discontinuity interfaces. Some preliminary tests on discontinuous functions are proposed, in order to assess the potential of such instruments.

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Non-intrusive model reduction of parametric frequency response problems via minimal rational interpolation

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Numerical methods for time-harmonic wave propagation phenomena e.g. in acoustics or elastodynamics, are often extremely computationally intensive, especially in mid- and high-frequency regimes. As such, in many cases a direct frequency response analysis has a prohibitive computational cost, and remains a major challenge. In this framework, model order reduction (MOR) methods are very promising: starting from few expensive solves of the problem, they can provide a reliable approximation of the frequency response of the system, very cheap to evaluate in a whole range of frequencies.

In many applications, the frequency response function $u : \mathbb{C} \ni z \mapsto u(z)$, which maps the frequency to (a functional of) the solution of the problem at hand, can be shown to be meromorphic, with poles at the *resonances* of the system. Accordingly, it is customary to seek a surrogate $\widetilde{u} \approx u$ among rational functions. In this talk we consider a MOR technique in this direction, *minimal rational interpolation* [1], which builds a rational approximation of the frequency response map by solving a constrained optimization problem based only on evaluations (*snapshots*) of u.

We discuss how minimal rational interpolation can be extended to problems with multiple parameters [2], for instance for frequency response analyses in presence of uncertain geometries and/or materials, where the quantity of interest is $u : \mathbb{C} \times \mathbb{R}^n \ni (z, \boldsymbol{\theta}) \mapsto u(\nu, \boldsymbol{\theta})$. The approach we describe is hybrid: for some values of $\boldsymbol{\theta}$, one builds approximate models *in z only*, by employing minimal rational interpolation; then a joint global surrogate is obtained by combining these models in $\boldsymbol{\theta}$-space.

We also describe some of the challenges of this technique. Most notably, combining frequency models in a sensible way is an extremely complex task, requiring an adequate theoretical understanding of how resonances can evolve as $\boldsymbol{\theta}$ changes. This is also linked to the obvious problem of determining how many frequency surrogates are required to achieve reasonable accuracy, an issue which becomes critical in the high-dimensional setting.

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Deep neural network surrogates in shape uncertainty quantification

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We consider the point evaluation of the solution to interface problems with geometric uncertainties, where the uncertainty in the obstacle is described by a high-dimensional parameter, as a prototypical example of non-smooth dependence of a quantity of interest on the parameter. We focus in particular on an elliptic interface problem and a Helmholtz transmission problem. The non-smooth parameter dependence poses a challenge when one is interested in building surrogates. Indeed, high-order methods show poor convergence rates, while methods which are able to track discontinuities usually suffer from the so-called curse of dimensionality. For this reason, in this talk we propose to build surrogates for point evaluation using deep neural networks. We provide a theoretical justification for why we expect neural networks to provide good surrogates. Furthermore, we present numerical experiments showing their good performance in practice. We observe in particular that neural networks do not suffer from the curse of dimensionality, and we study the dependence of the error on the number of point evaluations (which coincides with the number of discontinuities in the parameter space), as well as on several modeling parameters, such as the contrast between the two materials and, for the Helmholtz transmission problem, the wavenumber. This presentation is based on the work [1].

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A deep learning-based operator approximation for model order reduction in structural mechanics

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Solving inverse uncertainty quantification (UQ) problems governed by PDEs means to estimate unknown or uncertain model parameters from observations of suitable quantities of interest. In a Bayesian framework, Markov chain Monte Carlo methods (MCMC) are a popular way to sample the posterior distribution of the random inputs, however, requiring several queries to the forward problem. Relying on high-fidelity models, such as the Galerkin-Finite Element method, entails huge computational costs, thus making the solution to inverse UQ problems unfeasible as soon as the dimension of the underlying discrete PDE problem becomes too large. In this respect, we replace computationally expensive high-fidelity models with computationally inexpensive reduced-order models (ROMs), obtained through a Galerkin projection of the high-fidelity problem onto a low-dimensional space built, e.g., through proper orthogonal decomposition (POD). However, to make the assembling of the ROM independent of the FOM dimension, intrusive and expensive hyper-reduction stages are usually required [1].

To deal with nonlinear elastodynamics problems, and overcome the hyper-reduction bottleneck, we propose a novel strategy for learning nonlinear ROM operators using deep neural networks [2]. The resulting Deep-HyROMnet is a physics-based model, still relying on a POD-Galerkin strategy, but employing a deep neural network architecture to approximate reduced residual vectors and Jacobian matrices once a Galerkin projection has been performed. The proposed approach has been assessed in several scenarios dealing with fast simulations and parameter identification in nonlinear structural mechanics.

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MS-18
Trending topics in Uncertainty Quantification - Part II

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In many engineering applications the parameters of the underlying PDE model (e.g., coefficients, forcing terms, boundary and initial conditions, domain shape) are hampered by uncertainty. A very convenient framework is offered by probability theory: the unknown parameters can be effectively described as random variables or random fields with known probability laws. The goal of Uncertainty Quantification (UQ) is to estimate how the randomness in the input parameters affects the outputs of the PDE - typically its solution or related quantities of interest. Other related tasks are (i) to infer the probability density function of the input parameters exploiting measurements of the PDE output

(inverse problems); (ii) to achieve some target by controlling the PDE system subject to uncertainty (optimization problems).

UQ techniques often rely on sampling approaches, i.e. the repeated solution of the PDE at hand for various combinations of the input parameters, thus entailing a significant computational effort. Nowadays, the most promising strategies to reduce the computational complexity are: (i) Reduced Order Modeling, which aims at replacing the original high-dimensional PDE problem with a surrogate model for the sake of UQ analyses; this approach often requires some dimensionality reduction, where the parameters with limited impact on the quantity of interest are identified and neglected; (ii) Multi-fidelity paradigms, where most of the variability is explored by querying cheap computational models, still relying on a moderate use of the computationally intensive models to correct the predictions based on the cheap models. Last, but not least, artificial intelligence and machine learning techniques are also more and more employed in this context.

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Uncertainty quantification and continuous learning for real-time estimates of the remaining life of engineering systems

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Health monitoring and failure prognosis are key elements in the operation and lifecycle management of complex and safety-critical engineering systems. Common approaches to Prognostics and Health Management (PHM) aim at estimating the Remaining Useful Life (RUL) starting from the data measured from the monitored system. Usually, a two-steps approach is adopted, first estimating the current health status of the equipment and then leveraging this information to infer the remaining time to failure [1].

The estimation is commonly affected by multiple sources of uncertainty. The measurement of physical signals is limited by the accuracy of sensors and by the external disturbances inherent in field applications. Modeling the effects of incipient faults on the system behavior is difficult, and results in additional uncertainty when estimating the current health condition. Eventually, the propagation rate of the damages is hard to estimate accurately and may change in a hardly predictable manner. All these aspects pose major difficulties in achieving accurate, robust and computationally efficient failure prognosis [2, 3].

We propose and discuss a robust computational scheme for RUL prediction, able to deal with uncertainty. The use of model order reduction and machine learning helps reducing the computational burden associated with the failure prognosis, resulting in a fast and efficient estimation of Remaining Useful Life, suitable for real-time evaluation.

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Towards a integrated platform for the investigation of hemodynamics in thoracic aorta: UQ in simulations and experiments

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Techniques based on Computational Fluid Dynamics (CFD) have been extensively used in the last few years to investigate hemodynamics inside arteries in both healthy and diseased subjects at a patient-specific level. Indeed, CFD enables the investigation of pressure and flow fields at a time and space resolution unachievable by any *in-vivo* measurement and the computation of a variety of quantities and indicators that are difficult to be obtained from mesurements, e.g. wall shear stresses. On the other hand, different sources of uncertainties are present in CFD models, which can propagate and affect the hemodynamic quantities of interest. Among them are boundary conditions assumed at the inflow and outflow ([1]) of the computational domain and modeling of the vessel wall compliance properties.

The integration of patient-specific medical imaging data is necessary to reduce the modeling assumptions. In particular, 4D-Flow Magnetic Resonance Imaging (MRI) is a non-invasive technique that allows not only the geometry to be acquired, but also the velocity field to be measured at different points in space and at different time instants, although, as previously said, at a resolution significantly lower than that achievable in CFD simulations. MRI data can also be used to provide patient-specific inlet boundary conditions to numerical simulations (see e.g. [2]). A framework integrating *in-vivo* MRI data into the numerical simulation of a healthy thoracic aorta was presented in [3]. MRI data were used to provide/calibrate inlet and outlet boundary conditions, evaluate the elastic properties of the vessel walls, and validate the simulation results. The integration was all in all successful, but some discrepancies between numerical results, although calibrated, and *in-vivo* data were observed, which can be ascribed to limitations of CFD models and also to inaccuracies in MRI data. For instance, in *in-vivo* measurements it is difficult to characterize the rotation and translation movements of the inlet section. Recently, we have developed a fully controlled and sensorized circulatory mock loop able to reproduce the fluid dynamic physiological conditions for 3D-printed aortic models

([4]). The mock-circulatory loop is composed of an active component, i.e. a custom speed-controlled piston pump, and of a series of passive components to model the systemic resistances and compliances at each branch. This experimental setup allows a few uncertainties in measurements to be eliminated: the flow rate is controlled and it is the same for each cardiac cycle, the model is fixed and the wall model properties are known. In this way, clearer indications of the accuracy and possible improvements of CFD models can be obtained.

We focus herein on the effect of uncertainties in the inlet boundary condition both in numerical simulations and experiments. To this aim, we consider real healthy and aneurysmatic geometries acquired by MRI for which the experiments and numerical simulations are performed. We use the open-source software SimVascular to carry out the simulations, whereas we perform the experiments in the circulatory mock-loop. A systematic sensitivity analysis is carried out to the shape of the inlet flow rate waveform. We consider the cardiac cycle period and the stroke volume, i.e. the amount of blood pumped by the left ventricle of the heart in one cardiac cycle, as uncertain parameters to define the flow-rate waveform. Moreover, we also consider the spatial distribution of the inlet velocity. Because of the significant cost of each evaluation of the deterministic results, a stochastic approach is chosen, in which the selected parameters are considered as random variables with a given probability distribution. The uncertainty in the input parameters is propagated through the numerical model or the experiments by using the generalized Polynomial Chaos (gPC) approach and continuous response surfaces of the output quantities of interest in the parameter space are recovered through a "surrogate" model, which requires a limited number of deterministic evaluations. Among the selected input parameters, the stroke volume and the cardiac cycle period have the highest influence on the output quantities both in simulations and in experiments. In particular, the Time-Averaged Wall Shear Stresses (TAWSS) are highly sensitive to the shape of the flow rate waveform, especially in the aortic arch and in the descending aorta. The dominating parameter is the stroke volume, with a general increase of TAWSS with increasing the stroke volume. The stroke volume has also a strong impact on the velocity field in the regions characterized by large curvature, with highly distorted or recirculating flow appearing when the stroke volume is increased. Finally, the spatial distribution of the inlet velocity has a significant impact on the velocity distribution and wall shear stresses in the ascending aorta only, whereas lower effects are found in the aortic arch and the descending aorta.

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A Multi-fidelity Adaptive Gaussian Process for the Uncertainty Quantification of an Autonomous Surface Vehicle

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The Shallow Water Autonomous Multipurpose Platform (SWAMP) is a 1.24 m long autonomous surface vehicle designed for the acquisition of the environmental parameters in the extremely shallow waters of wetlands (e.g., rivers and lakes) [1]. The payload varies depending on the type and purpose of the survey. Therefore, the assessment of the performance (i.e., hydrodynamic resistance) needs to consider the uncertainty associated to the operating conditions. The objective of the present work is the uncertainty quantification (UQ) of the resistance, sinkage, and trim subject to stochastic payload weight and location of the center of gravity. A linear potential-flow solver (namely the WAve Resistance Program, WARP) coupled with the rigid body equations of motion is used for the performance prediction. A multi-fidelity (MF) surrogate model based on

Gaussian process (MF-GP) is used to build the response surface of the resistance versus the uncertain parameters. Finally, the UQ is achieved by a Monte Carlo sampling of the response surface. In this work, the fidelity level is defined by both the computational grid size and the convergence tolerance of the coupling solver between hydrodynamic loads and motions. Adaptive sampling methods are used to add training points where it is most informative, also selecting the most convenient fidelity level [2].

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Weighted Reduced Order Methods For Uncertainty Quantification Problems: State Of The Art And Applications In Fluids Dynamics and Optimal Flow Control

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This talk focuses on stochastic Partial Differential Equations depending on physical and/or geometrical parameters (PDE($\boldsymbol{\mu}$)s). In several scientific fields, stochastic models are used and analysed to guarantee more reliability in the simulations with respect to the deterministic ones. In this setting, the parameters carry uncertainties and, thus, the solution can be affected by this uncertainty as well. Furthermore, the classical statistical analysis based on Monte Carlo methods might lead to unbearable computational costs to deal with. The aim of the talk is to introduce weighted reduced order methods (w-ROMs) to accelerate standard Monte Carlo techniques. First, the reduced space is built taking into account the underlying parameters probability distribution and the influence of quadrature rules over the approximation [4]. Then, the problem is solved in this low-dimensional framework in a faster, but still accurate, way. We will test the methodology in several fluid dynamics applications: from linear advection-dominated phenomena [3] to nonlinear equations [2]. Furthermore, we successfully employed w-ROMs to Optimal Control problems in environmental sciences [1], building a reliable tool to bridge the gap between simulations and data.

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Bacteria transport within a riverbank filtration context under uncertainty

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MAR (Managed Aquifer Recharge) through riverbank filtration is an important method to ensure sustainable drinking water. The need for potable water has strongly increased over the recent years due to (i) population dynamics, (ii) increased urbanization, and (iii) climate and global changes. Yet, water quality related to transport of pathogens (such as bacteria) from the surface into groundwater systems is a matter of concern, especially in urbanized regions where the need for potable water is highest. We developed a reactive transport model to study bacteria transport at a riverbank filtration site (in Germany). The reactive transport model is characterized by a level of complexity which requires a significant parametrization through a large number of parameters, encompassing quantities driving flow as well as solute and bacteria transport (for a total of about 60 model parameters, which are typical affected by uncertainty). This high parametrization makes model calibration an arduous (if not impossible, considering the limited experimental data usually available) task. We show the benefit of using a Global Sensitivity Analysis (i) to identify the most relevant model parameters with respect to target variables of interest (such as pressure heads, concentrations of chloride, oxygen, coliforms, and Escherichia coli) and (ii) to guide the experimental activity as well as the model calibration workflow. The highest contributions to predict key features of bacteria transport (and the associated uncertainty) stem from inactivation coefficients, the colmation layer permeability as well as seasonal effects such as floods and changes of oxic to anoxic conditions. Finally, we calibrate the model within a stochastic framework, to provide model parameter estimates as well as to quantify their uncertainty and provide the ingredients needed for a risk-based management decision procedure.

Dealing with uncertainties in structural damage localization by reduced order modeling and deep learning-based classifiers

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Trying to localize structural damages, starting from online acquired data, is a complex task hampered by several sources of uncertainties. Indeed, the response of a structure is not affected just by the onset and propagation of damage, but also depends on loading and environmental conditions. To distinguish between the different sources of variability of a system, a statistics-based classifier is employed [1]. Its design is based on a deep learning architecture, featuring a three-layers fully convolutional network for sake of pattern recognition in the data [2]. The convolutional layers map the input data into linearly separable classes, each one featuring a possible damage state. The classification is done by associating a confidence level to each class. To train the classifier, a synthetic dataset is numerically generated in an offline phase by using a numerical model (playing the role of digital twin) of the structure. The more representative the training dataset of the damage and working conditions undergone by the structure, the better the prediction capability of the classifier on online acquired data. For this reason, it is extremely important to define the most plausible scenarios that might be experienced by the structure, and to include them in the training dataset in a statistically representative way. A certain number of parameters, controlling the working conditions and the material properties in different

subregions of the structure, are introduced with associated effective statistical distributions to attain this goal. Due to the adopted stochastic framework, the construction of the training dataset may require a great number of model evaluations, typically unaffordable from a computational point of view. Instead of relying on "expensive" full order models (e.g. based on the finite element method), a reduced order modelling approach is adopted to reduce the cost of each model evaluation, allow the creation of larger statistically-representative dataset and, at a later stage, ensure the effectiveness of the whole procedure [3]. Parametric model order reduction techniques are adopted to handle the dependency of the system on working and damage conditions, and, whenever this dependency implies the re-assembling of the full order model numerical operators, extremely expensive from a computational point of view, hyper-reduction is exploited [4].

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MS-19
New Mathematical Voices for Biomedicine and Neuroscience

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This minisymposium aims at giving an overview on new and innovative computational methods currently emerging in biomedicine and neuroscience. The main applications that will be addressed are magnetoencephalography, electrical impedance tomography, Terahertz microscopy, dMRI and brain structural connectivity analysis, while the math-

ematical techniques that will be described are concerned with inverse problems theory, numerical simulation, numerical optimization.

The speakers are promising young researchers with an excellent curriculum. The goal of the minisymposium is to promote their perspectives on this hot topic of applied mathematics as well as to stimulate discussions and exchange of ideas.

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Methods for analysing the statistical dependency between pairs of multi-dimensional neural time series

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The presence of functional interactions between pairs of human brain regions (the so-called "functional connectivities") is normally inferred by analysing the statistical dependency between the time series (e.g. functional magnetic resonance imaging, electroencephalographic or magnetoencephalographic signals) associated with each pair of regions. Given that each area is composed of multiple spatial locations associated with different scalar time series, we have that the data related to a region has a multi-dimensional nature. Since the standard statistical methods used in this field take as input scalar signals, the multi-dimensional data are usually reduced to representative one-dimensional

time series (e.g. through principal component analyses). Nevertheless, the application of a dimensionality reduction approach may lead to a loss of potentially important information regarding the complex dependencies between the regions [2]. This concern led to the definition of different "multi-dimensional connectivity methods" (MD-conn methods) that, as opposed to the standard approaches, allow to investigate the presence of neural interactions by directly relying on the multi-dimensional data [1, 3]. In my talk I will start by presenting the main MD-conn methods and, through a number of simulated and real data examples, by illustrating their strengths and weaknesses. Then, I will focus on a novel MD-conn method based on the polyspectral analysis, which can be used to investigate the presence of specific nonlinear interactions, and its application to real-time analysis. This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 810377). The content reflects only the authors′ view and the ERC Executive Agency is not responsible for the content.

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Computational framework for applying electrical impedance tomography to head imaging

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This work introduces a computational framework for applying absolute electrical impedance tomography (EIT) to head imaging without accurate information on the head shape or the electrode positions. In medical applications of EIT, the exact shape of the imaged object is usually unknown. Even if one has some generic information about the average shape of the imaged part of the human body, the natural variations between different subjects are often significant. Unfortunately, EIT is known to be a nonlinear, highly illposed inverse problem and extremely sensitive to geometric mismodeling of the imaged object. In this work, a library of fifty heads is employed to build a principal component model for the typical variations in the shape of the human head, which leads to a relatively accurate parametrization for head shapes with only a few free parameters. The modeling error is accounted for as an additive approximation error term in the measurement model. The actual inversion is then performed by reconstructing the deviation of the conductivity (inside the examined head) from an expected conductivity using the average head model, accounting for both the actual measurement noise and the approximation error noise within the Bayesian paradigm [1, 2].

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On the feasibility of random sampling for EEG inverse problem

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In the last years attention has growed toward non-invasive brain imaging techniques, the two most common being the magnetoencefalography (MEG) and the electroncefalography (EEG) [3]. In EEG brain's electrical activity is estimated using electric field sensed on the patient's scalp and, from this boundary data, the electric current density inside the brain is estimated as the solution of an ill-posed inverse problem.

Recently, sensor arrays used in EEG have become more and more portable, and they may soon be suitable for real time non-invasive brain-machine interface, but a portable implementation is still impeded by the high computational power required to compute the solution of the inverse problem.

Addressing the issue, a stochastic technique called RAMSET has been proposed [1] to reduce the dimensionality of MEG problem by uniformly sampling the source space, hence reducing the size of the problem accordingly.

In this conference talk, early results about the use of the RAMSET technique for the EEG problem are presented. Experimental evidence obtained through numerical simulations on synthetic EEG data shows that the reconstruction error of RAMSET is comparable to that of classical inversion methods [4, 3], but with a reduced computational load.

In these tests, RAMSET has been implemented in combination with different common solvers for EEG inverse problem and the results confirm that the source space sampling procedure, albeit reducing the dimensionality of the problem, does not seem to significantly affect the performances of those solvers. We also stress that RAMSET is very simple, if compared to other dimensionality reduction techniques.

As an additional test, the validity of RAMSET itself is investigated: the matrices representing the full and the reduced problem are compared using different metrics [4, 5, 6, 2], showing the strong relation that exists between them.

To conclude, although a complete study has not been conducted yet, experimental evidence suggests that RAMSET is also capable of locating deep sources, which is now one of the principal issues in M/EEG research.

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Scaled, adaptive and generalized FISTA algorithm for sparse image super-resolution problems

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Forward-backward (FB) algorithms have become standard tools for solving composite convex optimization problems arising in signal and image processing, thanks to their easy applicability and their fast convergence properties whenever endowed with appropriate inertial updates, as in the case of the popular FISTA algorithm [1]. However, their successful application relies on the accurate estimation of the Lipschitz constant of the gradient of the differentiable component; whenever such estimate is coarse, the practical effectiveness of FB methods may be limited. Possible remedies to solve this issue include the adoption of adaptive backtracking procedures [3] and suitable scaling approaches aimed at capturing some second-order information of the smooth component; the use of scaling approaches is particularly effective in the context of image reconstruction problems with signal-dependent Poisson noise in a variety of applications ranging from biological to astronomical imaging (see [2] and references therein).

In this talk we propose SAGE-FISTA [5] (SCaled Adaptive GEneralized FISTA) for the efficient solution of (possibly strongly) convex optimization problems. SAGE-FISTA couples a scaling strategy for the proximal–gradient step with an adaptive non-monotone backtracking procedure, which allows for the adjustment of the steplength along the iterations in order to improve the convergence speed. We prove a linear convergence result for the function values, which depends on both the strong convexity moduli of the two functions and the upper and lower bounds on the eigenvalues of the scaling matrices. The proposed algorithm is then validated on some image super-resolution problems where a sparsity-promoting regularization term is coupled with a weighted-ℓ_2 data fidelity [4]. Our numerical experiments show that SAGE-FISTA boosts the practical convergence rate in

function values with respect to a standard implementation of FISTA, as well as being an efficient inner solver for iteratively reweighted ℓ_1 algorithms.

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Convex Optimization Modeling for Microstructure Informed Tractography with anatomical priors

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Diffusion MRI is a noninvasive imaging technique that has been extensively used to study the neuronal architecture of the brain using tractography. However, recent studies highlighted that the anatomical accuracy of the reconstructions is inherently limited and challenged its appropriateness [3]. A number of solutions have been proposed to *improve the accuracy of tractography reconstructions*. The common idea consists of combining the reconstructed set of streamlines - i.e. curves connecting different brain regions forming the tractogram - with signal forward-models to assess their actual contribution to the acquired diffusion MR images and filter out the most implausible using global optimization techniques. Among them, the Convex Optimization Modeling for Microstructure Informed Tractography (*COMMIT*) [1] framework states that, given a set of streamlines, or tractogram, the acquired dMRI data can be modeled as $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \eta$, where $\boldsymbol{y}$ contains the dMRI signal, η is the noise and the matrix $\boldsymbol{A}$ encodes the possible signal contributions of each streamline to the voxels it passes through according to a given forward model. The actual contributions $\boldsymbol{x}$ of the streamlines can be conveniently estimated using non-negative least-squares: $\underset{\mathbf{x}\geq 0}{\operatorname{argmin}} ||\mathbf{A}\mathbf{x} - \mathbf{y}||_2^2$. This formulation assumes invariance of a microstructural parameter (e.g. intra-axonal signal fraction, axon diameters, ...) along a particular pathway and uses this prior to get more robust estimates of both the trajectory and microstructural properties of a fiber. However, although the filtered tractograms provide biologically more accurate estimates of connectivity, this method is not effective in reducing the presence of false positive bundles. Recently we have introduced a novel processing framework, named COMMIT2, for dramatically improving the specificity of the estimated brain networks without affecting their sensitivity [2]. It builds on COMMIT adding the fundamental observation that streamlines are not "just lines" but represent neuronal fibers and such neuronal fibers are naturally organized in bundles. Mathematically this is achieved with the *group lasso* regularization.The additional term in the cost function penalizes the contributions at the level of groups and promotes convergence towards a solution that explains the measured dMRI data with the minimum number of bundles. We will show the performances of COMMIT2 on both synthetic and invivo data highlighting possible new extensions.

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Optimal regularization approaches for estimating the cross-power spectrum from magnetoencephalographic data

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Magnetoecenphalography (MEG) is a modern neuroimaging technique that measures the magnetic field produced outside the scalp by the neural currents. Studying functional connectivity from MEG data consists in quantifying the statistical relationships between the activity estimated at different brain areas. Typical approaches for connectivity estimation consist of two steps [1]. First a linear ill-posed inverse problem is solved to reconstruct the time courses, $\mathbf{x}(t)$, of the neural sources that generate the recorded data. Then a proper connectivity metric is computed between the time series estimated at different brain locations. Due to the oscillatory nature of brain processes, many of these connectivity metrics are computed in the frequency domain starting from the cross-power spectrum of the neural sources, henceforth denoted as $\mathbf{S}^{\mathbf{x}}(f)$.

In this talk, I will consider Tikhonov regularization to solve the MEG inverse problem and I will investigate whether the regularization scheme that leads to the optimal estimate of the source time course also leads to an optimal estimate of the corresponding cross-power spectrum.

In detail, in a first scenario I will assume both the noise and the unknown source time courses to be realization of white noise Gaussian processes. Under these assumptions,

I will analytically prove that to minimize the ℓ_2-norm of the error in estimating $\mathbf{S}^{\mathbf{x}}(f)$ the Tikhonov regularization parameters needs to be lower than half of the value that minimize the ℓ_2-norm of the error for $\mathbf{x}(t)$ [2].

To model more realistic connectivity patterns, in a second scenario, I will assume $\mathbf{x}(t)$ to be the realization of a multivariate autoregressive model. By using simulated data I will show that also the spectral complexity of the source time–courses impact the value of the Tikhonov regularization parameter that returns the best estimate of $\mathbf{S}^{\mathbf{x}}(f)$ [3].

These results suggest that the standard two-step approach may by inherently sub-optimal. To overcome this limitations, a novel method to directly estimate $\mathbf{S}^{\mathbf{x}}(f)$ from the recorded data is proposed. In detail, by exploiting the linearity of the MEG inverse problem and of the Fourier transform, it is possible to write the cross-power spectrum of the data as the linear combination of the cross-power spectrum of the neural sources. In the last part of the talk, I will show some preliminar result on the lasso-based approach we implemented to solve this new linear inverse problem.

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Recent Results in Kinetic Theory and Applications Part I

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This minisymposium is concerned with innovative models and numerical methods having roots in kinetic theory. In recent years, this theory provided the backbone for the description of many phenomena at different scales. Similarly to the original gas dynamic setting, the exchange of distinctive properties can be reduced by suitable microscopic interaction rules whose evolution at the aggregate level is ruled by Boltzmann-type operators. Nowadays countless applications ranging from reactive mixtures to social interacting systems utilize this framework inspiring new frontiers both in the development of numerical methods and for theoretical investigations.

A survey of Monte Carlo methods for kinetic equations

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In this talk, we will give an overview of different direct simulation Monte Carlo (DSMC) methods for the numerical solution of kinetic equations. Particular emphasis is given to some recently developed hybrid and asymptotic preserving Monte Carlo methods for accelerating standard DSMC computations both in the case of BGK equations as well as in the more challenging case of the Boltzmann model.

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Stationary non-equilibrium solutions for coagulation equations

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Smoluchowski's coagulation equation, an integro-differential equation of kinetic type, is a classical model for mass aggregation phenomena extensively used in the analysis of problems of polymerization, particle aggregation in aerosols, drop formation in rain and several other situations.

In this talk I will present some recent results on the problem of existence or non-existence of stationary solutions to coagulation equations, for single and multi-component systems, under non-equilibrium conditions which are induced by the addition of a source term for small cluster sizes ([1]). The most striking feature of these stationary solutions is that, whenever they exist, the solutions to multi-component systems exhibit an unusual "spontaneous localization" phenomena. More precisely, the stationary solutions to the multi-component coagulation equation asymptotically localize into a direction determined by the source term ([2]). (Joint work with M.A. Ferreira, J. Lukkarinen and J.J.L. Velázquez)

References

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Boltzmann-type equations for multi-agent systems with label switching

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In this talk, we propose a Boltzmann-type kinetic description of mass-varying interacting multi-agent systems. Our agents are characterised by a microscopic state, which changes due to their mutual interactions, and by a label, which identifies a group to which they belong. Besides interacting within and across the groups, the agents may change label according to a state-dependent Markov-type jump process. We derive general kinetic equations for the joint interaction/label switch processes in each group. For prototypical birth/death dynamics, we characterise the transient and equilibrium kinetic distributions of the groups via a FokkerPlanck asymptotic analysis. Then we introduce and analyse a simple model for the contagion of infectious diseases, which takes advantage of the joint interaction/label switch processes to describe quarantine measures.

References

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Reaction–diffusion equations derived from kinetic models and their Turing instability

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We study a mixture composed by a polyatomic and a monatomic gas, that diffuse in a gaseous background and undergo elastic or inelastic scattering and chemical reactions. Inspired by [1], we perform the derivation of proper reaction–diffusion equations for the number densities of the constituents, from suitably rescaled kinetic Boltzmann equations. The elastic scattering with the host medium is the dominant process, while we consider two different scalings for the various chemical reactions: the first option leads to a system of three reaction–diffusion equations, while the second regime to two reaction–diffusion equations. This last system turns out to be similar to the classical Brusselator [2]. We discuss the Turing instability [3] properties of these macroscopic systems, showing their dependence on particle masses, on collision frequencies of the Boltzmann operators, and, above all, on particle internal energies.

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Kinetic and macroscopic models for epidemic dynamics

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We introduce a mathematical description of the impact of sociality in the spread of infectious diseases by integrating an epidemiological dynamics with a kinetic modeling of population-based contacts [2]. The kinetic description leads to study the evolution over time of Boltzmann-type equations describing the number densities of social contacts of susceptible, infected and recovered individuals, whose proportions are driven by classical compartmental models in epidemiology [1]. Explicit calculations show that the spread of the disease is closely related to moments of the contact distribution. We conduct numerical experiments which confirm the ability of the model to describe different phenomena characteristic of the rapid spread of an epidemic.

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MS-21
Recent Results in Kinetic Theory and Applications Part II

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This minisymposium is concerned with innovative models and numerical methods having roots in kinetic theory. In recent years, this theory provided the backbone for the description of many phenomena at different scales. Similarly to the original gas dynamic setting, the exchange of distinctive properties can be reduced by suitable microscopic interaction rules whose evolution at the aggregate level is ruled by Boltzmann-type operators. Nowadays countless applications ranging from reactive mixtures to social interacting systems utilize this framework inspiring new frontiers both in the development of numerical methods and for theoretical investigations.

A viral load-based model for epidemic spread on spatial networks

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We propose a Boltzmann-type kinetic model of the spreading of an infectious disease on a network. The latter describes the connections among countries, cities or districts depending on the spatial scale of interest. The disease transmission is represented in terms of the viral load of the individuals and is mediated by social contacts among them, taking into account their displacements across the nodes of the network. We formally derive the hydrodynamic equations for the density and the mean viral load of the individuals on the network and we analyse the large-time trends of these quantities with special emphasis on the cases of blow-up or eradication of the infection. By means of numerical tests, we also investigate the impact of confinement measures, such as quarantine or localised lockdown, on the diffusion of the disease on the network.

This talk is based on [2], which is part of a more extended research line comprising also works [1, 3].

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Mean-field optimal control problems with transient leadership

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A mean-field optimal control problem of multi-population dynamics via transient leadership is considered. The agents in the system are described by their spatial position and their probability of belonging to a certain population. The dynamics in the control problem is characterized by the presence of an activation function which tunes the control on each agent in a selective way, and according to the membership to a population, which, in turn, evolves according to a Markov-type jump process. This way, a hypothetical policy maker can select a restricted pool of agents to act upon based, for instance, on their time-dependent influence on the rest of the population. A finite-particle control problem is studied and its mean-field limits. Specific applications in the context of opinion dynamics are discussed with different numerical experiments

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Multistability and time-periodic spatial patterns in the cross-diffusion SKT model

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The Shigesada–Kawasaki–Teramoto model (SKT) was proposed to account for stable inhomogeneous steady states exhibiting spatial segregation, which describes a situation of coexistence of two competing species. Even though the reaction part does not present the activator-inhibitor structure, the cross-diffusion terms are the key ingredient for the appearance of spatial patterns. We provide a deeper understanding of the conditions required on both the cross-diffusion and the reaction coefficients for non-homogeneous steady states to exist, by combining a detailed linearised and weakly non-linear analysis with advanced numerical bifurcation methods via the continuation software `pde2path`. We study the role of the additional cross-diffusion term in pattern formation, focusing on multistability regions and on the presence of time-periodic spatial pattern appearing via Hopf bifurcation points.

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On a Multiscale Model for Glioma Invasion: the Effects of Acidity and Vasculature

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Glioblastoma are malignant brain tumors arising from the glia cells of the central nervous system. Their characteristics of highly aggressiveness and invasiveness are linked to the brain structure, that determines the typical infiltrative patterns in the tumor evolution. Here we propose a multiscale model for the description of the processes of glioma growth and invasion in the brain, with a specific focus on the effects of vasculature availability and hypoxia. Starting from the microscopic description of interactions between glioma, tissue, and protons, we consider a system of coupled kinetic transport equations for tumor cells, relying on the go-or-growth hypothesis, and for endothelial cells (ECs). Using a parabolic limit, we derive a macroscopic model describing both tumor and ECs evolution, as well as proton dynamics. Using real data about brain geometry, numerical simulations are performed to asses the role of vasculature, acidity, and phenotypic heterogeneity in influencing tumor proliferation and migration [1].

References

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Hydrodynamic equations for a mixture of monoatomic gases in different regimes

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We formally derive macroscopic (Euler and Navier-Stokes) equations for an inert gas mixture from a recent kinetic model of BGK-type [3]. The collisional process is described by a sum of binary relaxation operators, each of which involves the interactions of a pair of gaseous components. Such operator mimics the structure of Boltzmann operator for mixtures and allows to deal with different hydrodynamic regimes, accordingly to the dominant phenomenon.
In this presentation we derive macroscopic descriptions when the dominant phenomenon is constituted by the entire collision process and in presence of dominant intra-species interactions [2]. In particular, the latter leads to a multi-velocity and multi-temperature model, which can be very useful to investigate the dynamics of an $\varepsilon-$mixture of heavy and light components (e.g. a mixture of ions and electrons) [1].

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MS-22
New trends in tomography: From microscopy to astronomy

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Tomography has been one of the most important applications of mathematics since its development by Allan M. Cormack and Godfrey N. Hounsfield, in 1960s, when the first scanning device for X-ray computed tomography appeared (Nobel prize in 1979). In mathematical terms, it is related to the application of the so-called Radon transform, studied by Johann Radon in 1917. Currently the sector of tomographic imaging is still a fruitful field for the applied mathematicians, especially for those working on inverse problems and mathematical imaging. Therefore, it is of primary importance to provide and study new mathematical models, capable of explaining the physical experiments, and to develop sophisticated and efficient reconstruction algorithms which are especially able to handle big data. In Austria, the special research project "Tomography across the scales" consisting of six Institutes and more than 20 researchers (members and collaborators) is working in this direction to produce new mathematical tools for emerging imaging modalities. The aim of this workshop is to bring together experts and young researchers working in this field and discuss new and recent analytical and numerical techniques, related to adaptive optics, data-driven reconstructions algorithm, image processing and integral transforms. We would like to attract and stimulate the curiosity of young researchers, who started recently working on this field, and provide new insights into these topics.

Compressed sensing photoacoustic tomography reduces to compressed sensing for undersampled Fourier measurements

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Photoacoustic tomography (PAT) is an emerging imaging modality that aims at measuring the high-contrast optical properties of tissues by means of high-resolution ultrasonic measurements. The interaction between these two types of waves is based on the thermoacoustic effect. In recent years, many works have investigated the applicability of compressed sensing to PAT, in order to reduce measuring times while maintaining a high reconstruction quality. However, in most cases, theoretical guarantees are missing. In this talk, we show that in many measurement setups of practical interest, compressed sensing PAT reduces to compressed sensing for undersampled Fourier measurements. This is achieved by applying the theories of Riesz bases and nonuniform Fourier series.

References

[1] G. S. Alberti, P. Campodonico and M. Santacesaria, *Compressed sensing photoacoustic tomography reduces to compressed sensing for undersampled Fourier measurements*, SIAM J. Imaging Sci. (to appear).

Coherence enhancing variational image restoration

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In this talk we will propose a variational method for coherence enhancing image restoration, which is based on a non-convex, non-local integral functional. The functional penalises, locally around each point in the image, the size of the inner products of the gradients and thus enforces the reconstructed image to have locally coherent gradients. Because of the separate convexity of the integrand, one obtains lower semi-continuity of the resulting regularisation functional, and, as a consequence, the existence of minimisers. In addition, although the functional as a whole is non-convex, its particular structure allows for the application of exact line search methods, which reduces the chance of numerical algorithms converging to local minima.

The proposed idea is closely related to the PDE based method introduced by Weickert [1], where an image is evolved according to an anisotropic diffusion tensor, which is constructed by using local gradient information in terms of a non-linear transformation of the smoothed structure tensor. However, in contrast to Weickert's anisotropic diffusion, our method is based on the minimisation of a functional. Thus it lends itself easily to generalisation to arbitrary inverse problems.

References

[1] Joachim Weickert. *Anisotropic diffusion in image processing.* European Consortium for Mathematics in Industry. B. G. Teubner, Stuttgart, 1998.

Regularized Recycling Methods for Linear Inverse Problems

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Subspace recycling techniques have been used quite successfully for the acceleration of iterative methods for solving large-scale linear systems. These methods often work by augmenting a solution subspace generated iteratively by a known algorithm with a fixed subspace of vectors which are "useful' for solving the problem. Often, this has the effect of inducing a projected version of the original linear system to which the known iterative method is then applied, and this projection can act as a deflation preconditioner, accelerating convergence. In this talk we consider subspace augmentation-type iterative schemes applied to a linear ill-posed problems in a continuous Hilbert space setting, based on a recently developed framework describing these methods. We show that under suitable assumptions, a recycling method satisfies the formal definition of a regularization, as long as the underlying scheme is itself a regularization. We then develop an augmented subspace version of the gradient descent method and demonstrate its effectiveness, both on an academic Gaussian blur model and on problems arising from the adaptive optics community for the resolution of large sky images by ground-based extremely large telescopes.

Quantitative optical coherence elastography parameter reconstructions for a layered medium with random inclusions

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Quantitative information about optical parameters obtained via optical coherence tomography can be seen as an important indication factor in medical diagnosis.

Focusing on the refractive index as the parameter of interest, it has become clear that even for a layered medium, a (unique) quantitative reconstruction of the real and imaginary parts of the refractive index, representing the scattering and absorbative behavior, from a single optical coherence tomography measurement is not possible without any linking between the latter ones.

For this reason, elastography has been taken into account as a complementary method for optical coherence tomography. The idea is of this combination is stated as follows: by performing optical coherence measurements for different compressions states of the sample under investigation increases the dimensions of the data set and therefore ensures the well-posedness of the inverse scattering problem.

In this talk, the main goal will be to show the feasibility of this complementary approach for reconstructing the complex valued refractive index for the case of a dispersive layered medium. This approach is then completed by extending it to a layered medium with randomly distributed scattering inclusions.

MS-23
New trends in tomography: From microscopy to astronomy

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Tomography has been one of the most important applications of mathematics since its development by Allan M. Cormack and Godfrey N. Hounsfield, in 1960s, when the first scanning device for X-ray computed tomography appeared (Nobel prize in 1979). In mathematical terms, it is related to the application of the so-called Radon transform, studied by Johann Radon in 1917. Currently the sector of tomographic imaging is still a fruitful field for the applied mathematicians, especially for those working on inverse problems and mathematical imaging. Therefore, it is of primary importance to provide and study new mathematical models, capable of explaining the physical experiments, and to develop sophisticated and efficient reconstruction algorithms which are especially able to handle big data. In Austria, the special research project "Tomography across the scales" consisting of six Institutes and more than 20 researchers (members and collaborators) is working in this direction to produce new mathematical tools for emerging imaging modalities. The aim of this workshop is to bring together experts and young researchers working in this field and discuss new and recent analytical and numerical techniques, related to adaptive optics, data-driven reconstructions algorithm, image processing and integral transforms. We would like to attract and stimulate the curiosity of young

researchers, who started recently working on this field, and provide new insights into these topics.

Identification of cavities in a nonlinear model arising from cardiac electrophysiology via Γ-convergence

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Detecting ischemic regions from noninvasive (or minimally invasive) measurements is of primary importance to prevent lethal ventricular ischemic tachycardia. This is usually performed by recording the electrical activity of the heart, by means of either body surface or intracardiac measurements. Mathematical and numerical models of the cardiac electrophysiology can be used to shed light on the potentialities of electrical measurements in detecting ischemias. More specifically, the goal is to combine boundary measurements of (body-surface or intracavitary) potentials and a mathematical description of the electrical activity of the heart in order to identify the position, the shape and the size of heart ischemias and/or infarctions. The ischemic region is a non-excitable tissue that can be modeled as an electrical insulator and the cardiac electrical activity can be comprehensively described in terms of the monodomain model, consisting of a boundary value problem for a semilinear reaction-diffusion equation.
In my talk, I will analyze the case of an insulated heart neglecting the coupling with the torso and considering the steady-state version of the monodomain model. This results in the challenging inverse problem of detecting cavities for a semilinear equation with a single measurement of the endocardial potential. With minimal regularity assumptions on the cavities, I will first show well-posedness of the direct problem and then prove uniqueness of the inverse problem. Finally, I will propose a novel reconstruction algorithm by means of a phase-field approach rigorously justified via Γ-convergence.

References

[1] E. Beretta, M. Cristina Cerutti and D. Pierotti, *Detection of cavities in a nonlinear model arising from cardiac electrophysiology via* Γ*-convergence*, 2021 preprint

Verifying partial defects in spent nuclear fuel assemblies with Passive Gamma Emission Tomography

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In late 2017, the International Atomic Energy Agency (IAEA) approved passive gamma emission tomography (PGET) as a method for monitoring spent nuclear fuel assemblies (SFAs) as a part of the measures taken to deter the proliferation of nuclear weapons. The PGET instrument resembles a single photon emission computed tomography (SPECT) system that allows the reconstruction of axial cross-sections of the emission map of SFAs. The goal of SFAs monitoring is to detect even a single missing or tampered with fuel pin from an SFA [2, 3]. From a mathematical point of view, tomographic imaging of an SFA is very challenging because it contains materials with very different attenuation and emission properties. The fuel material strongly self-attenuates its gamma-ray emissions, so that correctly accounting for the attenuation is a critical factor in producing accurate images. Due to the nature of the inspections, it is desirable to use as little a priori information

as possible about the fuel, including the attenuation map, in the reconstruction process. Current reconstruction methods either do not correct for attenuation, assume a uniform attenuation throughout the fuel assembly, or assume an attenuation map based on an initial filtered back projection (FBP) reconstruction.

We propose a method to simultaneously reconstruct the emission and attenuation maps by formulating the reconstruction as a constrained minimization problem with a least squares data fidelity term and regularization terms. The performance of the proposed method, with two different regularizers, is evaluated on simulated data that includes missing rods and rods replaced with fresh fuel [1]. In addition, we present recent results on real data, measured during the last campaign at the Olkiluoto nuclear power plant in Finland in summer 2019. The method is shown to produce good results with simulated data when comparing the reconstructions to the ground truth by various numerical metrics, and when classifying the rods with the method currently employed by the IAEA. Results on real data are encouraging, but a more accurate physical modelling might lead to even more reliable reconstructions.

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Multispectral Fluorescence Lifetime Microscopy based on single pixel camera acquisition

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Multispectral Fluorescence Lifetime Microscopy (FLIM) is an optical technique for the study and characterization of samples with many different applications ranging from biological to material science. The possibility to merge spectral, temporal and spatial information at microscopic level provides fundamental insights on the photophysical processes. In particular the measurement of the fluorescence lifetime provides information on the fluorophore?s microenvironment being the lifetime strongly dependent on the local pH, temperature and molecular bindings etc [1]. However the measurement of a higher information content (spectrum, time and space) has the general drawback to significantly increase the acquisition time and this is quite critical especially for biological applications where the specimen is not static and its properties could change during the measurement time. Single-pixel camera scheme (SPC) is a novel and promising imaging technique which allows the acquisition of an image by spatially modulating the emitted (or illumination) light over a basis that is different from the pixels one and by exploiting a bucket detector. By applying proper algorithms the original image can be reconstructed and in particular by exploiting compressive sensing scheme it is possible to significantly reduce the acquisition time while preserving the information content [2]. In this work, we present a Multispectral Fluorescence Lifetime Microscope based on Single Pixel camera scheme implementing different reconstruction algorithms based on compressive sensing approaches. The system

is characterized and validated, by measuring fluorescent beads and cellular specimens, in terms of information content (spectral, temporal and spatial) and acquisition time. Moreover reconstruction algorithms and fitting strategy are presented to further reduce also the processing time.

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A fast stochastic algorithm for regularized PET reconstruction

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Positron Emission Tomography (PET) image reconstruction involves computing the solution of an inverse problem, which is typically expressed as the minimization of the sum of two functions: one corresponding to the data fit, and one corresponding to the regularizer. However, designing algorithms able to perform this task in a time compatible with clinical practice is currently challenging, especially for non-smooth priors which prevent the use of gradient-like methods. We present an algorithm which builds on the renowned Primal-Dual Hybrid Gradient (PDHG) algorithm [1], also known as Chambolle-Pock algorithm for convex optimization, with the added feature that it can randomly update partial variables. In the framework of PET imaging, the Stochastic Primal-Dual Hybrid Gradient (SPDHG) [2] algorithm is able to reconstruct images from sinograms with non-smooth priors like Total Variation, which promotes sharp boundaries. The algorithm proceeds by using only a randomly chosen subset of all views at a given iteration, hence using only partial forward and back-projections, which makes it much faster than PDHG. Furthermore, SPDHG converges almost surely under similar step-size conditions than PDHG [3]. We illustrate this on a variety of real patient datasets from Siemens and GE scanners.

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Photoacoustic Imaging of Viscoelastic Materials

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Photoacoustic tomography is a coupled physics imaging method where information on the optical absorption properties of a sample is gathered using the photoacoustic effect: By illuminating the sample with a laser beam, which is absorbed by the material, a local heating is caused, which in turn produces a local pressure distribution inside the object. This inequilibrium state then relaxes via an ultrasound wave, which is recorded around the object. For a more detailed description of this method, we refer to [5].

The corresponding inverse problem is then to recover from the measurements of the acoustic wave the initial pressure distribution, see [3]. For a simple acoustically homogeneous medium, where the ultrasound wave can be modelled by the linear wave equation with constant speed of sound, there are (depending on the measurement geometry) multiple explicit reconstruction formulas known for this problem, such as, for example, the universal back-projection formula, see [6, 4].

In real media, however, the acoustic waves typically also undergo attenuation effects and we have studied in [1] some of the common models for acoustic attenuation, see, for example, the survey in [2], and considered their effect onto the ill-posedness of the reconstruction problem.

We want to continue this analysis here by extending it to linearly viscoelastic media, in which next to the acoustic pressure waves also shear waves can propagate. To this end, we will present a model for a photoacoustic experiment of a viscoelastic sample and show how it can be decoupled for homogeneous media into separate equations for shear and pressure waves. To quantify the ill-posedness of the inverse problem, we will then analyse the asymptotic behaviour of the singular values of the forward operator.

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MS-24
Mathematical models for cell migration

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The understanding of mechanisms underlying the cell dynamics, as well as the interactions with the surrounding environment, are of particular interest in biology and medicine. In fact, cell migration plays a crucial role in several situations: from physiological development and reparation of multi-cellular organisms, to pathological situations as, for instance, tumoral growth and invasion. In the minisymposium, we will therefore present a series of mathematical models able to capture different phenomena, as shown by related numerical simulations. By focusing on the dynamics of a single cell we will address (i) the motion of engineered non adhering cells in artificial microchannels [3]; and (ii) the influence of environmental conditions on cell perception of external stimuli [4]. Dealing with multicellular systems, we will first discuss how the velocity of few individuals can control the overall dynamics of a cell aggregate immersed in a fluid. Then, (i) a general hybrid model for the collective motion of interacting cells under alignment and continuum chemotaxis [2]; and (ii) a multiscale model for glioma invasion and its interplay with the nervous tissue and therapy [1] will be presented.

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Cell Motility Without Adhesion: Mathematical And Numerical Modelling

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The different mechanisms allowing some animal cells to move are well understood when a flat substrate is involved, where adhesion plays a central role. It is much less so for complex environments, in the extracellular matrix for example. I will quickly present some of the experiments done at IST Austria, which shows that leukocytes can also move when adhesion to the substrate is prevented, if the latter has an adequate characteristic size. Based on these observations, one can write a mechanical model of this phenomenon, relying on simple physical considerations. The key ingredient is the asymmetrical renewal of the cell cortex which supports the membrane, creating a backward flow of material. Without renewal, the corresponding equation can be seen as the L^2 gradient flow of the energy functional corresponding to all contributions, and can be analyzed using general tools. If renewal is taken into account, it introduces a non variational term which breaks the gradient flow structure. On can however still show existence using an approach based on De Giorgi's. To conclude, I will present some numerical results showing the qualitative behaviour of this model, and in particular the impact of the structure size and the presence of the nucleus.

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Nonlocal kinetic models for cell-cell adhesion

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In this talk we present a nonlocal kinetic model for cell-cell adhesion, i.e. the tendency of cells to form junctions between their membranes. We will deal with a transport equation with a nonlocal quadratic interacting operator which implements a velocity-jump process, that is the typical microscopic stochastic dynamics that describes cell motion. Moreover, we have nonlocality because we suppose that cells sense the environment by extending their protrusions up to a maximum sensing radius. Furthermore, the model can be enriched with the volume filling effect also introducing physical limits of migration, that is when cells cannot move because of overcrowding. In order to obtain physical results, the sensing radius determining the nonlocality depends on time, position and direction of sensing. A linear stability analysis in the one dimensional case will be performed. We analyse how the actual possible sensing of the environment influences the dynamics by recovering the appropriate macroscopic limits and by integrating numerically the kinetic transport equation.

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Kinetic And Mean-Field Control Of Cells Through "Leaders"

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A model for the collective motion of N nearly spherical cells immersed in water is derived. We suppose that only a part of them, the so called *leaders*, is active, so that their velocity can be prescribed as a function of time, and thus used as a control. Because of the micro-scales of the cells, low Reynolds number regime applies together with far field approximation. The limit equation valid for *follower* cells [2] tending to infinity is derived both as a kinetic limit and using the mean-field approach, ending up with a similar PDE. Moreover the optimal control problem in the limit cases is stated starting from the solution for the finite dimensional one.

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Collective Motion Of Discrete Particles Under Alignment And Continuum Chemotaxis: A Hybrid Approach

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We propose a hybrid discrete-continuum mathematical model, with application to biological phenomena of collective motions of cells under mechanical and chemical interactions. The investigated system represents a simplified version of the models proposed in [1] and [2]. In these papers, authors investigate, respectively, the morphogenesis in the zebrafish lateral line primordium and the process of formation of cardiac stem cells. Both models take into account alignment, attraction-repulsion and chemotactic effects. Moreover, proliferation and differentiation phenomena in [2] depend on stochastic processes. In our study we investigate, both from an analytical and a numerical point of view, a second-order model, in which an alignment and chemotaxis effect act on a system of interacting particles. We rely on a hybrid description, in which the agents are discrete entities, while the chemoattractant is considered as a continuous signal. From a mathematical point of view, the dynamics of the units are described by second-order differential equations, whereas the evolution in time of the chemoattractant is regulated by a parabolic diffusion equation, with term of source and degradation. In order to investigate well-posedness results for our coupled system, we prove existence and uniqueness of global solutions in

the two-dimensional space. Moreover, we study the time-asymptotic behaviour [3]. Our results show that the migrating aggregate exponentially converges to a state in which all the particles have a same position with zero velocity. Finally, the analytical findings are compared to numerical simulations, based on finite-difference schemes, concerning the behaviour of the full nonlinear system.

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How Do Brain Fiber Tracts Influence Glioma Migration?

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The invasion of tumor cells into healthy tissue is a highly complex process involving several scales, from the microscopic to the macroscopic level. Furthermore, most of the events taking place on the various scales are still not completely understood. In this work, we focus on glioma, a particularly invasive brain tumor, whose evolution, owing to the peculiarities of the nervous tissue structures, is characterized by highly anisotropic diffusion and heterogeneous patterns. A multiscale mathematical model for glioma cell migration, proliferation and therapy, is proposed. Starting from the microscopic description of the binding process between tumor cells and ECM, we derive a macroscopic model, using the parabolic limit and the Hilbert expansions in the mesoscopic moment system [1]. To asses the role of the nervous fibers in tumor migration, we perform an extensive study about the fiber density function [2], comparing different possible expressions, intending to understand their specific capability in describing the actual fiber distribution. Finally, some numerical simulations, based on real data of brain geometry and cell diffusivity, show how tumor migration is influenced by the different modeled processes.

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MS-25
Advanced nonlinear optimization methods for image processing

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Image processing and analysis problems have become increasingly relevant in several areas of applied science, such as biology, astronomy, biomedicine or earth observation. In these applications, scientists and engineers are demanding for faster and more reliable numerical techniques to tackle some of the most challenging tasks, such as image denoising and deblurring, image segmentation and image super-resolution. The mathematical model underlying most of these image processing applications consists of a large-scale nonlinear optimization problem [1], in which the nonlinearity of the objective function might be due to either the acquisition model, the statistics of the noise corrupting the acquired image [2] or the regularization term adopted to impose some a priori properties on the unknown image [3]. Knowing the source of nonlinearity is then fundamental in order

to devise novel optimization strategies able to increase the reconstruction accuracy and reduce the computational time.
This minisymposium brings together researchers to present and discuss recent advances in nonlinear optimization for image processing, focusing both on theoretical and computational aspects, presenting innovative approaches and suggesting novel directions for future work in this field.

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New convergence results on forward–backward methods for nonconvex optimization

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The goal of image restoration is computing a good quality image from a given noisy data. Following the variational approach, the restored image is computed by solving an optimization problem where the objective function to be minimized includes both a data fidelity measure and a regularization term representing the *a priori* information. In the past few years, several numerical studies showed that nonconvex regularization can overcome the known drawbacks of the standard approaches, for example those based on the Total Variation [2]. On the other side, this leads to very challenging optimization problems, since nonconvexity, possibly combined also with the presence of nonsmooth terms in the objective function, is difficult to handle from both, theoretical and numerical point of view.

Forward-backward methods [3] are valid tools to solve optimization problems where the objective function is the sum of a smooth, possibly nonconvex term plus a convex, possibly nonsmooth function. The corresponding iteration is built on two main ingredients: the computation of the gradient of the smooth part and the evaluation of the proximity (or resolvent) operator associated to the convex term. A further difficulty in the implementation of forward–backward methods arises when the convex nonsmooth term has not a simple form and its proximity operator has to be computed in an inexact way.

The aim of this talk is to illustrate new convergence results about forward–backward methods with inexact computation of the proximity operator, under the assumption that the objective function satisfies the Kurdyka-Lojasiewicz property. This framework is very general and it applies also when the differentiable term is nonconvex. In particular, we adopt an inexactness criterion which can be implemented in practice, while preserving the main theoretical properties of the proximity operator. The strength of our approach is that its implementation results in algorithms with well established convergence guarantees, which, as the numerical experience shows, are also well performing on several relevant applications [1].

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Texture-driven methods for Image Segmentation

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Image segmentation is a central topic in image processing and computer vision and a key issue in many applications. According to the human perception, image segmentation is the process of dividing an image into non-overlapping regions. The division into regions is not unique, but it depends on the application, i.e., it must be driven by the final goal of the segmentation and hence by the most significant features with respect to that goal. Usually, a segmentation is obtained by minimizing an energy functional E containing a fidelity term $\mathcal{F}$ that measures the consistency of the candidate segmentation with the observed image, and a regularization term $\mathcal{R}$ that promotes solutions with suitable properties.
A well-known region-based variational model was introduced by Chan et al. [2], henceforth referred to as CEN model, and it is suitable for smooth images. In this talk we modify CEN model using a cartoon-texture decomposition [3] of an image into the sum of a smooth and nonsmooth (texture, noise, etc.) parts. We introduce nonsmooth information in the energy functional with the aim of preventing excessive regularization in piecewise-constant or smooth regions, and preserving spatial features in nonsmooth regions. One approach is to use a spatially adaptive regularization, where the regularization parameter is chosen according to the texture information [1]. Alternatively, we add to the objective function a Kullback-Leibler divergence term, that preserves the features of the texture part during the segmentation process of the cartoon. We solve the modified models by an alternating minimization method using split Bregman iterations. Numerical experiments show the effectiveness of our approaches on textural and noisy images.

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Scaled, inexact and adaptive generalised FISTA for (strongly) convex imaging problems

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We consider an inexact, scaled generalised Fast Iterative Soft-Thresholding Algorithm (FISTA) for minimising the sum of two (possibly strongly) convex functions, which we name SAGE-FISTA [1]. Here, the inexactness is explicitly taken into account so as to describe standard situations where proximal operators cannot be evaluated in closed form. The idea of considering data-dependent scaling in forward-backward splitting methods has furthermore been shown to be effective in incorporating Newton-type information along the optimisation via suitable variable-metric updates. Finally, in order to account for the adjustment of the algorithmic step-size along the iterations, we propose a non-monotone backtracking strategy which improves the convergence speed compared to standard Armijoo-type analogs. Analytically, a linear convergence result for the function values is proved. The result depends on the strong convexity moduli of the two functions, the upper and lower bounds on the spectrum of the variable metric operators and the inexactness/backtracking parameters. The performance of SAGE-FISTA is validated on convex and strongly-convex exemplar image denoising, deblurring and super-resolution problems where sparsity-promoting regularisation is combined with data-dependent weighted-ℓ_2 and Kullback-Leibler-type fidelity terms [2].

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Convex Non-Convex Variational Methods and Algorithms for Inverse Imaging Problems

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An important class of computational techniques to solve inverse problems in image processing relies on a variational approach: the optimal output is obtained by finding a minimizer of an energy function or "model" composed of two terms, namely the data-fidelity term and the regularization term. Much research has focused on models where both terms are convex, which leads to convex optimization problems. However, there is evidence that non-convex regularization can improve significantly the output quality for images characterized by some sparsity property. This fostered a lot of research towards the investigation of optimization problems with non-convex terms. Non-convex models are notoriously difficult to handle as classical optimization algorithms can get trapped at unwanted local minimizers.

To avoid the intrinsic difficulties related to non-convex optimization, the Convex Non-Convex (CNC) strategy has been recently proposed - see, e.g., [1], [2] - which allows the use of non-convex (sparsity-promoting) regularization while maintaining convexity of the total cost function. In this talk, after outlining the key ideas at the basis of the CNC strategy, a general class of parameterized non-convex sparsity-inducing separable and non-separable regularizers and their associated CNC variational models are presented [3]. Convexity conditions for the total cost functions together with suitable algorithms for their minimization based on a general forward-backward splitting strategy are discussed. Numerical experiments on the two classes of considered separable and non-separable CNC variational models are presented which show their superior performance versus the purely convex counterparts when applied to some inverse imaging problems.

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A variational approach to the suppression of MRI Truncation artefacts

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Magnetic resonance (MR) images obtained via the inverse Fourier transformation (iFT) of a finite k-space acquisition represent a classic case of Gibbs ringing. Because of scan time and SNR limitations, the k-space containing the high-frequency information of the image is generally not recorded. Correction techniques aim at recovering these missing data. Despite the intensive research into acquisition and reconstruction algorithms, the Zero Filling method (ZF) is still most commonly implemented on commercial MR imaging machines for reconstructing images from truncated k-space, since ZF method, although presenting truncation artefacts, is fast, stable and reliable. As a result, a considerable quantity of ZF-reconstructed images containing truncation artefacts are archived and re-exploited for the purpose of diagnosis, treatment evaluation and disease monitoring. Therefore, the development of an effective post-processing approach to removing truncation artefacts from these acquired images are highly desirable. In our approach, we propose to remove the truncation artefacts employing a variational approach. The enhanced image u_e is obtained by solving the following optimization problem:

$$u_e = \arg\min_{u\geq 0} \{\|sinc * u - f_0\|_2 + \lambda \mathcal{R}(u)\} \tag{1}$$

where $*$ is the discrete convolution operator and f_0 is the ZF-reconstructed image. The regularization term is represented by the product between the penalty parameter $\lambda \geq 0$ and the regularization function $\mathcal{R}$. In our approach we employed both the second order Total Generalized Variation function (TGV) [3] as well as the L_1 norm of the wavelet transform W, i.e.:

$$\mathcal{R}(u) = TGV(u), \quad \text{or} \quad \mathcal{R}(u) = \|W(u)\|_1$$

The Alternating Direction Method of Multipliers (ADMM) [4] is applied for the solution of problem (1). Numerical results on synthetic and real MR data show the effectiveness of the proposed approach compared to the literature methods [1], [2].

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Numerical optimization strategies for handling non-linearity in Electrical Impedence Tomography problems

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The inverse Electrical Impedance Tomography (EIT) problem involves collecting electrical measurements on the smooth boundary of a region to determine the spatially varying electrical conductivity distribution within the bounded region [1]. Effective applications of EIT technology emerged in different areas of engineering, technology, and applied sciences. However, the mathematical formulation of EIT is well known to suffer from a high degree of non-linearity and severe ill-posedness. Therefore, regularization is required to produce reasonable electrical impedance images. We discuss variational regularization methods which rely on the linearized model of the non-linear forward operator [2], and other optimization strategies for handling non-linearity in inverse EIT [3]. These optimization frameworks can easily integrate suitable penalties to enforce smooth or piecewise-constant conductivity reconstructions depending on prior information. In addition to these model-based approaches, deep learning has recently become a new frontier of EIT and, in general, of inverse problems in imaging. We finally present a model-based deep learning approach which aims to combine the advantages of model-based and data-driven paradigms to provide a parameter-free algorithmic approach to the non-linear EIT problem.

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MS-26
Advances in polygonal and polyhedral methods

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Recently, there has been a growing interest in the study of numerical methods for the approximate solution of partial differential equations (PDEs) on polygonal/polyhedral computational meshes. On the one hand, this is motivated by the geometric flexibility of polygonal/polyhedral meshes, allowing e.g. for hanging nodes, different cell shapes within the same mesh, non-matching interfaces, thus resulting in increased geometric flexibility to correctly represent complicated geometries, interfaces, and heterogeneous media. On the other hand, polygonal and polyhedral methods offer improved versatility for the accurate and efficient numerical approximation of a wide range of problems, including

fluid dynamics, mechanics, acoustics or electromagnetism. The goal of this MS is to discuss the recent developments and advances in the field of polygonal and polyhedral numerical methods. The proposed topics include (but are not limited to) recent advances on: *i)* the design and analysis of polygonal and polyhedral methods; *ii)* their applications in fluid dynamics, mechanics, and electromagnetism; *iii)* *h*-, *p*-, and *hp*-adaptivity; *iv)* fast solution techniques; *v)* the challenges in code development on modern architectures.

A polytopal discontinuous Galerkin method for the poro-elasto-acoustic problem

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In this talk, we focus on the numerical analysis of a polyhedral discontinuous Galerkin (PolyDG) scheme for the poro-elasto-acoustic differential problem modeling an acoustic wave impacting a poroelastic medium and consequently propagating through it. Coupled poro-elasto-acoustic models find application in many science and engineering fields. For instance, in acoustic engineering, for the simulation of sound propagation through acoustic panels; in civil engineering, for the study of passive control and vibroacoustics; in aeronautical engineering, where air-saturated porous materials are employed; in biomedical engineering, for the assessment of ultrasound propagation throughout bones and to model soft tissues deformation; and in computational geosciences, for the characterization of geologic formations through ultrasonic and seismic modeling [1].

In order to accurately simulate wave propagation in coupled poro-elasto-acoustic domains the numerical scheme should cope with the following issues: (i) in the low-frequency range the evolution problem become stiff and, as a result, time integration schemes might become computationally too demanding; (ii) the diffusive slow compressional waves are localized near the interfaces, and therefore, mesh refinements are needed to capture the phenomenon; (iii) an accurate geometrical description of the arbitrary complex interfaces is mandatory; (iv) a proper representation of the hydraulic contact at the interfaces is also crucial to correctly capture the physics of the problem. By taking into consideration the aforementioned difficulties, we propose in [2] a high-order PolyDG method for the space discretization of the coupled problem that, thanks to its appealing features, can be employed in real applications. We point out that the geometric flexibility due to mild regularity requirements on the underlying computational mesh together with the

arbitrary-order accuracy featured by the proposed PolyDG method are fundamental as they ensure a high-level of flexibility, precision, and scalability that are needed to correctly represent the solutions.

The starting point for the design of the numerical scheme is a *two-displacement* formulation of the poroelastic problem and an *acoustic potential* formulation in the fluid domain. The coupling between the two problems is realized through physically consistent interface conditions. This transmission conditions depend on the pores configuration at the interface, which is modeled by a scalar parameter $\tau \in [0, 1]$. One of the main contribution of the present work is the derivation of a unified and robust analysis with respect to the parameter τ. Well-posedness of the continuous problem is established by employing the semigroup theory and extending the results in [3]. A stability analysis for both the continuous and semi-discrete problem is presented and *hp*-error estimates for the energy norm are derived for the semi-discrete one. The spatial discretization is then coupled with Newmark-β time integration schemes to obtain the fully-discrete algorithm. The choice of employing an implicit time scheme is motivated by the fact that, in the case of low frequencies, a diffusive slow P-wave might become dominant and yield a drastic restriction on the stability condition for explicit methods [4]. A wide set of numerical results obtained on test cases with manufactured solutions are presented in order to validate the error analysis. Examples of physical interest are also presented to investigate the performances of the proposed method in practical scenarios.

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Bend mixed virtual element method

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We propose an extension of the Mixed Virtual Element Method (MVEM) for bi-dimensional polygonal meshes characterized by curved boundaries or interfaces starting from the idea described in the pioneering work [1].

This extension is a key aspect in the resolution of partial differential equations. Indeed, a "bad" approximation of the curved domain introduces a geometrical error on the numerical solution that can corrupt the expected convergence order of the numerical scheme itself.

A series of numerical experiments shows that the proposed approach does overcome this issue. Moreover, we observe that it is astonishly robust with respect to element distortion.

This work represents the first preliminary step of the wider project called *"Bend Vem 3D"* founded by *Gruppo Nazionale per il Calcolo Scientifico* whose main objective is to analyze and solve mixed problem characterized by curved boundaries in 3d.

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Refinement strategies for polytopal mesh

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Refinement strategies for general polytopal meshes preserving quality of the starting mesh, is still an open problem. In this talk we present several refinement strategies viable for polytopal elements suitable for VEM discretizations. In particular, for polygonal mesh, we analyse the behaviour of the error and the quality of the mesh produced with the L-shape domain problem. The proposed refinement strategies are tested on simple configurations in order to investigate the error decay and have been extended to develop a refinement strategy for polyhedral mesh.

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Refinement of polygonal grids using Convolutional Neural Networks with applications to polygonal Discontinuous Galerkin and Virtual Element methods

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We propose new strategies to handle polygonal grids refinement based on Convolutional Neural Networks (CNNs). We show that CNNs can be successfully employed to identify correctly the "shape" of a polygonal element so as to design suitable refinement criteria to be possibly employed within adaptive refinement strategies. We propose two refinement strategies that exploit the use of CNNs to classify elements' shape, at a low computational cost. We test the proposed idea considering two families of finite element methods that support arbitrarily shaped polygonal elements, namely Polygonal Discontinuous Galerkin (PolyDG) methods and Virtual Element Methods (VEMs). We demonstrate that the proposed algorithms can greatly improve the performance of the discretization schemes both in terms of accuracy and quality of the underlying grids. Moreover, since the training phase is performed off-line and is problem independent the overall computational costs are kept low.

Gradient discretization of two-phase flows coupled with mechanical deformation in fractured porous media

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In this talk, we consider a two-phase Darcy flow in a fractured and deformable porous medium for which the fractures are described as a network of planar surfaces leading to so-called hybrid-dimensional models. Fractures are assumed open and filled by the fluids, and small deformations with a linear elastic constitutive law are considered in the matrix. At matrix-fracture interfaces, phase pressures can be continuous or discontinuous, corresponding to two different models. Unlike single-phase flow, discontinuous pressure models for two-phase flows provide a better accuracy than continuous pressure models even for highly permeable fractures. This is due to the fact that fractures fully filled by one phase can act as barriers for the other phase, resulting in a pressure discontinuity at the matrix fracture interface. The model is discretized using the gradient discretization method, which covers a large class of conforming and non-conforming schemes. This framework allows for a generic convergence analysis of the coupled model using a combination of discrete functional tools. Numerical solutions provided by the continuous and discontinuous pressure models are compared on gas injection and suction test cases using a Two-Point Flux Approximation (TPFA) finite volume scheme for the flows and $\mathbb{P}_2$ finite elements for the mechanics.

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MS-27
Advances in polygonal and polyhedral methods

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Recently, there has been a growing interest in the study of numerical methods for the approximate solution of partial differential equations (PDEs) on polygonal/polyhedral computational meshes. On the one hand, this is motivated by the geometric flexibility of polygonal/polyhedral meshes, allowing e.g. for hanging nodes, different cell shapes within the same mesh, non-matching interfaces, thus resulting in increased geometric flexibility to correctly represent complicated geometries, interfaces, and heterogeneous media. On the other hand, polygonal and polyhedral methods offer improved versatility for the accurate and efficient numerical approximation of a wide range of problems, including

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Hybridization of VEM for Hellinger-Reissner elasticity problems

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The elasticity theory studies the deformation of bodies under the influence of applied forces. Considering the linear case, we take the Hellinger-Reissner functional as the basis of our discretization procedure, which means that the displacements and the stresses are the variables of our problems. Recently, some conforming Virtual Element schemes with a priori symmetric stress have been proposed and analyzed both for two-dimensional and three-dimensional problems [2, 3, 4]. In this talk, we present the hybridization procedure proposed in [1] to a low-order VEM scheme for these elasticity problems [2, 4]. This procedure consists of employing the Lagrange multipliers to impose the required continuity constraints across the inter-elements, rather than enforcing them directly in the approximation spaces, and using a static condensation technique to reduce the computational costs and obtain a symmetric and positive definite linear system. Moreover, exploiting the available information derived from multipliers, we also show how to design a better approximation of the displacement field using a straightforward post-processing procedure. Finally, some numerical experiments are provided to assess the validity and the potential of our analysis.

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A Quasi-optimal Variant of the Hybrid High-order Method for Elliptic Partial Differential Equations with H^{-1} Loads

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Hybrid High-Order methods for elliptic diffusion problems have been originally formulated for loads in the Lebesgue space $L^2(\Omega)$. In this paper we devise and analyze a variant thereof, which is defined for any load in the dual Sobolev space $H^{-1}(\Omega)$. The main feature of the present variant is that its H^1-norm error can be bounded only in terms of the H^1-norm best error in a space of broken polynomials. We establish this estimate with the help of recent results on the quasi-optimality of nonconforming methods. We prove also an improved error bound in the L^2-norm by duality. Compared to previous works on quasi-optimal nonconforming methods, the main novelties are that Hybrid High-Order methods handle pairs of unknowns, and not a single function, and, more crucially, that these methods employ a reconstruction that is one polynomial degree higher than the discrete unknowns. The proposed modification affects only the formulation of the discrete right-hand side. This is obtained by properly mapping discrete test functions into $H^1_0(\Omega)$.

On some error estimators for the *p*- and *hp*- versions of the virtual element method

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We present some error estimators for the *p*- and *hp*- versions of the virtual element method including: a residual error estimator that presents the usual suboptimality in terms of the polynomial degree in the efficiency; an error estimator based on the hypercircle of Prager and Synge, which is reliable and efficient; two error estimators based on local flux reconstruction techniques in the virtual element setting.

A three-dimensional Hybrid High-Order method for magnetostatics

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In this talk, I will present some co-joint works on the development and analysis of three-dimensional Hybrid High-Order (HHO) methods for the numerical approximation of magnetostatic problems; see [1, 2] . HHO methods are numerical methods of arbitrary order supporting fairly general meshes, whose construction relies on discrete unknowns based on mesh elements and faces. The well-posedness of the discretisations stems from a discrete version of the first Weber inequality on three-dimensional hybrid spaces.

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Performance of the mixed Virtual Element Method on complex grids for porous media flow

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The numerical simulation of flow in porous media, even in the simplest case of linear governing equations, entails challenges arising from the geometry and the data heterogeneity. For instance, in subsurface geological porous media, the shape of sedimentary layers and the presence of fractures/faults poses challenges in the discretization of the domain with traditional, conforming grids. Moreover, material properties can change abruptly in space, in particular across the aforementioned interfaces. The development of approximation schemes has recently focused on the overcoming of such difficulties with the objective of obtaining numerical schemes with good approximation properties. In this work we carry out a numerical study on the performances of the Mixed Virtual Element Method (MVEM) [1] for the solution of a single-phase flow model in fractured porous media. MVEM are selected thanks to their geometrical flexibility since they allow for general grid cells of polytopal type, and the mixed formulation is chosen to provide a locally mass conservative and accurate velocity field. The goal, presented in [4], is to assess the performance of the method on different types of grids that could be used in realistic workflows, for instance hybrid grids arising from quadrilateral grids cut by fracture networks, Voronoi grids, and grids generated by agglomeration. Numerical experiments are based on two well known benchmark problems, in particular: i) a 3D case with strongly heterogeneous permeability [3]; ii) a 2D case with a fracture network including small angles and "very close" fractures, [2]. Although the method proves, in general, to be robust with respect to both geometry and permeability distribution, some differences can be observed in matrix pattern, condition number, stabilization effectiveness for the different cell shapes.

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MS-28
Mathematical Models in Ecology and Epidemiology (Part 1)

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The minisymposium (in two parts) is devoted to a review of different mathematical models in the areas of ecology and epidemiology.

The first part is especially devoted to the spread of infectious diseases, including both theoretical topics, such as stochastic behavioural epidemiology, and applications to specific infections, such as measles and HIV.

Controlling OQDS (olive quick decline sindrome) outbreaks caused by *Xylella fastidiosa*.

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The motivation of our research has arisen by the outbreak of an epidemic, caused by the pathogen *Xylella fastidiosa* and known as olive quick decline syndrome (OQDS), which has been seriously affecting olive production of the Apulia region (Italy) since 2013, leading to dramatic socio-economic losses.

Current agronomic practices are mainly based on uprooting the sick olive trees and their surrounding ones, with later installment of more resistant olive cultivars. Unfortunately, both of these practices are having an undesirable impact on the environment (most of these trees were several hundred years old), and on the economy (e.g., costs of the new installments, the loss of production for some years and, the last but not less important the oil quality produced by more resistant cultivars may not match the high standards of the previous ones). Based on a mathematical model expressed in terms of a simplified reaction diffusion system, it has emerged that the best cost-effective practice consists of the removal of a suitable amount of weed biomass (reservoir of the juvenile stages of the insect vector - *P. Spumarius* - of *X. fastidiosa*) from olive orchards and surrounding areas, without requiring neither the removal nor the substitution of the existing olive trees. It has to be evidenced that the same kind of disease has been affecting most of the Mediterranean regions, wherever there is a large population of olive trees, in association with the fact that the pathogen *X. fastidiosa* can infect a large number of productive plants of relevant socio-economic importance (e.g., grapevines, almond trees, citrus plants).

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Behaviour-induced complex behaviours in spatiotemporal Epidemic Models

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Under voluntary vaccination, a critical role in shaping the level and trends of vaccine uptake is played by the type and structure of information that is received and used by parents of children eligible for vaccination. In this talk, which summarizes the paper *A. Lupica et al, Math Biosc Eng 17(2): 1090–1131 (2019)* we investigate the feedbacks of spatial mobility and the spatial structure of information on vaccination dynamics. We considered the simplest spatial setting, namely classical 'Fickian' diffusion, and focused on the important case where the infection is absent in the target population. We compared the effects of three main cases: (i) purely local information; (ii) a mix of purely local and global, country-wide, information due e.g., to country-wide media and the internet; (iii) a mix of local and non-local information. By representing these different information options through a range of different spatial information kernels, we investigated: the presence and stability of space-homogeneous, nontrivial, behavior–induced equilibria; the existence of bifurcations; the existence of classical and generalized traveling waves; and the effects of awareness campaigns enacted by the Public Health System to sustain vaccine uptake.

Novel frameworks for optimal control problems in SIR epidemic models

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Optimal control theory applied to Susceptible–Infected–Recovered (SIR) models has been widely used to identify effective strategies for minimizing the impact of infectious diseases. However, to the best of our knowledge, no attempts have been made to investigate two cases with significant real–world applications: i) the case that the costs of the epidemics are related not only to epidemic size, but also to epidemic duration. Indeed, the minimization of outbreaks duration is a priority when the imposed sanitary restrictions involve travel bans (in human diseases) and export bans (in livestock diseases) [1]; ii) the case that the infectious period is Erlang–distributed, implying that the chance for an infected individual to recover depends on the time since infection, as it has been documented for a wide class of infectious diseases [2]. For addressing the case (i), we built a *time–optimal* control problem for a SIR model using two alternative control strategies: vaccination of susceptible individuals or isolation of infected individuals. As regards the case (ii), we implemented the *method of stages* in an SIR model [3], by splitting the infected compartment in n fictitious stages in series ($n \in \mathrm{N}_+$); infected individuals at any stage are isolated at the rate that jointly minimizes the costs associated to the control efforts and the epidemic size. By applying the Pontryagin's minimum principle [4], we proved that both the optimal control problems admits only bang–bang solutions with at most two switches. The analytical results are supported by extensive numerical simulations obtained by a simple *ad hoc* numerical scheme.

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Modelling SARS-CoV-2 transmission from data collected in Vo', Italy

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In this talk I will present the analyses and modelling work that have been conducted on the data collected in Vo' since the start of the pandemic.

In February and March 2020, we conducted two mass swab testing campaigns and collected information on the demography, clinical presentation, hospitalization, contact network and the presence of SARS-CoV-2 infection in nasopharyngeal swabs for 85.9% and 71.5% of the population. From the first survey, which was conducted around the time the town lockdown started, we found a prevalence of infection of 2.6% (95% confidence interval (CI): 2.1–3.3%). From the second survey, which was conducted at the end of the lockdown, we found a prevalence of 1.2% (95% CI: 0.8–1.8%). Notably, 42.5% (95% CI: 31.5–54.6%) of the confirmed SARS-CoV-2 infections detected across the two surveys were asymptomatic (that is, did not have symptoms at the time of swab testing and did not develop symptoms afterwards). The mean serial interval was 7.2 days (95% CI: 5.9–9.6). We found no statistically significant difference in the viral load of symptomatic versus asymptomatic infections (P = 0.62 and 0.74 for E and RdRp genes, respectively, exact Wilcoxon–Mann–Whitney test).

In May 2020, we tested 86% of the Vo' population with three immuno-assays detecting antibodies against the spike (S) and nucleocapsid (N) antigens, a neutralisation assay and Polymerase Chain Reaction (PCR). Subjects testing positive to PCR in February or March or a serological assay in May were tested again in November 2020. Combining the results obtained with the three assays, we estimate a seroprevalence of 3.5% (95% Credible Interval (CrI) 2.8%-4.3%) in May. In November, all assays showed a reduction in antibody titres, though 98.8% (95% Confidence Interval (CI) 93.7%-100.0%) of sera still reacted against at least one antigen. Conversely, 18.6% (95% CI 11.0%-28.5%) showed a marked increase of antibody or viral neutralisation reactivity between May and November, linked to documented or likely re-exposures. We found significant differences in the magnitude and persistence of the antibody response by age group but not by symptom occurrence, hospitalisation, or sex.

Analysis of the serostatus of the members of 1,118 households indicated a 26.0% (95% CrI 17.2%-36.9%) Susceptible-Infectious Transmission Probability (SITP, which is the probability of SARS-CoV-2 transmission occurring between each susceptible-infectious pair of individuals, measured over the whole period of infectiousness of the infectious individual and in the case when the susceptible individual is not infected by a third party during that period), and that 79.1% (95% CrI 48.9 – 98.9%) of transmission could be attributed to 20% of infections. Contact tracing correctly identified 44% of the infected subjects. Our models suggest that contact tracing had a limited impact on the control of the epidemic.

Kinematics of COVID-19 at moderate levels of susceptible depletion: early growth, lockdown, unlocking,...

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The enaction and relaxation of interventions aimed to mitigate the harmful effects of the COVID-19 pandemic, have shaped the epidemic into a multi-phase form. Here, we provide a description of an epidemic whose time course is subdivided by mitigation interventions into a sequence of phases, on the assumption that interventions are effective enough to prevent the susceptible fraction to largely depart from 100% (or from any other relevant level). By applying this hypothesis to a general SIR epidemic model with age-since infection and piece-wise constant contact and recovery rates, we provide a unified treatment of multi-phase epidemics showing how they unfold over time. Subsequently, by exploiting a wide class of infectiousness and recovery kernels allowing reducibility to either ordinary or delayed differential equations, we investigate in depth a low-dimensional case allowing a non-trivial full analytical treatment also of the transient dynamics connecting the different phases of the epidemic. Finally, we illustrate our theoretical results by a fit to the overall Italian COVID-19 epidemic since March 2020 till March 2021 i.e., before the mass vaccination campaign started to display its effects. This show the abilities of the proposed model in effectively describing the entire course of an observed multi-phasic epidemic with minimal data and parameters, and in providing useful insight on the inertial phenomena surrounding the switch between different phases.

MS-29
Mathematical Models in Ecology and Epidemiology (Part 2)

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The minisymposium (in two parts) is devoted to a review of different mathematical models in the areas of ecology and epidemiology.

This second part is especially devoted to population dynamics, ecology and eco-epidemiology. Topics presented in the minisymposium will include the dynamics of spatially or phenotipically structured populations, with applications from movement ecology to the growth of multicellular systems.

Modelling carbapenem–resistant *Klebsiella pneumoniae* transmission in a hospital network

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The nosocomial spread of carbapenem–resistant *Klebsiella pneumoniae* (CRKP) represents a major threat to global public health [1]. However, the understanding of CRKP nosocomial transmission represents a challenging task due to the complex interactions between within-hospital and hospital-community dynamics [2].
Here, we considered an agent–based model of CRKP transmission over a real–world patient–to–patient contact network to infer nosocomial transmission and infection importation over actual incidence records. The contanct network is constructed using the hospitalization records spanning the years 2016–2017 from the public hospitals in the Italian region of Emilia-Romagna. We assumed that a link exists between two patients if they have shared a ward at a given time. The inference of epidemiological parameters is obtained by an iterated filtering algorithm, which involves the use of the Bayesian Ensemble Adjustment Kalman Filter [3, 4].
The estimate of within-hospital transmission and infection importation from the community in different wards and hospitals will provide a useful decision support tool for the Public Health Authorities in Emilia-Romagna for the prioritization of the intervention strategies to contrast CRKP infections.

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Data-informed modelling of movement may be key to properly describe important ecological and eco-epidemiological processes

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Movement plays a fundamental role in shaping major ecological and epidemiological processes. It can contribute to the decline of some populations that, along their long-distance migrations, may suffer from possible divergent effects of global changes (due to climate or land-use alterations) occurring at local scales along their path. A data-informed modelling of movement can also be key to map the unwanted dispersion of contaminants into the environment, a pollution that ends up impacting on the health of ecosystems and populations (which are themselves mobile according to their own different drivers). Not least, in complex eco-epidemiological systems, such as those of some infectious diseases involving humans, movement of both final and intermediate hosts is at the basis of the observed spatiotemporal patterns over which we would like to have control. The increasing availability of data allows us to develop more accurate models, not necessarily in terms of their mathematical formulation, but because they are run on the basis of information that is gathered from a variety of sources and/or because of the integration between models and data. In this talk, we will briefly discuss some of the methodologies we have developed to (1) try decrypting, thanks to data from geolocators placed on the wings of European barn swallows (*Hirundo rustica*), the still misterious trajectories

they follow during their recurrent, seasonal, long-distance migrations between Africa and Europe [1, 2], (2) understand the spatiotemporal patterns of plastic pollution in the ocean, with particular attention to the Mediterranean Sea, by linking in a novel modelling approach both pollution caused by plastic particles and by related chemical agents adsorbed/desorbed by them [3, 4], (3) detect the significant effects of movement of humans and parasites in determining the outcome of endemic diseases linked to poverty, such as schistosomiasis [5, 6].

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Modelling the Evolutionary Dynamics of Cancer Through Non-local Partial Differential Equations

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A range of mathematical models have been developed and used to gain a more in-depth theoretical understanding of the evolutionary dynamics that underpin cancer progression at the cellular scale. In this talk, deterministic, continuum models formulated as non-local partial differential equations will be considered. Analytical and numerical results summarising the behaviour of the solutions to the model equations will be presented and the biological insight generated by these results will be briefly discussed.

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Assessing SOC trends in Alta Murgia National Park with a novel non-standard discrete RothC model

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Trends of soil organic carbon (SOC) are significant indicators for land and soil degradation. Decrease in SOC compromises the efforts to achieve by 2030, a land degradation neutral world, as required by Target 15.3 of the Seventeen Sustainable Development Goals (SDGs) adopted by United Nations in September 2015. Differential models, as the Rothamsted Carbon model (RothC) [1], can be useful tools to predict SOC changes, taking into account the interactions among climate, soil and land use management.
In this talk, we illustrate some results on the application of a novel nonstandard discretization [2] of the continuous RothC model [3] for assessing the SOC indicator in Alta Murgia National Park, a protected area in Apulia region in the south of Italy. A procedure for determining the initial plant input necessary to run the model is described. Moreover, in order to detect the factors that determine the size and direction of SOC changes, a local sensitivity analysis based on the so-called *direct method* is performed.
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Optimal Resource Allocation for Controlling Invasive Species

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The introduction of invasive alien species is recognised as an important cause of the drastic loss of biodiversity that is affecting our planet, due to the alteration of ecosystems caused by the rapid proliferation of alien species. Invasive species cost billions of dollars a year in ecological damage and economic losses. The reduction or elimination of those alien species that threaten ecosystems, habitats or native species is a strategic objective to be carefully pursued with knowledge-based management practices.

Given the extent of the problems caused by invasive species and the limited resources available to control them, planning processes are required to identify cost-effective solutions that minimize the negative impacts of invasive species on colonized systems. Careful planning requires a high capacity for analyzing the extent of the invasion and an equally high capacity for predicting its evolution in time and space.

Starting from the results in [1] and [2], in [3] we develop a model capable to mimic the relevant features of the alien species invasion as well as the results of a control action when the species dynamics is influenced by external driving forces. We propose a parabolic optimal control model for both predicting the spread of the species and designing a strategy for the optimal spatiotemporal allocation of resources necessary to perform a control action, under a budget constraint. We show the analytical and numerical aspects of this approach.

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On the competition between red and grey squirrels: exotic species and Allee effect

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When an exotic species is introduced in a different ecosystem, even if the environment is similar to the one in which the population has grown, some diffculties can arise in reproduction, settlement and expansion, especially if the number of introduced individuals is small. Those problems could lead to exotic species extinction. The aim of this work is to investigate in which way the risk of the exotic species extinction could affect the possible outcomes of the mathematical model proposed in [1]. To describe the risk of its extinction, a strong Allee effect is considered in the dynamics of the exotic species. The possible stable outcomes are reduces to three: the invasion, the undisturbed original system, and a total coexistence. The conditions under which the system evolves towards one of them still relate to the level of competition: if it is too intense for native populations, then the invader replaces them, while if there is a balanced competition all the populations coexist. The outcome in which exotic population cannot settle and disappears is unconditionally stable thanks to the introduction of Allee effect, so it can be realized starting from suitable initial populations sizes regardless their characteristics.

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MS-30
Numerical modeling of cardiac function and vascular circulation - part I

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In this minisymposium, we aim at presenting some recent contributions in the numerical modeling of the cardiovascular system. In particular, we want to address the modeling

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Numerical Modeling of Cardiac Reentry in the Presence of Infarct Scars and Border Zones

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We investigate, by means of numerical simulations, the role of infarct scar dimension, repolarization properties and anisotropic fiber structure of scar tissue border zone (BZ) in the genesis of ventricular tachycardia (VT). The simulations are based on the Bidomain model, a reaction-diffusion system of Partial Differential Equations, discretized by finite elements in space and implicit-explicit finite differences in time. The computational domain adopted is an idealized left ventricle affected by an infarct scar extending transmurally. We consider cases with transmural scars having either a central sub-epicardial channel BZ region (CBZ) or an epicardial BZ region covering the scar (EBZ). In CBZ simulations, the results have shown that: i) the scar extent is a crucial element for the genesis of reentry; ii) the repolarization properties of the CBZ, in particular the reduction of IKs and IKr currents, play an important role in the genesis of reentrant VT. In EBZ simulations, since the possible reentrant pathway is not assigned a-priori, we investigate in depth where the entry and exit sites of the cycle of reentry are located and how the functional channel of reentry develops. The results have shown that: i) the interplay between the epicardial anisotropic fiber structure and the EBZ shape strongly affects the propensity that an endocardial premature stimulus generates a cycle of reentry; ii) reentrant pathways always develop along the epicardial fiber direction; iii) very thin EBZs rather than thick

EBZs facilitate the onset of cycles of reentry; iv) the sustainability of cycles of reentry depends on the endocardial stimulation site and on the interplay between the epicardial breakthrough site, local fiber direction and BZ rim.

A Novel Numerical Model of the Action Potential of Atrioventricular Node Cell

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The development of computational electrophysiology and numerical modeling allows nowadays to reproduce the action potential (AP) in a variety of cardiac cell types and species. The atrioventricular node (AVN) is a small cardiac tissue at the border of right atrium and right ventricle, which acts as a subsidiary pacemaker and controls impulse conduction between the atria and ventricles. Despite its physiological importance, limited experimental data are available for computing AVN cellular electrophysiology.Further,

the ionic mechanisms underlying the automaticity of AVN myocytes are incompletely understood. To date, only two numerical models of AVN have been developed in the last decades (one for rabbit [1], the other for mouse but without calcium handling [2]). We aimed to develop a new mouse model AVN model.

We thus build on the preliminary AP mouse AVN model published by Marger et al.[2], which has been updated and improved, by implementing more realistic cellular compartments and calculation of dynamics and handling of intracellular Ca^{2+}. The equations describing calcium handling are based on the AP mouse SAN single-cell model from Kharche's work [3]. The cell's compartmentalization has been updated as follows: the sarcoplasmic reticulum, divided into junctional and network spaces (JSR and NSR, 1.12% and 11.6% of the whole cell volume, respectively), the subsarcolemmal calcium subspace (1% of the total cell volume), and the cytosol. The calcium subspace is considered as an independent intracellular compartment because of the transient local calcium accumulation taking place upon release from the SR. The Hodgkin-Huxley formulations for the membrane ionic currents were taken from the preliminary mouse AVN single-cell model [2]. Experimental data [2, 4], as current-to-voltage (I-V) curves from mouse AVN single cells, were used to reformulate the following ionic currents in the new model to obtain a more realistic description: I_{Na_r} TTX-resistant component of Na^+ current, I_{Na_s} TTX-sensitive component of Na^+ current, I_{Ca_D} Ca^{2+} current through L-type Cav1.3 channels, I_{Ca_L} Ca^{2+} current through L-type Cav1.2 channels, I_{Ca_T} Ca^{2+} current through T-type Cav3.1 channels, I_{K_r} rapid delayed rectifier K^+ current, I_{to} transient outward K^+ current, I_f Na^+ and K^+ currents activated by hyperpolarization. The pacemaking was simulated for 300s to ensure reaching of steady-state.

The new model reproduces almost all the AVN AP hallmarks (beating rate, maximum diastolic potential, AP amplitude, and AP duration) and has been used to simulate the effects of blockade of ionic currents (I_f, I_{Ca_D}, I_{CaL}, and I_{Kr}) involved in AVN pacemaking. Despite the lower density of the "funny" current in AVN compared to the SAN, I_f significantly contributed to AVN pacemaking. Indeed, a slowing in rate is obtained followed by the arrest of cell beating under the condition of the current block. I_{Ca_D} was also found to be important for AVN pacemaking since its blockade arrests automaticity. In conclusion, our work proposes a new updated version of a mouse AVN single-cell AP. This model reproduces experimentally measured AP hallmarks and can be used to simulate the blockade of ionic currents to help understand the pacemaking mechanisms in mouse AVN.

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Parallel solvers for cardiac electro-mechanics and applications

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The spread of the electrical impulse in the cardiac muscle and the subsequent contraction-relaxation process are quantitatively described by the cardiac electro-mechanical coupling (EMC) model, which consists of the following four components:

- the quasi-static finite elasticity model of the deformation of cardiac tissue, derived from a strain energy function which characterizes the anisotropic mechanical properties of the myocardium;
- the active tension model, consisting of a system of non-linear ordinary differential equations (ODEs), describing the intracellular calcium dynamics and cross bridges binding;
- the electrical current flow model of the cardiac tissue, called Bidomain model, which is a degenerate parabolic system of two non-linear partial differential equations of reaction-diffusion type, describing the evolution in space and time of the intra- and extracellular electric potentials;
- the membrane model of the cardiac myocyte, i.e. a stiff system of ODEs, describing the flow of the ionic currents through the cellular membrane.

The numerical approximation and simulation of the cardiac EMC model is a very demanding and expensive task, because of the very different space and time scales associated with the electrical and mechanical models, as well as their non-linear and multiphysics interactions.

In the first part of this talk, we present the finite element solver that we have developed to simulate the cardiac electro-mechanical activity on parallel computational platforms. The solver is based on a Multilevel Additive Schwarz preconditioner for the linear system arising from the discretization of the Bidomain model and on a Newton-Krylov-BDDC method for the non-linear system arising from the discretization of finite elasticity.

In the second part, we present an application of the electro-mechanical solver to the *in silico* evaluation of the performance of conventional biventricular and multipoint pacing in cardiac resynchronization therapy.

Deep learning-based reduced order models for the real-time approximation of parametrized PDEs

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Conventional reduced order models (ROMs) anchored to the assumption of modal linear superimposition, such as proper orthogonal decomposition (POD), may reveal inefficient when dealing with nonlinear time-dependent parametrized PDEs, especially for problems featuring coherent structures propagating over time. To enhance ROM efficiency, we propose a nonlinear approach to set ROMs by exploiting deep learning (DL) algorithms, such as convolutional neural networks. In the resulting DL-ROM, both the nonlinear trial manifold and the nonlinear reduced dynamics are learned in a non-intrusive way by relying on DL algorithms trained on a set of full order model (FOM) snapshots, obtained for different parameter values. Performing then a former dimensionality reduction on FOM snapshots through POD enables, when dealing with large-scale FOMs, to speed-up training times, and decrease the network complexity, substantially. Accuracy and efficiency of the DL-ROM technique are assessed on different parametrized PDE problems in computational mechanics and fluid dynamics, possibly accounting for fluid-structure interaction (FSI) effects, where new queries to the DL-ROM can be computed in real-time.

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A fast cardiac electro-mechanics model with blood circulation using the Eikonal equation

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In this work we present a cardiac electro-mechanics (EM) model coupled with blood circulation with the aim of reducing the computational costs to evaluate significant mechanical outputs in view of clinical practice. For the electrophysiology (EP) part, we started from the strategy of the Reaction-Eikonal model [1], proposing an efficient way to solve the reaction problem. We couple EP with a physics-based active force model [2] to better characterize the coupling with respect to a phenomenological model. We finally couple the 3D EM model with a windkessel model for blood circulation. We show the capability of the model to accurately reproduce physiological PV loops. We also analyze numerical results to show the validity of the method in reproducing significant mechanical outputs (PV loops, ejection fraction) comparing them with the ones obtained with the full EM model with blood circulation using the monodomain model for EP.

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MS-31
Numerical modeling of cardiac function and vascular circulation - part II

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In this minisymposium, we aim at presenting some recent contributions in the numerical modeling of the cardiovascular system. In particular, we want to address the modeling

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Vortex formation across the tricuspid valve in the right heart

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The function of the human heart is that of creating and sustaining blood motion. Studies on cardiac flow were principally focused on the left heart; however both sides of the heart are arranged in series and pump the same volume of blood during one heartbeat. Indeed, the function of the right ventricle (RV) is central in several cardiac dysfunctions including congenital heart diseases. The RV presents a peculiar shape that is elusive to visualizations, only the advent of 3D imaging technology permitted a more comprehensive evaluation of RV structure. It presents a streamlined geometry, which led to various suggestions about its function in fluid mechanical and physiological terms [2]. To date, the role of fluid dynamics in RV function is largely unknown.

Studies on RV fluid dynamics evidenced the formation of a diastolic 3D vortex across the tricuspid valve inlet, that eventually allows an efficient transfer of energy to the outflow with limited muscular effort. The RV streamlined geometry may undergo to compensative changes in presence of a disease that reduce efficiency and lead to progressive worsening of RV function. However, numerical studies [4] were performed with a sharp orifice in place of the actual tricuspid valve (TV), and *in vivo* observations are limited by the time-space resolution of current imaging technology [3].

This study will present a numerical study of RV with TV. Geometries are obtained by 3D echocardiography; the TV is modeled by a fluid-structure-interaction technique that substitutes the specification of tissue material properties, not available *in-vivo*, with measures of valvular motion that can be extracted from imaging [1]. Results aim to associate the 3D fluid dynamical pattern with the fundamental functional properties of the right heart.

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Modeling cardiac thermo-electro-viscoelasticity: The role of nonlinear diffusion

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Cardiac functions depend on local temperature and the associated mechanical properties. The underlying multiscale mechanisms are complex and consequence of the nonlinear character of the thermo-electro-mechanical coupling. In such a context, recent studies highlighted the role of nonlinear coupling in voltage diffusivity [1, 2]. In the present contribution, we discuss a new class of mathematical models for the active contraction of cardiac muscle, featuring thermo-electric, nonlinear conductivity and viscoelastic properties. The set of governing equations consists of a nonlinear viscoelastic orthotropic active strain framework coupled with a four-variable phenomenological model for human myocyte electrophysiology. Thermo-electric couplings are experimentally imposed and electric conductivities are modified according to stress, e.g. stress-assisted diffusivity, enhancing the multiscale and multiphysical couplings occurring at the cell-cell interface. We evaluate the influence of the new terms in the electromechanical model through a sensitivity analysis, and we provide numerical validation through a set of computational tests using a novel mixed-primal finite element scheme [3].

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Incorporating Heart Valves Using a Varying Permeability Approach

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Simulating the total heart function includes CFD blood flow models which serve as the hydrodynamic load imposed on cardiac mechanics. Heart valves play a pivotal role in filling and ejection of cardiac chambers such as the left ventricle (LV). Thus, their functional representation in CFD simulations of hemodynamics in the LV and the attached aorta is vital. Usually this task is achieved using fluid-structure-interaction (FSI) where valves are modeled as thin structures.

We investigate the suitability of an alternative approach: A fictitious domain method is realized by extending the Navier-Stokes equation with a linear permeability term, which results in the Navier-Stokes-Brinkman equation. In this setting the permeability parameter is used to model a valve as a fictitious solid domain. The (fast) opening and closing of the valve is realized by changing the permeability within the finite elements which are covered by the moving valve in its current configuration. The underlying mesh representing the blood pool remains unchanged but the equations contain a volume fraction parameter denoting the degree of partial coverage of finite elements in the blood pool by the valve. To deal with turbulence occurring at higher Reynolds numbers the residual based variational multiscale (RBVMS) turbulence model [1, 2] was employed.

The RBVMS formulation has the additional property of stabilizing our method, which allowed the use of lowest equal order finite elements reducing also the implementation work in the cardiac modeling framework *CARPentry*. In this talk we will present ongoing validation work and applications stemming from clinical datasets.

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Modelling cardiac muscle fibers in electro-mechanical simulations

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A crucial issue in simulating heart electro-mechanics (EM) is accounting and modelling the arrangement of myocardial fibers that characterizes the cardiac tissue. Aggregations of myofibers, namely the results of cardiomyocytes orientation, plays a key role in the electric signal propagation and in the myocardial contraction. This motivates the need to accurately include cardiac fibers in EM computational models. Laplace-Dirichlet-Rule-Based-Methods (LDRBMs), which provide a surrogate of myocardial fibers field, are one of the most used strategy to prescribe fiber orientation in EM models. In this work, we review existing bi-ventricular LDRBMs presented in a unified description. We perform their numerical comparison in terms of meaningful electrophysiological and mechanical biomarkers computed as output of numerical simulations. Furthermore, we study how different configurations in cross-fiber active contraction, that surrogate the myofibers dispersion, affect EM simulations. We also propose a novel bi-atrial LDRBM which is able to qualitatively reproduce the main atria fiber bundles. Finally, we show numerical results including LDRBM fiber generations for a computational domain of the whole heart.

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Computational Fluid Dynamics of Blood Flow in the Human Heart

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Blood flows in the heart are usually studied and analysed through experimental techniques and imaging processes. However, these approaches suffer from a lack of resolution into the spatial and temporal scales of blood flow. Computational fluid dynamics stands as a tool to complement such techniques to provide a detailed description of the physiological condition, as well as for an in-depth analysis of pathological scenarios. From a numerical point of view, CFD modeling of heart's flows faces several challenges. In fact, the fluid problem is defined in geometrically complex domains which undergo very large deformations, moreover, the dynamic of valves makes the topology of the domain changing over the heart-cycle and the flow behaviour is the result of a complex electro-mechanical-fluid problem. In addition to this, the blood flow regime is known to be not laminar, nor fully turbulent but rather transitional [2]. In this work, we develop a mathematical and numerical framework for the numerical simulation of blood flows in the whole human heart. In our CFD model, we adopt the Navier-Stokes equations in Arbitrary Lagrangian Eulerian (ALE) framework, in order to account for the endocardium displacement. We use a Variational Multiscale - Large Eddy Simulation (VMS-LES) model [5, 3] to get a stable formulation of the Navier-Stokes equations discretized by means of Finite Element Method and, then, to account for turbulence modeling within the framework of LES; we also aim to consider typical transitional effects of blood flows. We mimic the presence of cardiac valves by means of the Resistive Immersed Implicit Surface (RIIS) method [4]. We propose a computational model on the haemodynamics of an idealized left atrium and we study the role of the VMS-LES model in such transitional flows showing that VMS-LES model is more accurate to predict transitional blood flow indicators than the standard SUPG stabilization technique [8]. We then present a multiscale computational model for the simulation of the whole left heart, using a realistic geometry and a realistic displacement. The latter is obtained suitably lifting to the whole boundary the left ventricle's displacement, result of an electromechanical simulation previously run [6, 7]. Our 3D-CFD model is coupled to a 0D circulation model of the whole cardiovascular

system [1, 6], in order to prescribe realistic and physiological boundary conditions that are respectful of the closed-loop circulation model of the whole cardiovascular system. Finally, advances regarding a CFD multiscale model of the whole human heart coupled with the circulation model will be introduced and discussed.

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MS-32
Numerical modeling of cardiac function and vascular circulation - part III

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In this minisymposium, we aim at presenting some recent contributions in the numerical modeling of the cardiovascular system. In particular, we want to address the modeling

of both the cardiac function and the vascular circulation. In the first case, main core functionalities like electro-physiology, active and passive mechanics, blood dynamics and valve dynamics will be considered, together with their coupling . Regarding the vascular circulation, both the arterial and venous systems blood dynanics and/or wall mechanics will be addressed. Together with the numerical approximation of standard forward problems, also the case of inverse problems, including uncertainty and applications to cases of clinical interest will be considered.

Determination of the total effective compliance of a global mathematical model for the cardiovascular system

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Vascular compliance is an index used in cardiovascular physiology to describe the relation between changes in blood volume and changes in circulatory pressure. In humans, the Total Effective Vascular Compliance (TEVC) can be defined as the ratio between changes in total blood volume and central venous pressure, obtained by simultaneous recording of right atrial pressure changes induced by transfusion/bleeding and added/subtracted blood volumes. In mathematical models of the cardiovascular system, vascular compliance is usually modelled by means of physical parameters that are in turn inferred from experimental data. In this work, we determined the TEVC of a global closed-loop model [1] by performing a blood infusion test reported in [2]. The underlying model [1] used here includes all the main cardiovascular compartments (arteries, veins, vascular beds, heart and pulmonary circulation), a physiological distribution of vascular compliance parameters and total blood volume, a nonlinear representation of venous resistances and compliances, and main mechanisms by which the body regulates blood pressure. We show that the TEVC is the result of the interaction between the assigned constant physical vascular compliance and the capacity of the cardiovascular system to adapt to new situations via regulatory mechanisms. Moreover, we provide an example in which simply assigning a value to a physical model parameter strongly limits the applicability range of a model if main physiological aspects are not considered.

In order to be able to perform the infusion experiment proposed in [2] and to obtain physiologically sound results, the following modifications to our model were necessary:

- introduction of unstressed volumes, total blood volume and blood volume distribution;
- non-linear dependence on compartment volume for resistances and compliances of venule/vein vascular districts;

- low- and high-pressure baroreflex modelling.

Table 1 shows main cardiovascular indexes for the modified model showing that the overall description of cardiovascular haemodynamics is maintained after model modifications (which include baroreflex models working at a baseline state). Moreover, Figure 1 shows the resulting blood volume distribution among main vascular districts, as well as literature data.

Figure 2 shows TEVC of our model obtained for the infusion test reported in [2] and different model configurations, as well as changes in main cardiovascular variables for the different model configurations considered.

Index	**Current Value**	**Ref. Value**	**Ref.**
SBP [mmHg]	107.48	105 ± 8, 129 ± 3	[4, 2]
DBP [mmHg]	76.18	71 ± 7, 76 ± 2	[4, 2]
MBP [mmHg]	91.19	89 ± 8, 97 ± 2	[4, 2]
PP_{Aorta} [mmHg]	31.31	30 ± 6	[4]
$PP_{Brachial}$ [mmHg]	38.01	49 ± 9	[4]
$PP_{Amplitude}$ [mmHg]	1.21	1.7 ± 0.14	[4]
CO [ml/s]	88.64		
C_a [ml/mmHg]	1.91	1.7	[5]
CVP [mmHg]	4.21	4.2 ± 0.8	[2]
H [beats/min]	75	76 ± 4	[2]
E_{es} [mmHg/ml]	4.61	4.5	[6]
E_a [mmHg/ml]	2.80	2.3	[6]
Ea/Ees	0.60	0.58	[6]
LV_{max}	116.66	150 ± 67	[7]
LV_{EF}	0.62	0.68 ± 0.12	[7]
max. $\frac{dP_{LV}}{dt}$	1511.27	1915 ± 410	[7]
min. $\frac{dP_{LV}}{dt}$	-2632.04	-2296 ± 530	[7]

Table 1: Cardiovascular indexes. Current Value: computed numerical value; Ref. Value: literature reference value with mean and standard deviation. (S/D)BP: systolic/diastolic aortic blood pressure; MBP: mean blood pressure; PP: pulse pressure in aortic root and in brachial artery; PP*Amplitude*: ratio between pulse pressure in brachial artery and aortic root; CO: cardiac output; C_a: arterial compliance evaluated as the ratio between stroke volume and brachial pulse pressure [5]; CVP: central venous pressure; H: heart rate; Ea: arterial elastance; Ees: left ventricle elastance; Ea/Ees: arterial-ventricular coupling index; $LVmax$: maximum left ventricle volume; $LVEF$: averaged left ventricle volume; max. $\frac{dPLV}{dt}$: maximum pressure rate of left ventricle; min. $\frac{dP_{LV}}{dt}$: minimum pressure rate of left ventricle.

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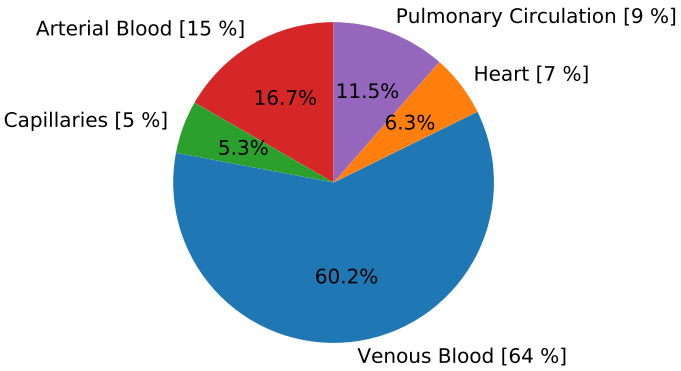

Figure 1: Total blood volume distribution among different vascular compartments. In square brackets, reference blood volume distribution [3]. Total blood volume is set to be 5520 ml. Arterial blood: 1D arteries and arterioles; Venous Blood: 1D veins and venules; Heart: sum of volume of the four cardiac chambers; Pulmonary circulation: arterial, capillaries and venous blood of pulmonary compartments.

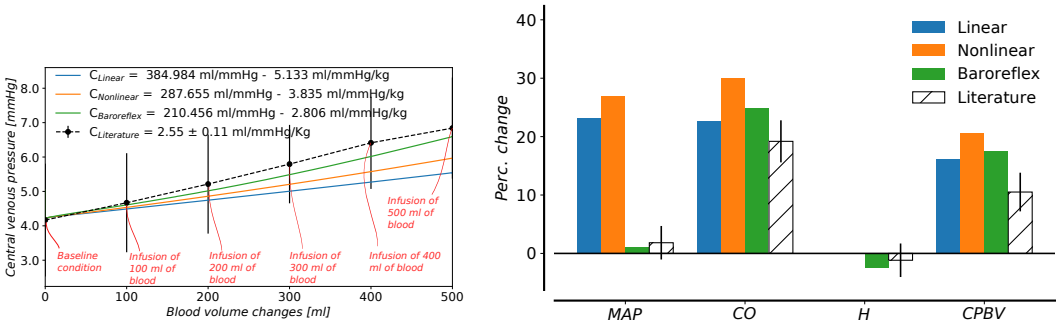

Figure 2: In the left picture we show computed ETVC by means of an infusion test of 500 ml of blood in 4 minutes. Changes in mean central venous pressure are plotted against changes in total blood volume and the inverse of the slope of their linear relationship is the value of the effective compliance. Linear : linear relationship for resistances and compliances in venules compartments; Nonlinear : nonlinear resistances and compliances in venules/vein compartments; Baroreflex : nonlinear resistances and compliances and baroreflex control; Literature : London et al. [2] experimental results on 9 controls subjects (mean value of the group and ± 1 standard deviation). Right figure shows changes in hemodynamic parameters before and after expansion for different model configurations. Literature data from [2]. MAP: mean arterial pressure; CO: cardiac output; H: heart rate; CPBV: cardiopulmonary blood volume.

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Large Eddy Simulation Model for Patient-Specific Aortic Hemodynamics

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Aortic diseases, such as aneurysms and dissections, are calling for biomechanical assessment of their onset and developments. Proper boundary conditions and turbulent flow modeling should be considered in computational fluid dynamic (CFD) simulations to get reliable results. As for the treatment of boundary conditions, the main problem is the occurrence of backflow numerical instabilities when prescribing Neumann conditions. Moreover, blood flow in aorta is difficult to simulate and assess due to large Reynolds number at the systolic peak, and complex geometry for aortic diseases [2]. Both these factors may trigger a disturbed or even turbulent flow. In this scenario, Direct Numerical Simulations (DNS) to solve the small significant scales of the flow may require high computational costs, not compatible with a large number of patients, like in a Computer-Aided Clinical Trial. We are focusing on Large Eddy Simulation (LES) models, which are proved to be more accurate than the Reynolds-Averaged Navier-Stokes (RANS) models [1], and, in particular, on the Smagorinsky-Lilly model. This work aims to prove numerically that the Smagorinsky-Lilly model is able to both treat flow disturbances and suppress the occurence of the backflow instability with a proper selection of the Smagorinsky-Lilly constant, C_S. Three geometries of patient-specific aorta with aneurysm in the vicinity of aortic arch were considered. We prescribed the no-slip condition on the wall of the domain, three-elements Windkessel model at the outlets, and patient-specific flow, as extracted from PC-MRI of each patient, at the inlet. Simulations run for six heart-beats to reach periodicity with a constant time-step set to 0.001 s. Both qualitative and quantitative analysis were performed comparing the results obtained from the LES model with those

given by the DNS, in terms of velocity streamlines, time-averaged wall shear stress, oscillatory shear index, and local normalized helicity. Our preliminary results prove that the LES model well controls both flow disturbances and the numerical backflow instability, by tuning the value of C_S.

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Non intrusive data-driven reduced order model for biomedical applications

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Despite the significant increase of computational power occurred in recent years, the numerical resolution of Partial Differential Equations (PDEs) based on classical discretization, e.g. finite volume and finite element methods (the so-called Full Ordel Models (FOMs)), when several configurations have to be investigated, could require a prohibitive computational cost. In this context, Reduced Order Models (ROMs) (see, e.g., [1]) have been proposed a useful tool able to provide accurate solution at a significantly reduced computational cost.

Non intrusive data-driven ROM approach is a highly active area of research. It is based only on data and does not require knowledge about the governing equations that describe the system. Moreover, no modification of the simulation software is carried out.

In this work, we apply Proper Orthogonal Decomposition (POD) for the computation of reduced basis space. On the other hand, for the evaluation of the modal coefficients, we use two different methodologies, the one based on interpolation with Radial Basis Functions (RBF) [3] and the other one based on Artificial Neural Network (ANN) [2]. In this framework, both physical and geometrical parametrization are considered.

We test the performance of our approach through the application of two different biomedical problems: (i) POD-RBF is used for the investigation of the modifications to aortic blood flow patterns induced by the presence of the outflow cannula of a Left Ventricular Assist Device; (ii) POD-ANN is used for the modelling of the blood flow in the coronary system when an isolated stenosis of the left main coronary artery occurs. In both cases, the accuracy and efficiency of the ROM is assessed against results obtained with the FOM.

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A multiscale poromechanics model integrating myocardial perfusion and systemic circulation

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The importance of myocardial perfusion at the outset of cardiac disease remains largely understudied. To address this we present a mathematical model which considers systemic circulation, coronary vessels, myocardium, and the interaction between these components. The core of the whole model is the description of the myocardium as a multi-compartment poromechanics system [1]. A novel decomposition of the poroelastic potential involved in the poromechanics model [2] allows for a quasi-incompressible model which adequately describes the physical interaction between all components in the porous medium.

To reduce the computational cost of our model we propose decoupling the mechanics and systemic circulation from the myocardium and coronary vessels, which allows us to apply the model also in combination with pre-computed cardiac displacements, obtained form other models or medical imaging data. We test the methodology through the simulation of a heartbeat in healthy conditions, in which we are able to capture the systolic impediment phenomenon, a unique feature of myocardial perfusion.

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Electromechanical modeling of human ventricles with ischemic cardiomyopathy: numerical simulations in sinus rhythm and under arrhythmia

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We developed a novel patient-specific computational model for the numerical simulation of ventricular electromechanics in patients with ischemic cardiomyopathy (ICM). This model reproduces the activity both in sinus rhythm (SR) and in ventricular tachycardia (VT). The presence of scars, grey zones and non-remodeled regions of the myocardium is accounted for by the introduction of a spatially heterogeneous coefficient in the 3D electromechanics model. This 3D electromechanics model is firstly coupled with a 2-element Windkessel afterload model to fit the pressure-volume (PV) loop of a patient-specific left ventricle (LV) with ICM in SR. Then, we employ the coupling with a 0D closed-loop circulation model [1, 2] to analyze a VT circuit over multiple heartbeats on the same LV. We highlight similarities and differences on the solutions obtained by the electrophysiology model and those of the electromechanics model, while considering different scenarios for the circulatory system. We observe that very different parametrizations of the circulation model induce the same hemodynamical considerations for the patient at hand. Specifically, we classify this VT as unstable. We conclude by stressing the importance of combining electrophysiological, mechanical and hemodynamical models to provide relevant clinical indicators in how arrhythmias evolve and can potentially lead to sudden cardiac death.

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MS-33
Mathematical Modelling for Urban Planning

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The minisymposium aims at gathering researchers working on multidisciplinary aspects of urban planning. Urban issues are increasingly prominent in national policy agendas and urban development policies seek to address a range of topics, from managing urban expansion and congestion to fostering competitiveness, innovation, social inclusion and environmental sustainability [1].
A particular focus will be placed on resilience and safety of the natural and built environment. Urban resilience refers to the ability of an urban system and of all its socio-ecological and socio-technical constituents to maintain or rapidly return to desired functions in presence of a disturbance, to adapt to change and to quickly transform systems that limit current or future adaptive capacity.
Resilience is not just about a recovery, it is also about transformation: new research

questions, new operative needs and a new interdisciplinary approach are now required by the scientific community.

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Dynamical Models for Monitoring and Assessing Complex Environmental Systems

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Today Decision Makers ever more require reliable assessment models to support the building of winning strategies, of medium-long term, that may guarantee over time both the resilience and sustainability of cities and territories. The antropogenic impacts, the ongoing climate-change negatively influence the environment health and therefore the citizens life quality. In light of this worrying scenario, it is necessaire to build suitable strategies to arrest the climate change irreversibility and compensating the impacts by human activities. Dynamic models play a very important role in measuring the performance over time, especially when they are combined within decision supporting frameworks to design sustainable choices that do not compromise resilience of the environment [1, 2].
This contribution aims to illustrate the usefulness of mathematical models within decision supporting frameworks for assessing the performance of complex environmental systems, with particular regard to the family of cooperative Lotka-Volterra models [3]. These models applied to the discipline of Landscape Ecology are able to understand the ecological dynamics and to predict possible future ecological scenarios as support in the field of environmental monitoring and assessment [4, 5].
Some applications are illustrated of selected cases study of large scale with rural vocation. The first application employs a PANDORA mathematical model and considers both the ecological and economic states of a case study in Northern Italy [6], whereas the second integrates ecological value within a decision supporting model to assess the resilience of a wine region in Portugal [7]. These mathematical models and the proposed applications may be of interest of planners, Decision Makers, technicians and freelances to envision both sustainable and resilient strategies.

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Spatial agent-based models for sustainable policies and urban transformation scenarios

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Cities are considered complex systems, characterized by the interrelations and conflicts of multi-dimensional aspects, multi-scalar effects, and multi-stakeholders' perspectives. These considerations have assumed even more importance with the increasing awareness of the role of sustainability issues and the urgency of a resilient transition of urban areas. Consequently, the evaluation of urban transformations and policies needs to consider the variety of elements in play, spanning environmental, economic and social impacts, as well as the interaction among people and stakeholders. The comprehension of actors' views and needs is crucial for an effective decision-making process since people represent one of the main catalysts for the diffusion or inhibition of strategies and policies in urban areas. The present work investigates the role of the agent-based model (ABM) in supporting the definition of sustainable policies and transformation scenarios in urban contexts. It is increased interest in the challenge of this model in real-world decisions, compared to more traditional mathematical models, such as differential equations, statistical forecasters or system dynamics. ABM is considered an alternative and "right" way [2, 4] in socio-related studies, since it is able to capture emergent phenomena through a bottom-up approach, i.e. from the analysis of individual behaviors of its constituent units, the agents. Moreover, ABM considers the relationships among agents in an environment, from which and to which exchange information and resources. Geographical data, such as income disparity, buildings' quality, infrastructures and services distribution, have to be incorporated into the evaluation model through the adoption of Geographic Information System (GIS), in order to model the social system with its real local characteristics of individual and surrounding space [5]. More specifically, the present application proposes a mixed hybrid ABM, which combines the small world network (SWN) theory [7] and the relative agreement (RA) opinion formation dynamics [3, 6] into an adapted theory of planned behavior (TPB) [1] using a rich set of real-world data and a spatial representation through the integration of GIS maps. This multi-methodology perspective makes possible

the simulation of individual household preferences for the adoption of the photovoltaic system in a centric neighborhood of the city of Torino (Italy).

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A cellular automata for e-planning sustainable urban forms

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A cellular automata-like model, twinned with interactive intelligent geographical systems, is presented to drive planning process toward sustainable urban forms. The use of algorithms and mathematical approaches for the study of urban forms [1] becomes increasingly useful and sometimes indispensable for the understanding of social, economics, behavioural and spatial urban phenomena, and, when possible, for their guidance toward objectively desired patterns. A vast literature using cellular automata for urban growth processes [2] succeeded earlier cellular automata models of three decades ago [3]. Urban morphogenesis is a critical theme due to the exceptional magnitude and speed of world urbanisation which urge novel models of cities if we want a pleasant life and sustainable growth [4]. Isobenefit Urbanism [4] is a libertarian paternalistic approach whose morphogenetic code induces a particular green/built spatiality and a 15-minute walking city where one can reach within 1km natural land, shops, amenities, services and places of work. It does so by leaving free the actual urban development and growth to follow spontaneous random – or locally desired – patterns of functional locations and density across the urban planimetry liberally driven by market forces and genius loci. The outputs are in fact infinites, though all satisfying the code design objective function which can generate interesting urban environmental, planning and economic impacts [5].

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Sequential and Interdependent Investments in Urban Development Projects: a Real Option Approach

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Investments in urban development involve high irreversible sunk costs and are affected by significant uncertainties over future demand and returns. It is generally argued that significant initial capital outlays and uncertainty over future payoffs make de facto these investments irreversible and extremely risky, specifically in boom-and-bust cycles. Ambitious urban regeneration projects are characterized indeed by high operational flexibility, in the form of multiple real options, as they can be expanded by sequential investments and modified over time, in order to adapt to changes in state variables (e.g. demand, construction costs, market prices, etc.). The multiple interacting options or compounded options thus generated can increase projects Net Present Value. Nowadays, both academics and practitioners fully acknowledge that traditional Discounted Cash Flow (DCF) analysis fails to capture the strategic impact of urban development projects and the additional value deriving from real options embedded. As new information is made available and uncertainty about future cash flows is gradually resolved, developers may have valuable flexibility to alter their initial operating strategy in order to capitalize on favourable future opportunities [3]. Indeed, operating options becomes of crucial importance when the environment is highly volatile as in a bust, but planning is flexible, thus permitting developers' and/or planners' intervention at limited cost. This flexibility gives e.g. developers the opportunity to decide strategically the optimal construction schedule and can significantly contributes to limiting economic and financial losses, hedging of investment risks and increasing urban resilience. Nonetheless, the value of this flexibility is strongly dependent on developers' ability to change their planned course of action, given then-available information [2].

This paper investigates the value of flexibility embedded in large urban regeneration projects. In detail, we model the value of flexibility to proceed by sequential investments [1]. Sequential investments can actually be viewed as a sequence of compound and growth options, where an earlier investment guarantees the right but not the obligation to continue operating the project until the next stage comes due. Compoundness within the same multi-stage project generates de facto a series of decision nodes at which the project can be discontinued, if market conditions turns out to be unfavourable. In detail, we analyse the optimal investment strategy of a developer willing to invest in urban development programs. We take into account not exclusively the value of the immediate investment, but rather the value of subsequent investment opportunities and real options interactions. When future payoffs are volatile and market conditions are uncertain, real estate developers can decide to invest firstly in a smaller scale project and then wait to invest in a larger scale project until new information arrives and uncertainty about future cash flows is gradually resolved.

The model is tested on an Italian case study to show the potential of implementing

dynamic stochastic optimization models in the context of urban development projects.

Keywords: Urban Development, Property Investments, Real Options

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System Dynamics Model for Urban Resilience Assessment

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World is actually exposed to several stresses and hazards, both man-made and natural. Cities have thus to face with these pressures, such as population growing, earthquakes, floods and economic crisis. Therefore, the main challenge of the current urban agenda is improving and maintain the resilience of urban systems, in order to make them able to face both with the pressures and the uncertainty of the future development.

Within the introduction of the paradigm of "urban resilience as transformative approach", both new research questions and operative needs have been arisen. The main question is "How to create resilient cities starting from the current situation? Which can be the most suitable strategy?. Thus, new evaluation tools are required. They should be able to assess the urban resilience performance of the urban system in the future, according both to the evolution of the current conditions and to development strategies.

Within this scenario, the present contribution proposes an integrated evaluation framework, based on the combination of the System Dynamics Model (SDM) [1, 5] with the Multi-Criteria Analysis (MCA). The main objective is providing an operative decision-support tool, able to assess urban resilience within its multidimensionality, its complexity and its dynamic behaviour over time [6]. In details, the proposed evaluation framework is grounded on the employment of different urban resilience indicators, that represent different and multidimensional variables of urban system [4]. In fact, these indicators are firstly employed to structure the SDM model. Secondly, to simulate the behaviour of urban system over time, according to the mathematical equation that describe both the variables and their relationships. Thirdly, they are employed to calculate the synthetic urban resilience index through the MCA. This assessment framework method has been firstly applied to different case studies, within a simplified structure [2, 3]. Actually, it is employed within its complete and complex structure to evaluate the urban resilience index over time of two different European cities.

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A framework for the management of territorial resilience

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This mini-symposium is dedicated to the approach to the territorial resilience developed within the R3C Responsible Risk Resilience Centre of Politecnico di Torino. The problem here addressed is the evaluation of the resilience of territories exposed to multiple stressors and opportunities, of anthropic and natural origin, keeping into account the vulnerabilities and the coping capacities, to obtain a GIS map able to support the resilience based decision making in the identification of planning and technical measures to enhance it. The intervention will explore the maturity level of the proposed framework, the pro's end con's identified thanks to the ongoing applications and the solutions devised to address the identified shortcomings and to enhance positive aspects. The functionalities of the method will be exemplified and visualized through the application to a territory used as a sample.

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MS-34
Variational Methods in Materials Science: Mathematics and Mechanics – Part I

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These three MiniSymposia concern the application of the Calculus of Variations to Materials Science, in particular to Continuum Mechanics. Scientists working in different fields will contribute by presenting results of theoretical, numerical, and experimental nature, fostering collaboration between engineers and mathematicians.

The talks will address two main research directions:

- Approximation and optimization of complex energies
- Variational models for material defects

Approximation and optimization of complex energies. Variational methods are successfully employed to detect stationary energetic configurations, to optimize them under proper boundary conditions, to approximate complex energies, and to validate their effective expressions. Some problems discussed in the session will be the passage from discrete to continuum in atomistic systems, the study of optimal configurations and of microstructures, the derivation of effective energies suitable to numerical simulation, as in phase-field approximation. Presentations will cover new and recent methods for the description of fracture and damage phenomena.

Variational models for material defects. The prediction of the occurrence and of the motion of defects in materials is of fundamental importance in applications. This requires an analytical validation of evolutionary models for material defects. Energetic criteria have been largely employed to study evolutions of both rate-dependent and rate-independent type. The session will present different approaches to these problems, mainly in the context of continuum mechanics and with variational methods. The talks will deal with phenomena taking place at different scales, ranging from quasi-static, viscous, gradient flows, to inertial dynamic evolutions.

Asymptotic analysis of deformation behavior in high-contrast composites: rigidity and anisotropy

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Rigidity results in general are powerful statements that allow to derive global properties of a deformation from local ones. The classical Liouville theorem states that every local isometry of a domain corresponds to a rigid body motion, but if connectedness of the set fails, global rigidity is no longer true. In this talk, we discuss two new asymptotic rigidity results in the context of nonlinear elasticity, showing that if an elastic body contains sufficiently stiff connected components arranged into fine parallel layers or fibers, then its effective deformation behavior is restricted by global, anisotropic constraints. In mathematical terms, we characterize the weak limits of sequences of Sobolev maps whose gradients on the stiff components lie in the set of rotations. Besides their theoretical interest, these findings facilitate the homogenization via Γ-convergence of variational problems modeling high-contrast fiber-reinforced and bilayered composite materials. We present explicit formulas for the Γ-limits and discuss examples of attainable limit deformations.

This is joint work with Fabian Christowiak (University of Regensburg), Dominik Engl (Utrecht University), and Antonella Ritorto (KU Eichstätt-Ingolstadt).

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Endow Griffith's brittle fracture theory with the ability to describe fatigue cracks

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Fracture mechanics is nowadays a consolidated theory within the realm of continuum mechanics, that has been developed starting from the pioneering work of Griffith [1], where the key concepts of energy release rate and fracture toughness (surface energy) has been established. A remarkable variational extension of such a theory has been proposed by Francfort and Marigo in [2]. A lacking feature of Griffith's brittle fracture criterion, including its variational extensions, is the inability to capture and describe fatigue cracks, that is cracks evolving due to repeated loads that singularly would be too small to cause the material failure.

In this contribution, we will propose a phenomenological model that endows Griffith's brittle fracture criterion with the ability to describe fatigue cracks. The key idea of the present model is to consider the fracture toughness not as a material parameter anymore but rather as a material function, assumed to be decreasing as a an accumulated energy based measure increases. Analytical and numerical examples will shown the capability of the present model to recover Paris fatigue law and many other key features of fatigue cracks propagation.

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Uniform distribution of dislocations at semi-coherent interfaces

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We will introduce variational models for edge dislocations at semi-coherent interfaces between two heterogeneous crystals, and prove the optimality of uniformly distributed edge dislocations. Specifically, we prove that, in the large interface limit, the elastic energy Γ-converges to a limit functional comprised of two contributions: one is given by a constant gauging the minimal energy induced by dislocations at the interface, and corresponding to a uniform distribution of edge dislocations; the other one accounts for the far field elastic energy induced by the presence of further, possibly not uniformly distributed, dislocations. After assuming periodic boundary conditions and formally considering the limit from semi-coherent to coherent interfaces, we show that the optimal configuration consists in evenly-spaced dislocations on the one dimensional circle. This is joint work with M. Ponsiglione and R. Scala, based on [1].

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Topology optimization in inelastic structures

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Topology optimization aims at detecting the optimal distribution of a material within a fixed region given applied loads and volume or shape constraints, with the scope of maximizing the performance of the resulting object. In the framework of linearized elastoplasticity, we will show how to recast such a problem as an optimal control problem, where the density of the material acts as a control parameter. We will prove existence of optimal configurations and compute their first-order optimality conditions.

Modeling of fatigue crack growth phenomena using the variational phase-field approach

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Fatigue failure is one of the major cause of structural failures, however most of the studies available are based on empirical laws that lack of generality and predictive capabilities. In general, a framework that covers both the mechanics of the monotonic fracture and the fatigue behavior is missing.

The present work aims at proposing a framework to model fatigue in brittle materials based on the variational phase-field approach to fracture [1]. The standard phase-field free energy functional is modified similarly to [2] so as to allow the fracture toughness of the material to decrease as a fatigue scalar history variable increases. The reduction rate is governed by a fatigue degradation function and takes as argument only the fatigue history variable. Two definitions of the cumulated variable and two fatigue degradation functions are proposed, allowing to reproduce the major fatigue characteristics of brittle materials. The obtained results show the capability of the approach to reproduce the major features of the fatigue behavior including the crack nucleation, stable and unstable propagation phases. Also, the Paris law and the Wöhler curve are obtained naturally, while the Palmgren-Miner rule and the monotonic behavior are encompassed as special cases.

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Soap films spanning elastic rods

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The Kirchhoff-Plateau problem concerns the equilibrium shapes of a system in which a flexible filament in the form of a closed loop is spanned by a liquid film, with the filament being modeled as a Kirchhoff rod and the action of the spanning surface being solely due to surface tension. We establish the existence of an equilibrium shape that minimizes the total energy of the system under the physical constraint of non-interpenetration of matter, but allowing for points on the surface of the bounding loop to come into contact. In our treatment, the bounding loop retains a finite cross-sectional thickness and a nonvanishing volume, while the liquid film is represented by a set with finite two-dimensional Hausdorff measure. Moreover, the region where the liquid film touches the surface of the bounding loop is not prescribed a priori. Our mathematical results substantiate the physical relevance of the chosen model. Indeed, no matter how strong is the competition between surface tension and the elastic response of the filament, the system is always able to adjust to achieve a configuration that complies with the physical constraints encountered in experiments. In this seminar I will present some results concerning the Kirchhoff-Plateau problem obtained in collaboration with Eliot Fried and Giulio Giusteri [3], Giulia Bevilacqua and Alfredo Marzocchi [1, 2].

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MS-35
Variational Methods in Materials Science: Mathematics and Mechanics – Part II

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These three MiniSymposia concern the application of the Calculus of Variations to Materials Science, in particular to Continuum Mechanics. Scientists working in different fields will contribute by presenting results of theoretical, numerical, and experimental nature, fostering collaboration between engineers and mathematicians.

The talks will address two main research directions:

- Approximation and optimization of complex energies
- Variational models for material defects

Approximation and optimization of complex energies. Variational methods are successfully employed to detect stationary energetic configurations, to optimize them under proper boundary conditions, to approximate complex energies, and to validate their effective expressions. Some problems discussed in the session will be the passage from discrete to continuum in atomistic systems, the study of optimal configurations and of microstructures, the derivation of effective energies suitable to numerical simulation, as in phase-field approximation. Presentations will cover new and recent methods for the description of fracture and damage phenomena.

Variational models for material defects. The prediction of the occurrence and of the motion of defects in materials is of fundamental importance in applications. This requires an analytical validation of evolutionary models for material defects. Energetic criteria have been largely employed to study evolutions of both rate-dependent and rate-independent type. The session will present different approaches to these problems, mainly in the context of continuum mechanics and with variational methods. The talks will deal with phenomena taking place at different scales, ranging from quasi-static, viscous, gradient flows, to inertial dynamic evolutions.

Mathematical models of chemical and mechanical damage in cultural heritage

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In this talk I present some recent models of coupled mechanical and chemical damage in materials used in historical building as stones, but also concrete. These models are derived by using a mixed evolutionary-stationary formulation. Some modelling assumptions and numerical simulations will presented and discussed. Work in progress in collaboration with Francesco Freddi (Università di Parma).

Topological singularities in periodic media: Ginzburg-Landau and core-radius approaches

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I will describe the emergence of topological singularities in periodic media within the Ginzburg-Landau model and the core-radius approach. In particular I will investigate, through a multi-scale analysis, the interaction between the oscillation period of the composite and the length scale parameter of the Ginzburg-Landau functionals.

Asymptotic analysis of 3d nonlinear elastic models for dislocations

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We derive a line tension model for dislocations in 3d through the asymptotic analysis, as the amplitude of the Burgers vectors (proportional to the lattice spacing) tends to zero, of a geometrically nonlinear elastic energy.
More precisely we introduce a so called semidiscrete model, that represents a continuum approximation of an interaction energy between particles in a lattice in the presence of defects. Here the relevant variable is a strain field that shows topological incompatibilities near the defects and as consequence the corresponding continuum energy blows up near the singularities. Therefore a regularisation in the region close to the defects is required. We discuss different types of regularisations: the first is a truncation of the energy using mixed growth conditions, the second is instead the so called core cut-off regularisation, and the third is a regularisation by mollification. We show that these regularisations, in the case of dilute dislocations, are all equivalent, in the sense that they produce the same limit.
The latter is given by the contribution of two terms, a volume term, that represents the linearised elastic energy, and a line tension, that represents the plastic energy. These results were obtained in collaboration with A. Garroni and R. Scala in [2] and with A. Garroni and S. Conti in [1].

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Rotations with constant curl are constant

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It is a classical result in nonlinear elasticity due to Liouville that a curl-free field of rotations $\beta : \Omega \subseteq \mathbb{R}^n \to SO(n)$ is locally constant. However, in the continuum theory of dislocations the strain fields β are not curl-free. In this talk we address a natural extension of Liouville's theorem to the theory of dislocations. We show in three dimensions that a field $\beta : \Omega \to SO(3)$ such that $\operatorname{curl} \beta$ is constant, is again necessarily locally constant. As a byproduct, we discuss the regularity of the field $\beta : \Omega \to SO(3)$ in terms of the regularity of $\operatorname{curl} \beta$.

Multi-phase field approach to tensile and compressive failures in brittle materials

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In classical phase field models for brittle fracture, the damage is usually associated to tensional stress states [1]. However, in many porous materials, like rocks or bones, failure is the result of a combination of both tensional and compressive damages [2]. These materials exibith very different damage mechanisms in tension and compression with brittle fracture in tension and crushing in compression. Here, a novel strain energy decomposition method is intruduced in a multi-phase field approach to nonlocal damage to consistently simulate failures involving the interaction between tensile cracks and damage in compression responsible for crushing. To this purpose, the following decomposition of the energy density is assumed $\psi(\boldsymbol{\varepsilon}, s_1, s_2) = (1 - s_1)^2\psi_+(\boldsymbol{\varepsilon}) + (1 - s_2)^2\psi_-(\boldsymbol{\varepsilon})$, where $0 \leq s_i \leq 1,\ i = 1, 2$ are the phase field variables associated respectively to tensile and compressive damage, being ε the infinitesimal strain tensor and ψ_+ and ψ_- the positive and negative parts of the strain energy density.
A finite element procedure has been proposed in FEniCS [3] to numerically solve the coupled nonlinear variational problem. The model is exploited to simulate fracture in porous materials under compression for different specimen shapes and porosities, and it is capable of representing damage patterns ranging from diagonal cracks to crushing failures.

Acknowledgements
Support from the Italian Ministry of Education, University and Research (MIUR) to the project PRIN 2017 "XFAST-SIMS: Extra-fast and accurate simulation of complex structural systems" (CUP: D68D19001260001) is gratefully acknowledged.

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On a Rate-Independent Damage Model for Hybrid Laminates with Cohesive Interface

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In this talk we present a rate-independent model for hybrid laminates described by a damage phase-field approach on two elastic layers glued together and subjected to a horizontal loading in a one-dimensional setup; we assume the adhesive interface connecting the two layers follows a cohesive law. The analysis is based on the concept of (globally stable) energetic evolution introduced by Mielke, Roubicek and Theil to deal with rate-independent problems. Due to the presence of the cohesive zone, compactness mathematical issues usually lead to the introduction of a fictitious variable replacing the physical one which represents the maximal opening of the interface displacement reached during the evolution. We illustrate a novel strategy which allows to recover the equivalence between the fictitious and the real variable under general loading-unloading regimes. The argument is based on temporal regularity of energetic evolutions, achieved by means of a careful balance between the convexity of the elastic energy of the layers and the natural concavity of the cohesive energy of the interface.

MS-36
Variational Methods in Materials Science: Mathematics and Mechanics – Part III

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Γ-convergence and stochastic homogenisation of singularly-perturbed elliptic functionals

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In this talk we analyse the limit behaviour of the general elliptic functionals of Ambrosio-Tortorelli given by

$$F_k(u,v) = \int_A v^2 \, f_k(x, \nabla u)\, dx + \frac{1}{\varepsilon_k} \int_A g_k(x, v, \varepsilon_k \nabla v)\, dx\,,$$

where u is a vector-valued Sobolev function, $v \in [0,1]$ a phase-field variable, and $\varepsilon_k > 0$ a singular-perturbation parameter, *i.e.*, $\varepsilon_k \to 0$, as $k \to +\infty$.

Under mild assumptions on the integrands f_k and g_k, we show that if f_k grows superlinearly in the gradient-variable, then the functionals F_k Γ-converge (up to subsequences) to a *brittle* energy-functional, *i.e.*, to a free-discontinuity functional whose surface integrand does *not* depend on the jump-amplitude of u. This result is achieved by showing that volume and surface term in F_k *decouple* in the limit.

As an application of the abstract Γ-convergence result as above, the case of *stationary random* integrands will be also discussed.

Morphable structures inspired by the pellicle of euglenids

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Structures capable of reconfiguring themselves, hence adapting their properties to changing demands on the functions they have to perform, are attracting increasing interest. To achieve such reconfigurations, previous studies have considered the use of soft active materials and fiber-reinforced composites. Along this research line, a number of design principles are being explored, such as those based on the buckling-induced rearrangement of material micro-architectures, origami, and kirigami. Here, we draw inspiration in the pellicle of euglenids, a family of unicellular protists whose unique shape-morphing principle is based on the relative sliding between the pellicle strips that comprise their cytoskeleton [1, 2]. The resulting kinematics has been previously examined in a continuum limit, where we mapped the broad range of shapes accessible by this mechanism [3], but not the underlying mechanics. While the regulation of shape in euglenoid cells is provided by the activity of molecular motors that exert forces in the overlap region between adjacent strips, it is unclear how the elasticity of the strips controls the overall mechanical properties of a biomimetic material inspired by the pellicle. We introduce a mathematical model based on rod's theory to discuss adaptive geometry and mechanical properties of an assembly of helical elastic strips [4, 5]. For the case of cylindrical deformations, we address the problem of computing the external equilibrium forces (axial force, axial torque, pressure on the lateral walls) necessary to drive and control the shape changes resulting from the uniform sliding between adjacent strips. In carrying out the analysis, we neglect inter-strip friction and boundary layer effects, while retaining in full the geometric nonlinearities and the discreteness of the structure. Under these assumptions, the equilibrium response of the composite structure is described by explicit formulae that

we obtain by exploiting analytical techniques based on energetic arguments. Despite its simplicity, the structure displays a complex and highly nonlinear mechanical behaviour that can be tuned by the spontaneous curvature or twist of the strips, as illustrated in Fig. 1 for the prototypical case of an assembly of rods subject to an axial vertical force. We believe that our findings highlight the remarkable potential in engineering

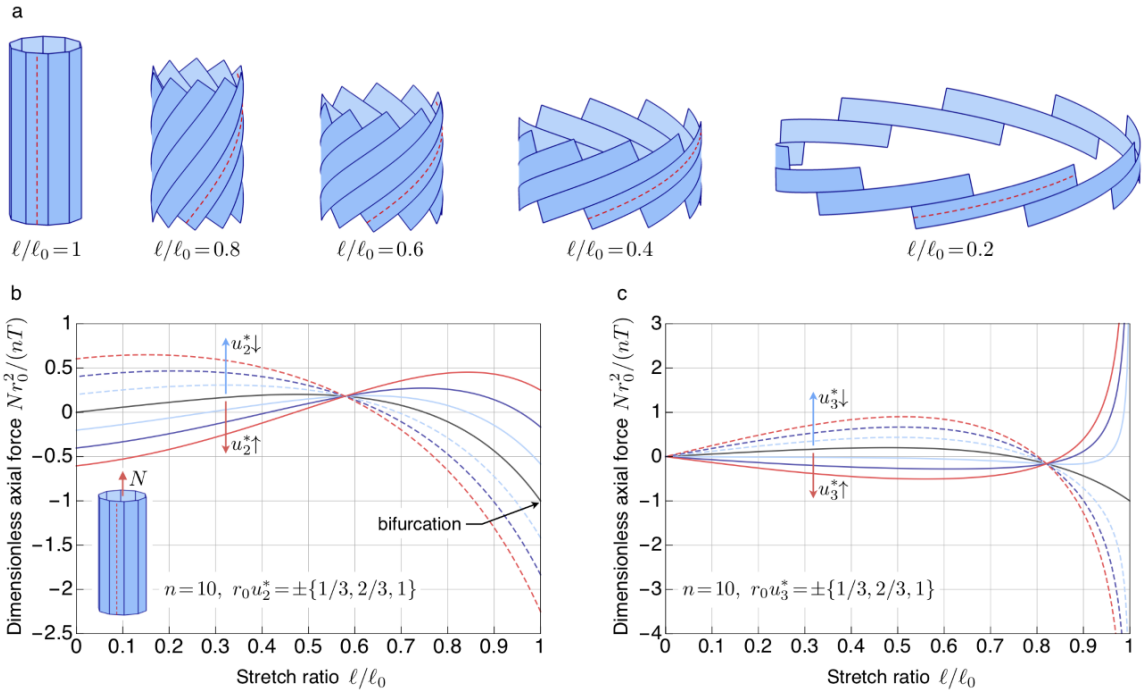

Figure 1: (a) Deformed configurations of a structural assembly of ten rods at distinct levels of axial stretch. Effect of spontaneous curvature (b) and of spontaneous twist (c) on the axial-force versus vertical-stretch mechanical response of the composite system. Solid and dashed curves correspond to positive and negative values of the spontaneous curvature u_2^* or twist u_3^*, respectively. The black solid curve corresponds to the reference conditions of $u_2^*=u_3^*=0$.

and robotics of structural systems inspired by the euglenoid pellicle. Current studies by the authors include the analysis of the impact of inter-strip friction on the response of such mechanical systems. We also plan to validate our theoretical findings by carrying out physical experiments on biomimetic structures realized by means of multi-material additive manufacturing techniques.

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Vectorial phase field approximation of cohesive fracture models

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We pursue the study started in [1], where a cohesive fracture model, depending on scalar-valued displacements, was obtained as Γ-limit of damage models. We focus here on the case in which the displacement variable is vector-valued. Precisely, we obtain a cohesive fracture model as Γ-limit, as $\varepsilon \to 0$, of damage models in which the elastic coefficient is computed from the damage variable v through a function f_ε of the form $f_\varepsilon(v) = \min\{1, \varepsilon^{1/2} f(v)\}$, with f diverging for v close to the value describing undamaged material. The resulting fracture energy, depending on the opening z of the jump set and on the normal vector ν to the jump set, is given in terms of an asymptotic cell formula. It is one-homogeneous in the opening z at small values of $|z|$ and has a finite limit as $|z| \to \infty$.

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Microscopical justification of solid-state wetting and dewetting

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The continuum model related to the Winterbottom problem, i.e., the problem of determining the equilibrium shape of crystalline drops resting on substrates, is derived by means of a rigorous discrete-to-continuum passage performed by Gamma-convergence from atomistic models. Such atomistic models are introduced by taking into account both the interactions of the drop particles among themselves and with the fixed substrate atoms. In particular, previous results in the literature are generalized to the presence of a half-plane substrate and, as a byproduct of the analysis, effective expressions for the drop anisotropy at the free surface and the drop wettability at the contact region with the substrate are characterized in terms of the atomistic potentials, which are chosen of Heitmann-Radin type. Furthermore, a threshold condition only depending on such potentials is determined distinguishing the wetting regime, where discrete minimizers are explicitly characterized as configurations contained in a one-atom thick layer on the substrate, from the dewetting regime. In the latter regime, also in view of a proven conservation of mass in the limit as the number of atoms tends to infinity, proper scalings of the discrete minimizers converge to a bounded minimizer of the Winterbottom continuum model satisfying a nonzero volume constraint.

Characterization of quasi-static evolutions generated by alternate minimization

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We consider separately convex phase-field energies $\mathcal{F}_\epsilon(t,u,v)$ and we assume that a Dirichlet boundary condition $u = g(t)$ on $\partial_D\Omega$ is imposed on the displacement u, for $t \in [0,T]$. We employ with a time-discrete approach with step τ and discrete times $t_m = m\tau$, in which, for each t_m, the evolution is obtained by an alternate minimization scheme, like

$$\begin{cases} u_{m,k} \in \operatorname{argmin}\big\{\mathcal{F}(t_m, u, v_{m,k-1}) : u = g(t_m) \text{ on } \partial_D\Omega\big\}, \\ v_{m,k} \in \operatorname{argmin}\big\{\mathcal{F}(t_m, u_{m,k}, v) : v \le v_{m,k}\big\}. \end{cases}$$

In this way we build a "two scale" time discrete evolution in which the intermediate steps $u_{m,k}$ and $v_{m,k}$ provide some information on the transition from (u_{m-1}, v_{m-1}) to (u_m, v_m) which give the configurations at time t_{m-1} and t_m respectively.

In the limit as $\tau \to 0$ the time-discrete solutions obtained by the staggered scheme converge to an evolution (u,v) which presents both steady-state (continuous) and unsteady-state (discontinuous) regimes; note that this is actually a general feature of quasi-static evolutions for non-convex energies. Qualitatively, steady-state and unsteady-state regime have respectively the following features: if (u,v) is continuous in a time interval then the evolution is simultaneous in u and v, the system is in equilibrium, Griffth's criterion holds (in phase-field form), energy identity holds, thermodynamic consistency between monotonicity and dissipation holds; if (u,v) is discontinuous in a certain time t then the transition between (u^-, v^-) and (u^+, v^+) is still staggered in u and v.

The latter feature can be observed also in the time-discrete setting. In particular, if t_m is a discontinuity (or unsteady-state) time it takes a huge number of staggered iterations to converge. In the latter case, the step length $\|v_{m,k} - v_{m,k-1}\|_{L^2}$ as a function of the iteration index k presents a long "tail" of small steps followed by a plateau of long steps and a peak, corresponding to complete failure. On the contrary, when t_m is a continuity (or steady-state) time the scheme converges in few staggered iterations.

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Variational approaches for crack tracking based on the concept of eigenfracture

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The eigenfracture scheme of [1] provides a regularization of the energy functional attending the propagation of fracture according to Griffith's criterion. Regularization is achieved by means of eigendeformations, i.e., deformations that are not associated to energy and allow to develop displacement jumps with no energy cost. A particular implementation of eigenfracture leads to an element erosion scheme, which we refer to as *eigenerosion*. Eigenerosion is derived from the general eigenfracture scheme by restricting the eigendeformations in a binary sense: they can be either zero, in which case the local behavior is elastic; or they can be equal to the local displacement gradient, in which case the corresponding material neighborhood is failed, or *eroded*. When combined with a finite-element approximation, this scheme gives rise to *element erosion*, i. e., the elements can be either intact, in which case their behavior is elastic, or be completely failed —or eroded— and have no load bearing capacity [2].

Thus eigenerosion (EE) stands as a discretization approach to fracture alternative to the popular phase-field (PF) method. Phase-field is a very general method that can be used to model material discontinuities and interfaces. Contrariwise, eigenerosion has been developed explicitly to model fracture. Phase-field and element erosion methods have a common variational structure: an elastic energy-release mechanism, namely, progressive damage in the case of PF and abrupt damage in the case of EE; and an energy cost of damage, derived from the phase-field and its gradients in the case of PF and from an estimate of the fracture area in the case of ER. In both cases, the static equilibrium configurations of the solid follow from global energy minimization. In addition, crack propagation is modeled in both cases by means of a rate-independent gradient flow that balances elastic energy-release rate and dissipation.

In this work we want to compare eigenerosion and phase-field in a very general form, pointing out similarities and differences, and focusing on the accuracy and convergence properties to reveal the advantages and the drawbacks of both approaches [3].

This research has been developed in collaboration with Michael Ortiz and Kerstin Weinberg.

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MS-37
Trends in nonlinear PDEs and applications

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In the last fifty years the analysis of nonlinear partial differential equations (N-PDEs) has become a fundamental tool in the modeling of real life phenomena, due to the wide range of applications that N-PDEs present in applied sciences. From theoretical physics to biology, from economics to engineering, each field of natural and social sciences gives rise to always new and challenging questions concerning N-PDEs, whose investigation requires to draw upon several branches of mathematical analysis. As a consequence, interdisciplinarity is a deep-seated feature of the discussion on N-PDEs, given by its twofold nature: the variety of the applications and the multiplicity of the techniques necessary to such discussion.

The aim of the minisymposium is to bring together recognized experts in the study of nonlinear PDEs alongside with young mathematicians working on the topic. A

major goal is to gather people coming from different mathematical communities, foster interactions, promote the exchange of ideas and methods, and contribute to the diffusion of new interesting problems. Among the main topics that will be represented in the minisymposium are the analysis of nonlinear dispersive equations such as Schrödinger and Dirac Equations, the Calculus of Variations and the study of Geometric Flows.

Action versus energy ground states in nonlinear Schrödinger equations

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We consider the stationary nonlinear Schrödinger equation

$$\Delta u + |u|^{p-2}u = \lambda u$$

in $H_0^1(\Omega)$, where Ω is a (possibly unbounded) open subset of $\mathbf{R}^N$ and λ is a real parameter.

The existence of positive solutions can be addressed by variational methods in at least two different ways: either by minimizing the action functional on the Nehari manifold or by minimizing the energy functional on the set of functions having a prescribed L^2 norm. In the former case, we speak of action ground states, and in the latter of energy ground states.

Action ground states have a prescribed value of the frequency λ and an unknown value of the mass (the L^2 norm), while energy ground states have a prescribed value of the mass and an unknown frequency.

These two approaches are clearly intertwined, since any action ground state is also a critical point of the energy with the appropriate mass constraint and, conversely, any energy ground state is also a critical point of the action, with the appropriate value of λ.

Despite these relationships, however, the precise interplay between the "action approach" and the "energy approach" (in particular, the question whether an action ground state is necessarily also an energy ground state, or the other way round) has not been thoroughly investigated yet, and the present talk aims at taking a first step in this direction.

Our first general result is that the "ground state levels" are strongly related by the following duality result: the (negative) energy ground state level is the Legendre–Fenchel transform of the action ground state level. Furthermore, whenever an energy ground state exists at a certain frequency, then all action ground states at that frequency have the same mass and are energy ground states too. We prove that the converse is in general false and that the action ground state level may fail to be convex. Next we analyze the differentiability of the ground state action level and we provide an explicit expression involving the mass of action ground states.

Effective theories for many-body quantum systems

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A central challenge in many-body quantum mechanics is to understand how the microscopic Schrödinger equation manifests in the macroscopic world. In certain regimes the many-body theory can be approximated by an effective theory describing the macroscopic properties of the system in terms of fewer degrees of freedom. A renowned example is the nonlinear Schrödinger equation emerging from the many-body dynamics of Bose-Einstein condensates. Static properties instead are described by Bogoliubov's effective theory. We consider Bose-Einstein condensates in a dilute limit (Gross-Pitaevskii limit) and determine the low-energy excitation spectrum, providing a rigorous proof of Bogoliubov's effective theory. To achieve this, we go beyond Bogoliubov's ideas and combine second quantization techniques with a new description of quantum correlations.

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Normal Form and Existence Time for the Kirchhoff Equation

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In this talk I will present some recent results on the existence time for solutions of the Kirchhoff equation

$$\partial_{tt} u - \left(1 + \int_{\mathbb{T}^d} |\nabla u|^2 \, dx\right) \Delta u = 0$$

with periodic space boundary conditions (i.e. $x \in \mathbb{T}^d$). Computing the first step of quasilinear normal form, we erase from the equation all the cubic terms giving nonzero contribution to the energy estimates for the time evolution of Sobolev norms; thus we deduce that, for small initial data of size ε in Sobolev class, the time of existence of the solution is at least of order ε^{-4} (which improves the lower bound ε^{-2} coming from the linear theory). After the second step of normal form, there remain some resonant terms (which cannot be erased) that give a non-trivial contribution to the energy estimates; this could be interpreted as a sign of non-integrability of the equation. Nonetheless, we show that small initial data satisfying a suitable nonresonance condition produce solutions that exist over a time of order at least ε^{-6}.

Spatially inhomogeneous multi-agent dynamics with label switching: mean-field limits and optimal control

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Multipopulation agent systems model realities where multiple individuals with *labels* evolve in time. These labels, that define the population each agent belongs to, can adapt to a number of different situations, according to the meaning given to them: evolutionary population dynamics, economics, chemical reaction networks, and kinetic models of opinion formation are just a few of the possible applications.

Starting from a mean-field limit result for evolutionary games [3], we will extend the functional setting of evolution equations in Banach spaces to include label switching [4] to model realistic cases in which transitions from one population to another one are allowed. Finally, we discuss the case in which selective optimal control is added to the system [1], allowing for a potential policy maker to act specifically on a targeted subgroup of agents. In [2], a multi-step discretization scheme is proposed, that is appropriate for numerical discretizations.

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Fine properties of weak solutions of Burgers equation and applications to a singularly perturbed variational problem

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We consider bounded weak solutions to the inviscid Burgers equation

$$\partial_t u + \partial_x \left(\frac{u^2}{2} \right) = 0.$$

A pioneering result in the theory of conservation laws establishes the well-posedness of the associated Cauchy problem in the class of bounded entropy solutions, namely bounded functions satisfying

$$\mu_\eta := \partial_t \eta(u) + \partial_x q(u) \leq 0 \qquad \text{in } \mathcal{D}' \tag{1}$$

for every convex entropy $\eta : \mathbb{R} \to \mathbb{R}$ and corresponding flux $q : \mathbb{R} \to \mathbb{R}$ defined up to constants by $q'(v) = \eta'(v)v$. We are interested in the more general class of weak solutions with finite entropy production, where the distribution μ_η in (1) is only required to be a locally finite Radon measure (without constraints on its sign). Although weak solutions with finite entropy production are not locally of bounded variation, they share with BV functions most of their fine properties: in particular a one dimensional rectifiable set J of shocks is identified in [DLOW03, Lec05]. The main result of this talk is that the measure μ_η is concentrated on this shock set J.

The motivation of this result is the study of the asymptotic behavior as $\varepsilon \to 0^+$ of the following functionals:

$$F_\varepsilon(u, \Omega) := \int_\Omega \left(\varepsilon |\nabla^2 u| + \frac{1}{\varepsilon} \left| 1 - |\nabla u|^2 \right|^2 \right) dx, \qquad \text{where } \Omega \subset \mathbb{R}^2.$$

Limits of functions u_ε with uniformly bounded energy solve the eikonal equation $|\nabla u| = 1$, which can be interpreted as an $\mathbf{S}^1$-valued conservation law. In particular the notion of entropy can be introduced also in this setting and it turns out that the candidate Γ-limit F_0 can be described in terms of the entropy dissipation measures. Although a full rectifiability result as in the case of Burgers equation is still not available, we can prove some partial results in this direction. As a consequence we prove that if Ω is an ellipse and u_ε are minimizers of $F_\varepsilon(\cdot, \Omega)$ under appropriate boundary conditions, then

$$u_\varepsilon \to \bar{u} := \operatorname{dist}(\cdot, \partial\Omega).$$

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MS-38
Non-standard time integration of evolutionary problems – Part I

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The minisymposium is focused on providing recent advances in the numerical time integration of evolutive problems, mostly based on differential operators, by non-standard schemes. These problems normally arise as models of time-space evolutionary phenomena and usually require a large computational effort in order to provide accurate solutions. A particular emphasis will be given to efficiently computing accurate solutions, as well as on preserving qualitative properties of the operator also along discrete solutions and solving problems in presence of stochastic terms affecting the overall dynamics. The theoretical analysis of the problems of the resulting schemes will be supported by the numerical evidence obtained on non-trivial selected problems of interest in the applications.

The minisymposium is scheduled in two parts. The scientific work of young researchers will also be emphasized through dedicated talks given by themselves. The minisymposium

is organized within the activities of the PRIN2017-MIUR project "Structure preserving approximation of evolutionary problems".

Long-term stable integration of stochastic systems subjected to small random forces

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Often, in various models of real applications, fluctuations affecting the system are small and state-independent. To study the behavior of these systems many times it is needed to integrate over very long time intervals (e.g. when we aim to compute statistical quantities with respect to invariant laws of the system). Unfortunately, in this case, many of the available methods in the literature show explosive behavior or are inefficient. In this work we develop a technique that allows the construction of efficient integrators with valuable long-term properties for this kind of systems. Their convergence and stability are studied, and computer simulations are carry out to illustrate the practical performance of the proposed integrators and their advantages in comparison with other existing ones.

Stiffness, order reduction and fake news: multivalue numerical modeling and applications

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Our lives have significantly been influenced by the birth of social networks, which provide a large reservoir of news. The veracity of this information and the spread of fake news certainly requires a special attention [5] and mathematical modeling for the diffusion of fake news has attracted the attention of many authors (see, for instance, [1, 2, 4] and references therein). We emphasize in this talk the role of the stiffness ratio that characterize differential problems modeling the diffusion of fake news. In particular, we show that the stiffness ratio allows to understand how fast is the transit of fake news in a given country, providing a numerical evidence based on real data [2]. Moreover, for an efficient numerical modeling of stiff problems, we also introduce a theory of multivalue collocation methods free from order reduction [3], which is typical of Runge-Kutta (RK) methods. The theoretical analysis, examples of methods as well as numerical experiments on a selection of stiff problems are presented in this talk.

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Some trends in the numerical computation of matrix functions in the integration of differential problems

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The numerical computation of matrix functions is an extensively analyzed topic in numerical linear algebra. The interest in matrix functions lies in the diverse important roles they play in the solution of problems in science and engineering. Starting from the classical paper by Moler and Van Loan [5] in 1978 about the matrix exponential, many works have been devoted to the numerical computation of $f(A)$, being A an order n complex matrix and f an analytic complex valued function. Different functions have been then considered (i.e. trigonometric functions, pth root function, sector functions, sign matrix and others, see [3]): some of them could be used in integration schemes of matrix differential systems or, as recently discovered, in the numerical integration of fractional differential equations [1].

Severe challenges arise in these contexts: here we consider applications, for example, in which the numerical approximation of a matrix function must belong to a given group (see for example [4]), or requiring that the numerical approximation preserves some features of the matrix function, as the stochasticity when computing the matrix pth root [6], or the sparsity [2]. Moreover, some recent trends in the integration of differential problems will be discussed.

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On the stability of linear stochastic differential equations with non-normal drift

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In the framework of the mean-square asymptotic stability of the equilibria of linear stochastic systems, we study the impact on the stability of the introduction of a hypothesis of strong non-normality of the drift matrix. In particular, inspierd by the work [3], we start from non-normal homogeneous linear systems of ODEs, which are stable, but become unstable when an "exponentially small" amount of linear multiplicative noise is introduced. We proceed by employing tools provided in [2] to study the ε-pseudospectrum of a matrix, and the structural analysis derived in [1] on the asymptotic mean-square stability for multi-dimensional linear stochastic differential systems, to provide results and considerations both on the continuous problem and on the difference equations deriving from the application of numerical methods.

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Numerical Methods That Preserve Conservation Laws

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The solutions of a PDE that arises as a realistic model of a physical phenomenon, typically satisfy a set of conservation laws. Conservation laws usually refer to some quantity with an important physical meaning such as mass, momentum, energy or charge. They state that within an arbitrary small volume the amount of the conserved quantity can only change by the amount of quantity which flows in or out of the volume in the considered interval of time.

From a mathematical point of view, conservation laws are among the most important geometric properties of a PDE and preserving them in the discrete setting confers very strong constraints on the behaviour of the numerical solutions and yields better accuracy on long times. Moreover, numerical methods that satisfy conservation laws are often paramount for the physical significance of the model.

A new strategy for developing bespoke finite difference methods that preserve conservation laws has been recently introduced in [3] and further refined in [4].

The schemes obtained in this way typically feature certain free parameters that can be arbitrarily chosen without compromising the preservation of the conservation laws. A convenient choice of the parameters generally yields very accurate approximations. However, the optimal values of the parameters are not known a priori and depend heavily on the initial conditions.

In this talk we will discuss some new techniques for improving the accuracy of the schemes by minimizing an estimate of the local error. We will also remark on the possibility of adapting the schemes to solutions whose oscillatory behaviour can be speculated from the formulation of the problem [1, 2]. Numerical tests showing the effectiveness and efficiency of the new approach will be presented.

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MS-39
Non-standard time integration of evolutionary problems
Part II

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The minisymposium is focused on providing recent advances in the numerical time integration of evolutive problems, mostly based on differential operators, by non-standard schemes. These problems normally arise as models of time-space evolutionary phenomena and usually require a large computational effort in order to provide accurate solutions. A particular emphasis will be given to efficiently computing accurate solutions, as well as on preserving qualitative properties of the operator also along discrete solutions and solving problems in presence of stochastic terms affecting the overall dynamics. The theoretical

analysis of the problems of the resulting schemes will be supported by the numerical evidence obtained on non-trivial selected problems of interest in the applications.

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Stirring, mixing, growing: numerical challenges to phytoplankton modeling

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Understanding climate change requires modeling processes that are both physical and biological, spanning many spatial and temporal scales. In particular, any satisfactory description of marine systems must take into account plankton dynamics that occurs at sub-centimeter scales, and turbulent stirring, which may involve all scales from the size of the basin down to the Kolmogorov length. These biological and physical processes are coupled by irreversible mixing, which, in nature, is negligible except than at the smallest scales.

Current Eulerian biogeochemical ocean circulation models are anchored to the eddy diffusion paradigm, where unresolved scales are parameterized as more or less complicated irreversible mixing *effective* terms. While this approach, if properly executed, may give excellent results in the description of turbulent flows, in the presence of nonlinear reaction terms describing biological growth, it generally introduces uncontrollable biases, as we shall illustrate with some simple examples.

As a way out we propose a family of Lagrangian numerical methods that allows for a clear separation between stirring (that is, transport) and mixing (that is, irreversible changes of concentration). With these methods the amount of mixing is fully controllable, and is independent from numerical stability requirements.

We illustrate the potentiality of the method by studying the phenology of phytoplankton blooms in the open ocean. Our Lagrangian approach reproduces the observed natural patchiness of the planktonic field. This, in turn, affects the timing and intensity of the seasonal bloom.

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Self-oscillating deterministic systems in geosciences

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Self-oscillations have been introduced as explanatory model in many complex systems. This work shows their role for many phenomena in a geophysical context, from volcanoes to earth tides. The noteworthy correlation of volcanic tremor to external forces, such as earth tides, is discussed and synchronization mechanism is advocated. Seismicity observed on active volcanoes is characterized by a variety of manifestations (Long-Period (LP), explosions, volcanic tremor, etc.) that operate on different time and space scales. Understanding the pre/co-eruptive seismicity scheme, identifying the growth processes of gas bubbles and the motions of internal fluids are priorities to be investigated because they are associated with the source mechanisms. The coupling between fluid phases and vibrating solid structures associated with the source in volcanic areas in the non-paroxysmal phase generate self-oscillations similar to those produced in self-sustained musical instruments. The interaction involves the synchronization, also in the tidal band, between the space-time scales on which the dynamics of the fluids takes place (mixture of magma/gas or hydrothermal) and those, which the "resonance" of ducts is installed on. Permanent flow in a cavity produces mechanical vibrations only if there is a suitable impact geometry and if the convective flow scales agree with the viscous ones. The increase in flow / pressure then causes, for example, LPs and/or explosions to appear. Specifically, the physical processes associated with the generation of volcanic tremor and explosions in volcanic areas such as at Stromboli, Campi Flegrei and Ischia are studied. At Stromboli, the distribution of tremor amplitudes is Gaussian while the intertimes between the maxima in a suitable scale are described by a Poisson clustered process. Starting from these analyses, we proposed a first approximate model for volcanic tremor field. The recorded seismic tremor can be described by a nonlinear equation, which gives limit cycles. This equation is governed by a time-dependent threshold which represents the variability of bubble flux. We take into account some inelasticity in the medium perturbing the elastic potential with a Gaussian function on a suitable scale. It acts as a radiance function modulating the frequency of the limit cycle. The model is able to reproduce waveform, Fourier spectrum, and phase space dimension of one of the extracted nonlinear wave packets. In addition, Campi Flegrei seismicity shows a correlation between the diurnal solar solid tide and the energy released by the long period signals, indicating that the whole mechanism is modulated on a tidal scale. Finally the background seismic noise, at Ischia Island, is interpreted as the persistent whisper of the shallow circulation of fluids, which are a mixing of sea and meteoric water and thermal fluids of the hydrothermal reservoir. In the conceptual scheme of the self-sustained musical instruments, we hypothesize that the solid structure of the shallow hydrothermal system of Ischia is formed by a network of channels, continuously excited by the circulating hydrothermal fluids, which produce a whispered sound (i.e. the seismic noise).

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Nonlinear stability analysis of stochastic time integrators

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In this talk, we focus our attention on the nonlinear stability property of stochastic time integrators, such as stochastic ϑ-methods and stochastic Runge-Kutta methods, when applied to the exponential mean-square dissipative stochastic differential equations [4]. This property consists in the preservation of the mean-square contractivity along the numerical solutions provided by the aforementioned methods. In particular, for the stochastic ϑ-methods, we provide suitable restrictions of the stepsize of the numerical discretization in order to retain the contractivity behavior along the numerical dynamics [1, 3]. For the class of stochastic Runge-Kutta methods, the analysis leads to conditions on the coefficients of the methods that make mean-square dissipativity visible overall the numerical dynamics [2]. Finally, numerical evidence on selected test problems, also coming from applications [5], is provided to confirm our theoretical results.

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On the perturbative analysis of the time-discretization for stochastic Hamiltonian problems

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Stochastic Differential Equations (SDEs) are excellent models used to describe several natural and real-life phenomena, when they are subject to random perturbations. This is the case, for example, of weather forecasts, turbulent diffusion or investment finance. Indeed, SDEs provide a key tool for a "mesoscopic" approach to describe the effects of external environments to a physical model. The irreversible character of a stochastic dynamics destroys the idea of isolate systems, since the particles are repeatedly influenced by small unpredictable perturbations of the external environment.
In this talk, specifically, we focus on the study on the dynamics of stochastic Hamiltonian problems because they represent a suitable candidate to conciliate the canonical character of the evolution equations, with the non-differentiability of the Wiener process, that describes the continuous innovative character of stochastic diffusion.
Our analysis focuses on the study of stochastic Runge-Kutta methods developed by Burrage and Burrage, obtained through a stochastic perturbation of symplectic Runge-Kutta methods, in order to understand if they maintain the linear drift visible in the expected Hamiltonian of the system. In particular we observe that stochastic Runge-Kutta methods exhibit a remarkable error that increases with the parameter ε, describing the amplitude of the diffusive part of the problem. Through a perturbative analysis, in terms of ε expansions, we investigate the reason of this behaviour and exhibit the presence of a secular term $\varepsilon\sqrt{t}$ that destroys the overall conservation accuracy. The theoretical results are also confirmed by selected numerical experiments.

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Synchronization scenarios due to the insertion of time delay in a communication ODEs model for chemical oscillators

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The Oregonator system, consisting of three Ordinary Differential Equations (ODEs), can be used for modeling the Belousov-Zhabotinsky (BZ) chemical reaction. The behavior of this phenomenon is interesting, given the oscillatory character of the related chemical components. For this reason, the use of techniques such as Exponential Fitting (EF) can be very effective in solving the Oregonator system, and D'Ambrosio et. al. have conducted studies related to this purpose. In fact, given the oscillation experimental frequency of the components, they used adapted numerical methods to follow the qualitative a-priori known behavior of the solution.

In a recent work, Budroni et. al. considered a modified version of the Oregonator model, inserting an additional ODE within the original system and slightly altering the others. This version was used to model a network of diffusively coupled inorganic oscillators, confined in micro-compartments by means of a flow-focus microfluidic technique. Such networks allow to understand and predict the communication modalities between different individuals, regulated by the exchange of activatory or inhibitory signals. However, there are some compartmentalization constraints that can affect the communication between consecutive micro-oscillators.

Therefore, in order to improve the model from this point of view, we have introduced a constant time delay inside the coupling term of the ODEs system. We show how the new Delay Differential Equations (DDEs) model thus obtained can be used not only to quantitatively improve the correspondence between numerical and in-silico experimental results, but also to represent other types of real phenomena. In fact, as the delay varies, different synchronization scenarios occur for the micro-oscillators involved in the system. For example, there are similarities between the observed phase transition dynamics and synchronization scenarios characterizing the coordination of oscillatory limb movements.

Furthermore, we analyze and compare the efficiency of numerical methods used to solve the DDEs system, also discussing techniques that can be used to improve experimental results.

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GPU accelerated solution of time fractional diffusion systems

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Fractional diffusion systems model a number of important applications, as for example water diffusion magnetic resonance imaging, since the biological tissues are heterogeneous and the signal exhibits a heavy tail which is characteristic of anomalous diffusion [3]. In this talk, we consider a time-fractional diffusion system discretized by a mixed method, consisting of a spectral method along time and a finite difference scheme along space [1]. As the spatial mesh becomes finer, the computational cost becomes very large and prevents getting high accuracy. In this context, our contribution is a suitable parallel implementation on GPUs (Graphics Processing Units) of this model. This massively multi-processors architecture has been recently used in several scientific applications to improve performance of software [4] and to get accurate and accelerated solutions in similar fractional diffusion problems [2]. Experiments show the gain of performance in execution time and accuracy terms of the parallel implementation.

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MS-40
New numerical tools for poro-fractured media simulations - Part I

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Research on numerical tools for effective simulations in porous and fractured media is currently very active, driven by the interest from many practical activities and by the lack of established, industry-ready solutions. One of the major sources of complexity is related to the generation of the computational mesh on typically non trivial domains, characterized by multiple intersecting interfaces. Among the various strategies, two approaches are gaining increasing popularity in the field. On one side we find so-called non-conforming methods, which allow the use of meshes non conforming to the interfaces, and thus easily generated, and requiring specialized numerical schemes for problem resolution, and, on another side, polygonal methods, which instead allow to generate conforming meshes of polygonal/polyhedral elements of intricate domains, which can be then used in conjunction with more conventional and well established numerical approaches. The minisymposium aims at collecting the latest contributions in the field of numerical simulations of porous and fractured media, mainly focusing on such kind of innovative strategies.

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Solving flow in large scale discrete fracture networks with the hybrid high-order (HHO) method.

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We are interested in efficient numerical methods for solving flow in large scale fractured networks. Fractures are ubiquitous in the subsurface. Flow in fractured rocks are of interest for many applications (water resources, geothermal applications, oil/gas extraction, nuclear waste disposal). The networks are modeled as Discrete Fractures Networks (DFN) [3]. The main challenges of such flow simulations are the uncertainty regarding the geometry and properties of the subsurface, the observed wide range of fractures length (from centimeters to kilometers) and the number of fractures (from thousands to millions of fractures). In natural rocks, flow is highly channelled, which motivates to mesh finely the fractures that carry most of the flow, and coarsely the remaining fractures. But independent triangular mesh generation from one fracture to another yields non matching triangles at the intersections between fractures. Mortar methods have been developed in the past years to deal with non matching grids [1, 5]. In this presentation, we propose an alternative based on the recent HHO method which naturally handles general meshes (polygons/polyhedral) and face polynomials of order $k \geq 0$ [2, 4]. We will show how these features are useful to save computational resources in large scale DFN flow simulations. Different benchmarks will be presented.

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An Improved Embedded Method for Flow in Fractured Porous Media with Numerical Upscaling and Machine Learning

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The study of flow in fractured porous media is a key ingredient for many geoscience applications, such as reservoir management. Modelling and simulation of these highly heterogeneous and geometrically complex systems require the adoption of non-standard numerical schemes.

Embedded Discrete Fracture Models (EDFMs) are a simple and effective way to account for fractures with coarse and regular grids, but they suffer from some limitations: they assume a linear pressure distribution around fractures, which holds true only far from the tips and fracture intersections, and they can be employed for highly permeable fractures only.

We aim at overcoming these limits computing an improved coupling between fractures and the surrounding porous medium by a) relaxing the linear pressure distribution assumption, b) accounting for impermeable fractures modifying near-fracture transmissibilities.

These results are achieved by solving different types of local problems with a conforming method and computing new transmissibilities for connections between fractures and the surrounding porous medium and those through the porous medium itself near to the fractures.

The local problems for transmissibility computation are inspired from numerical upscaling techniques present in the literature.

Numerical tests, comparing the new EDFM solution with a reference solution, confirm the aforementioned improvements, even in the case of impermeable fractures.

To speed up an otherwise costly procedure, local problems are solved in an offline stage, where different fracture configurations are examined. Then, machine learning techniques are adopted to exploit the previous results to build models that provide an efficient, yet accurate description of the near-fracture flow for any fracture configuration.

A stabilization free Virtual Element Method

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In this talk, we present a Virtual Element Method that has the interesting property of allowing a definition of bilinear forms that do not require a stabilization term. We introduce and analyse the first order of this method in [1], we have named it Enlarged Enhancement Virtual Element Method (E^2VEM). It is based on the use of higher order polynomial projections in the discrete bilinear form with respect to the standard one [2], and on a modification of the discrete VEM space to allow the computation of such projections, maintaining the same set of degrees of freedom. We provide a proof of well-posedness and optimal order a priori error estimates. Finally, we present some numerical tests on convex and non-convex polygonal meshes, which confirm the theoretical convergence rates.

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A Virtual Element Approach to the Numerical Simulation of Immiscible Incompressible Two-Phase Flow in Porous and Poro-Fractured Media

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The Virtual Element Method (VEM), firstly introduced in [1], is a very recent extension of the Finite Element Method that allows the resolution of partial differential equations using general polygonal tessellations of the domain. This is a very attractive feature in tackling problems characterized by geometric complexity such as the numerical modelling of realistic flow processes in porous and in poro-fractured media. In the present contribution we investigate the potentialities of the VEM in the framework of the two-phase flow of immiscible incompressible fluids in porous media [2] and, as a further extension, in porous-fractured media. The problem is mathematically described by a system of time-dependent coupled nonlinear partial differential equations. In this work, we discretize the governing equations in time and in space combining an iterative Implicit-Pressure-Implicit-Saturation method with a primal conforming virtual element discretization. Moreover, exploiting the potentiality of the VEM, we further extend this formulation to a Discrete Fracture Network model (DFN) characterized by a local and global conforming mesh. We analyse the performance of the resulting scheme testing it on both regular and more realistic test cases and showing its potentialities in terms of mesh flexibility.

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MS-41
New numerical tools for poro-fractured media simulations - Part II

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Research on numerical tools for effective simulations in porous and fractured media is currently very active, driven by the interest from many practical activities and by the lack of established, industry-ready solutions. One of the major sources of complexity is related to the generation of the computational mesh on typically non trivial domains, characterized by multiple intersecting interfaces. Among the various strategies, two approaches are gaining increasing popularity in the field. On one side we find so-called non-conforming methods, which allow the use of meshes non conforming to the interfaces, and thus easily generated, and requiring specialized numerical schemes for problem resolution, and, on another side, polygonal methods, which instead allow to generate conforming meshes of polygonal/polyhedral elements of intricate domains, which can be then used in conjunction with more conventional and well established numerical approaches [1, 2]. The minisymposium aims at collecting the latest contributions in the field of numerical simulations of porous and fractured media, mainly focusing on such kind of innovative strategies.

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Virtual Element Method applied to the prediction of long-term dynamics of transitional environments

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The simulation of the long-term dynamics of a transitional environment can be used to reproduce many physical phenomena, as lagoon evolution, salt-marsh growth or river delta progradation. Modelling these processes plays a key role for the reconstruction of the sea-level evolution and distribution over time and space of the sediment deposition occured, for example, during the Holocene. The numerical simulation of the two main processes driving the dynamics of these environments, that is accretion and consolidation, suffers from a significant geometric non-linearity. The standard Finite Element (FE) approaches used to solve this type of problems may encounter some difficulties in adapting to the pronounced domain distorsion. Remeshing strategies can be applied, but with a computationally expensive efforts, especially on consideration of the domain modification in time[6].

We present an alternative to avoid the drawbacks associated to the requirement of a topologically consistent grid, by applying the Virtual Element Method (VEM).

The VEM is a Galerkin method such as the FE method where the approximation space in every element of the grid is composed by the solutions of a differential problem[1]. The basis functions of such Galerkin formulation are *virtual* as they are never built explicitly and the bilinear forms associated to the variational formulation are approximated by using special polynomial projections that are computable from the degrees of freedom. The VEM can be applied on very irregular meshes consisting of a free combination of different polyhedral elements. Significant application have been successfully developed, for instance, in elasticity, geomechanics and flow in discrete fracture network [2],[4] and [3].

In this work, we present the VEM to solve the groundwater flow equation, coupled to a geomechanical module based on Terzaghi's principle, in a large deformation setting. In the governing equations, the pore pressure evolution within a compacting/accreting vertical cross-section of the landform is coupled to a geomechanical module computing the vertical large deformation of the porous medium. To take into account the geometric nonlinearity, we apply an adaptive polyhedral grid, where new elements are added to follow the sedimentation and distorted elements are automatically joined to adiacent cells according to the deposits consolidation. In particular, the last feature is guaranteed by the VEM flexibility in the element management, avoiding the numerical difficulties due to strongly distorted grids.

Finally, we apply the proposed approach to a real-world example, simulating the long-term evolution of the Mekong river delta, Vietnam[5].

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3D-1D coupling on nonconforming meshes using a Three-Field PDE-constrained optimization approach

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A new numerical approach is proposed for the coupling of three-dimensional and one-dimensional elliptic equations (3D-1D coupling). Possible applications concern all those cases in which small tubular inclusions are embedded in a much wider three-dimensional porous matrix, as a capillary network interacting with the surrounding tissue, tree roots in the soil, or a system of wells in a reservoir. For all these examples, if one-dimensional modeling assumptions can be applied, it can be extremely convenient to reduce the vessels to their centerline, avoiding the generation of a 3D mesh inside the small inclusions and lowering the computational cost of solving the discrete problem. For these reasons we propose a novel framework for 3D-1D coupling [1], based on a well posed mathematical formulation and ending up in a method which is highly robust and flexible in handling geometrical complexities. This is achieved resorting to a three-field domain decomposition [2] to decouple the reduced 1D problems from the bulk 3D problem. The resulting formulation is then recast into a PDE-constrained optimization problem, by the introduction of a cost functional accounting for the error committed in the fulfillment of the matching conditions. This functional is minimized subject to the 3D and the 1D equations, following an approach similar to the one used to couple 2D problems in [3] for Discrete Fracture Networks. Thanks to the structure of the functional, the method does not require the 3D mesh and the 1D partition of the centerlines to be conforming, thus making the mesh generation an easy task. In order to extend the method to a huge number of possibly intersecting inclusions, a gradient based method is proposed [4].

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Efficient reordering of conforming virtual element dofs for large scale parallel solvers

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Numerical simulations on DFNs are performed by several discretization approaches. The number of mesh cells required for a DFN simulation depend on the number of fractures, the density of the network, and the range of length scales generated by the network. We briefly introduce the Discrete Fracture Network problem, following [2], considering an impervious rock matrix and modeling fractures as planar polygons. The generation of a mesh conforming to fracture intersections in a DFN is often a complicated process. We present a VEM discretization on a conforming polygonal mesh approach [1]. In this context the problem is solved on progressively refined meshes being the refinement based on the information provided by an a posteriori error estimator.

The discrete structure of a DFN naturally implies several graph representations. In order to balance the computations in DFN flow simulations two main partitioning strategies are possible: the mesh-based partitioning and the DFN-based ones. In computing, load balancing is a technique used to spread work load among many processes. A mesh partitioning strategy involves the degrees of freedom aiming at balancing the computation. The DFN partitioning strategy subdivides the fractures among processes arising communicating data where two fractures on different processes intersect between them.

In this work we focus on three different DFN-based graph partitioning strategies. We describe fractures, traces and multiple intersections (cross points in the following) as nodes or edges in different ways according to the graph representations. Then, the METIS graph partitioning toolkit is used. Once the DFN is divided among the processes, auxiliary sub-networks are created in order to suitably manage the communications between processes.

The neighborhood of each degree of freedom includes the dofs of its adjacent cells. The sparsity of the matrix operator depend on the way the neighborhood is indexed. Most of the dofs on fractures have a neighborhood within the fracture: dofs on traces and cross points have adjacent cells on different fractures. The neighborhoods of the degrees of freedom of traces and cross points are relevant during the partitioning strategies presented in the following as long as, when the connected fractures lie on different processes, they are related to the part of the solution that requires communications between processes.

We propose a reordering of the degrees of freedom in order to set the communicating degrees of freedom in the first part of each local stripe of the matrix conferred to each

process; this approach ensures a communicating part of the matrix to each process balancing the communications required by the solver at each iteration. Moreover the degrees of freedom of local communicating traces are handled by the process that owns them. This reordering aims at obtaining a speed-up during the PETSc resolution.

We conclude this talk with numerical results confirming the performances in the dofs reordering and the DFN partition strategies.

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Efficient preconditioners for Discrete Fracture Network models

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Discrete Fracture Networks (DFN) models allow for an explicit representation of the fractures and their properties. These models are particularly useful in the simulation of fluid motion in the subsoil, especially when the presence of underground fractures have a dominant impact on it [5]. The main issues of DFNs include the complexity of the models and the multi-scale geometry, that reflect in the limited applicability of the conventional discretization approaches. Exploiting the capabilities of the parallel computing, an optimization-based formulation has been recently developed for the simulation of flows in large scale DFNs on non conforming meshes by [2] and [3]. The solution of the algebraic problem arising from such formulation of the DFN model can be written in a compact form as $\mathbf{Kx} = \mathbf{f}$, where $\mathbf{K}$ is a symmetric saddle-point matrix with a possibly rank-deficient leading block. Many applications give this kind of problem, and thus it has been object of several works, that are summarized for instance in [1].
Here, exploiting the peculiarities of the specific problem, we focus on the development of an ad-hoc preconditioning framework for the system resulting in [2] and [3], that is:

$$G^h\mathbf{h} - \alpha B\mathbf{u} + A^T\mathbf{p} = \mathbf{0}, \quad \text{(energy minimization)} \tag{1}$$
$$-\alpha B^T\mathbf{h} + G^u\mathbf{u} - C^T\mathbf{p} = \mathbf{0}, \quad \text{(energy minimization)} \tag{2}$$
$$A\mathbf{h} - C\mathbf{u} = \mathbf{q}, \quad \text{(mass balance)} \tag{3}$$

where $\alpha \in \mathbb{R}$ is a user-specified parameter, generally on the order of 1, $\mathbf{h} \in \mathbb{R}^{n^h}$ is the hydraulic head, $\mathbf{u} \in \mathbb{R}^{n^u}$ is the flux on the fracture traces, and $\mathbf{p} \in \mathbb{R}^{n^p}$ are Lagrange multipliers. Usually, $n^p = n^h$, while according to the problem n^u can be either larger or smaller than n^h. The matrices $G^h \in \mathbb{R}^{n^h \times n^h}$ and $G^u \in \mathbb{R}^{n^u \times n^u}$ are symmetric positive semi-definite (SPSD), usually rank-deficient, $B, C \in \mathbb{R}^{n^h \times n^u}$ are rectangular coupling blocks, whose entries are given by inner products between the basis functions of the main unknowns along the fracture traces, while $A \in \mathbb{R}^{n^h \times n^h}$ is symmetric positive definite (SPD) with a block diagonal structure.
Following the results obtained in [4], we define a decoupling operator $\mathbf{E} = \mathbf{GF}$ for the matrix $\mathbf{K}$ after a proper permutation of its rows and columns. The factorization of the matrix $\mathbf{K}$ through the decoupling operator $\mathbf{E}$ is used to build an inexact application of the inverse of $\mathbf{K}$ that can be used as a preconditioner in a Krylov subspace method. Thanks to the block structure of these matrices, the application of such preconditioner results particularly efficient in a parallel computational environment.

In this work, we investigate different choices of approximations for the construction of the preconditioner. The computational efficiency is evaluated considering both theoretical benchmarks and real DFN applications. Numerical results show that the use of an appropriate block preconditioner allows for an acceleration of the iterative solver, with promising potentials for its application in real-world DFN problems.

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MS-42
European High-Performance Scientific Computing: Opportunities and Challenges for Applied Mathematics

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High Performance Computing (HPC) is at the core of significant advances in scientific discoveries and innovation in industrial design and society needs, and is therefore a strategic

resource for Europe's future. In recent years, European Union (EU) has considerably increased its investments in the HPC ecosystem, making available resources to set up large facilities capable of reaching the peta/exascale rate of computation ($10^{15} - 10^{18}$ floating-point operations per second) and data centers with many exa-bytes of secondary storage, as well as to support the development of a European technology and pursue excellence in application development. Regarding this last objective, the Horizon 2020 program has supported the creation of 10 Centers of Excellence (CoEs) for computing applications, in areas such as environmental science, renewable energies, new materials, bioscience, etc., whose scientific challenges motivate the need for exascale-class computing resources. Predictive simulation capabilities in the different domain science are the main goal of the CoEs, so that computational results can be used not only to increase scientific knowledge and understanding but also for design and decision. In the above context, applied mathematics research is a critical component, indeed Mathematics permeates the activities from the formulation of the problems to the analysis of the results. New models and algorithms to be integrated in new science application codes are required in order to fully exploit the significant advances in computational capability that will be soon available. This mini-symposium aims to cover some of the most critical research areas of the system of CoEs, highlighting topics such as physical-mathematical modelling, numerical algorithms and scientific libraries, mixed-precision arithmetic for scientific computing, data assimilation and uncertainty quantification, pointing out how CoEs activities and applications result in tangible benefits to address scientific, industrial or societal challenges. The mini-symposium is supported by the EU project FocusCoE, an initiative funded to promote the CoEs services and findings to ever more partners from science and industry, with particular focus on small and medium-sized enterprises (SMEs), and thereby reinforce the positive impact of HPC in all of the areas covered by the CoEs.

E-CAM: A path to extreme-scale computing for industry and academia

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The goals and activities of the E-CAM Center of Excellence for Computing Applications (www.ecam2020.eu), funded via the H2020 program and coordinated by the Centre Européen de Calcul Atomique et Moléculaire, will be presented.

E-CAM supports the development of scientific software with clear industrial and societal interest, in view of exploiting HPC resources. The developed software targets efficient implementation of existing algorithms and optimal first deployment of new methods across areas including rare events, electronic structure, quantum dynamics, and meso and multiscale modelling. E-CAM benefits from input and coordinated actions within the CECAM network, which includes leaders in each of these areas therefore providing a unique access point to broad simulation expertise. The capabilities of the network are demonstrated by the range of successful pilot project with academic and industrial partners that currently span applications in materials, quantum computing, and biophysics.

Through application co-design for HPC technologies, the provision of libraries and frameworks in domains relevant to exascale computing, such as high throughput computing and load-balancing, and delivery of the respective training, we push the community to exploit the HPC resources available at a European level. Relevant interactions with industry through pilot projects and scoping workshops support the transfer of HPC best practices into industry.

Parallel block low-rank sparse direct solvers with applications

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Low-rank approximation techniques have recently gained considerable interest in the world of scientific computing thanks to their ability to reduce the asymptotic complexity of linear solvers at the price of a reliably controlled loss of accuracy. Among the proposed approaches, block low-rank (BLR) have proved to offer a robust and efficient alternative to the better-known hierarchical matrices (and other related approaches such as HODLR or HSS) especially in the case of sparse direct solvers; indeed, when combined with the sparsity of the problem, BLR allows for achieving a considerable reduction of the operation count and memory consumption and an asymptotic complexity which is comparable to what obtained with hierarchical formats. BLR has been implemented in several sparse direct solvers. In this talk we will provide a brief introduction of the BLR format, the related factorization algorithm and its complexity. Then we will focus on its implementation within the MUMPS solver and how it can benefit, in this framework, from distributed and shared memory parallelism and robust pivoting. This leads to a very versatile tool that can be used either as a direct solver or as an approximate one and combined with iterative or multigrid methods. We will finally present experimental results on different classes of problems, including some from the European EoCoE center of excellence, in different use cases and settings.

HPC & BigData for Nanotechnology

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HPC (High Performance Computing) and BigData technologies are revolutioning how computational materials science is addressed. In a few years the new generation of supercomputers will be capable of delivering a computational power in the range of about 1018 floating point operations per second. The availability of this tremendous computational power opens new ways to face challenges in nanotechnology research. Materials science will be greatly affected since a new kind of dynamics between theory and experiment will be established, with the potential to accelerate materials discovery to meet the increased demand for task-specific materials. Moreover HPC will be able to analyze very large amount of data (BigData) giving access to unforeseen interpretations of both experimental and computational data. The heightened demand for automation, advanced analysis and predictive capabilities inherent to these new methods put it in an especially exciting crossroads between chemistry, mathematics and computational science. In the European sphere, the transversal multidisciplinary approach is the key ingredient of the Horizon2020 Energy oriented Centre of Excellence (EoCoE) which aims to accelerate the European transition to a reliable low carbon energy supply exploiting the ever-growing computational power of HPC. This session aims to bring together researchers in materials science and computer science to discuss new approaches and explore new collaborations in the theoretical discovery of materials.

Scalable AMG Preconditioners for Computational Science at Extreme Scale

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The challenge of exascale requires rethinking numerical algorithms and mathematical software for efficient exploitation of heterogeneous massively parallel supercomputers. In this talk, we present some activities aimed at developing highly scalable and robust sparse linear solvers for solving scientific and engineering applications with a huge number of degrees of freedom (dof) [1]. We discuss algorithmic advances and implementation aspects in the design of Algebraic MultiGrid (AMG) preconditioners based on aggregation, to be used in conjunction with Krylov-subspace projection methods, suitable to exploit high levels of parallelism of current petascale supercomputers. These activities are carried on within two ongoing European Projects, the Energy-oriented Center of Excellence (EoCoE-II) and the EuroHPC TEXTAROSSA project, having the final aim to provide methods and tools for preparing scientific applications in facing and successfully grasping the near future exascale challenge. Beyond possible advances in base software technology to make available programming environments that tend to hide the details of the hardware, we still need to rethink and redesign numerical methods and applications, especially for irregular computations and memory-bound kernels, like sparse solvers. Algorithms that express a high level of data parallelism should be preferred to algorithms that induce data dependency even though, sometimes, the former may have worse convergence properties; extra computations are often well tolerated and balanced by a very efficient execution on multi/many-core architectures. Such is the case, for example, of some smoothers and coarsest solvers in AMG cycles or sub-optimal maximum weight matching algorithms employed in the setup of the AMG matrix hierarchy, which avoid intrinsically sequential computational kernels. Memory footprint, measured in terms of hierarchy complexity, is also a key issue in pursuing scalability in AMG preconditioners; balancing hierarchy complexity and convergence property of the final AMG is another main challenge in the current research on the topic. We discuss the above tasks while presenting a software

framework for Parallel Sparse Computations (PSCToolkit [2]), which has recently been selected by EU Innovation Radar as Excellent Innovation. Results obtained with our algorithms and software, on some of the most powerful European supercomputers, for solving systems with tens of billions of dof arising from isotropic and anisotropic scalar elliptic PDEs, will be presented.

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The transition to Exascale in Solid Earth Sciences

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The transition to exascale computing offers to Solid Earth Sciences the opportunities for a new paradigm shift: more physics, more resolution, more data, larger domain, less uncertainty. However, the exploitation of the disrupting exascale technologies requires a step forward in the design, implementation and application of numerical codes, simulation workflows, and analysis procedures. To do that, a synergy between scientists and technologists in different research fields, from geophysical sciences, to mathematics, engineering and information technology, has to be enforced. The ChEESE Centre of Excellence for Exascale in Solid Earths aims at promoting and consolidating such a transformation.

ChEESE's Pilots have been designed to demonstrate that some of the main scientific and societal challenges associated with the modelling of catastrophic phenomena (volcanic eruptions, earthquakes and tsunamis) can be addressed by exascale computing, both in terms of enhanced capability (i.e., using the maximum computing power to solve a single large problem in the shortest amount of time) and capacity (i.e., the ability to use exascale computer architectures to run large ensembles of simulations). In particular, enhanced simulation capability is required to increase the physical model complexity, the spatial/temporal resolution or the domain extent (by improving the application's weak scaling), or to achieve a shorter execution time (by improving the application's strong scaling). On the other hand, enhanced simulation capacity allows the enlargement of the simulation ensambles (to better quantify epistemic and aleatoric uncertainty and assess probability distributions) and the assimilation of larger datasets.

These features will represent the necessary ingredients needed to exploit HPC numerical simulations in very constrained operational environments before, during and after the occurrence of natural catastrophes, when strict time requirements (Urgent Computing and Early Warning applications) and rigorous probabilistic uncertainty quantification (Long- and Short-Term Hazard Assessment) are needed to inform decision-makers.

MS-43
Charge transport in low dimensional structures: Part I

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The minisymposium will be concerned with the mathematical modeling and simulation of charge transport in semiconductors, graphene and other 2D materials and in structures, like double gate MOSFETs, nano-ribbons, nano-wires, where the presence of confinement effects allows for the formal description of the carrier flow as that of a two dimensional or one dimensional electron gas [1]. Graphene, thanks to its peculiar electrical and mechanical properties, is considered as one of the most promising materials for future electron devices. Lately, it has also been realized that, by increasing the miniaturization of devices, hot-spots are observed, that is zones with very high crystal temperature due to the release of energy by high energetic electrons. The effect is particularly relevant in materials with reduced dimensionality and confined structures. For these reasons, the mini symposium will foresee the discussion of the following arguments: ab initio calculations

to furnish the correct band structures for the materials, e.g. doped graphene or graphene nanoribons; thermal effects in the crystal lattice; rippling in suspended graphene as result of coupling between elasticity and Dirac fermions; analytical properties of the Schrödinger equation; Monte Carlo simulations; Wigner transport equation; nonlinear dynamics in charge transport; numerical schemes for the charge carrier transport equation; fluid models deduced from the kinetic transport equations.

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A hydrodynamical model for charge transport in graphene nanoribbons

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Since its first isolation as a single layer of carbon atoms graphene has appeared as one of the most promising material for the new era of electronic devices [1]. It presents high electronic mobility at room temperature and high current density, nevertheless the absence of a band gap in its band structure does not make it a good solution for controlling the current flux. For solving the drawback the pristine graphene can be substituted by graphene nano-ribbons, narrow strips of graphene that exhibit a band gap depending on the width of the strip [2, 3].
Here we propose a hydrodynamical model for the charge transport in graphene nano-ribbons that takes into account the gap in band structure and the electron scattering with the lattice structure and with the edge [4].

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The Pauli principle in the Monte Carlo Method for charge transport in graphene

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The Monte Carlo method has become a standard tool for the study of transport problems in electronic devices [1], together with the semiclassical Ensemble Monte Carlo method (EMC) [2]. When the Pauli principle is no longer negligible, however, the EMC suffers from some drawbacks regarding the correct reconstruction of the carrier distribution. Many attempts were made over the years to overcome this problem until a new Monte Carlo scheme which takes into account the Pauli principle correctly was developed (see [3] and references therein). Almost all of these works were based on some convenient approximations in the description of the distribution function or of the scattering terms, with no attention on the free-flight step. Earlier on [4], a novel procedure was developed for silicon, which added the Pauli principle also at the end of the free flight, and which could be used when the degeneracy effects are predominant. Here, we address the question of the correctness of representing the free flight in a quantum perspective, with the application of the Pauli principle, or if it is more appropriate to represent it in a semiclassical way with the Liouville operator. We carry out this study by performing a numerical comparison of the various approaches by looking at the effects on the electron distribution function and on the mean values of energy and velocity in the case of a suspended monolayer graphene. This problem is fundamental in the study of new materials, as graphene, where degeneracy effects are important.

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Thermal and electro-thermal properties of suspended graphene

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We investigate some thermal and electro-thermal properties of suspended monolayer graphene. In particular, by means of a numerical experiment, made using a macroscopic model for charge and energy transport in graphene [1], we analyse how fastly a suspended graphene sheet heats up when it is subject to a constant homogeneous electric field and how it reaches the equilibrium state when the electric field is turned off. We consider all phonon branches and show that the influence of the out-of-plane acoustical phonons on the final equilibrium temperature is notable, due to their big heat capacity. While, the influence of the electrons on the final temperature is through the energy that they gain on account of the work of the electric field. This energy is greater at higher Fermi energy, since the number of electrons in the conduction band increases with the latter. We also analyse the physical meaning of two local phonon temperatures, which are commonly used in the literature, and we provide a theoretical justification of the behaviour of the system, which is based on the conservation of the total energy and on the total entropy of the electron-phonon system, of which we give an almost explicit expressions.
Eventually, we furnish an expression of the graphene thermopower as functions of the Fermi energy and of the temperture.

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Simulation of graphene field effect transistors

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Metal Oxide Semiconductor Field Effect Transistor (MOSFET) is the backbone of the modern integrated circuits. In the case the active area is made of traditional semiconductor materials such as, for example, silicon or gallium arsenide, a lot of analysis and simulations have been performed in order to optimize the design.

Lately, a great attention has been devoted to graphene [2] on account of its peculiar features and, in particular, from the point of view of nano-electronics, for the high electrical conductivity. It is highly tempting to try to replace the traditional semiconductors with graphene in the active area of electron devices like the MOSFETs (cfr. [1, 3, 5, 8]).

Here, graphene field effect transistors, where the active area is made of monolayer large-area graphene, are simulated including a full 2D Poisson equation and a drift-diffusion model with mobilities deduced by a direct numerical solution of the semiclassical Boltzmann equations for charge transport by a suitable discontinuous Galerkin approach (cfr. [4, 6, 7]).

The critical issue in a graphene field effect transistor is the difficulty of fixing the off state which requires an accurate calibration of the gate voltages. We propose and simulate a graphene field effect transistor structure which has well-behaved characteristic curves similar to those of conventional (with gap) semiconductor materials. The introduced device has a clear off region and can be the prototype of devices suited for post-silicon nanoscale electron technology. We compare numerical results with the simulation of standard GFET structures.

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Simulation of Graphene Field Effect Transistors by directly solving the semiclassical Boltzmann equation

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In the last years an increasing interest has been devoted to graphene field effect transistors (GFETs) as potential candidates for high-speed analog electronics, where transistor current gain is more important than ratio current ON/current OFF. Several types of GFETs have been considered in the literature [7]: top-gated graphene based transistors, obtained synthesizing graphene on silicon dioxide wafer, and double gate GFETs. The current-voltage curves present a behaviour different from that of devices made of semiconductors, like Si or GaAs. Because of the zero gap in monolayer graphene, the current is no longer a monotone function of the gate voltage but there exists an inversion gate voltage [7].

Lately, some attempts to simulate Graphene Field Effects transistors (GFETs) have been performed (see for example [1, 6, 2, 3, 5]) with simplified models like drift-diffusion. The latter contains several functions to be fitted by experimental data such as mobilities and generation-recombination terms. Often adaptations of the expressions used for standard semiconductors are adopted and a reduced 1D Poisson equation is coupled to the equations for the charge transport. It is therefore warranted to have a confirmation of the obtained results by a direct solution of the semiclassical Boltzmann equation for charge transport in graphene. Here a discontinuous Galerkin method, already developed in ([4]), is used to simulate some challenging geometries for future GFETs by numerically solving the Boltzmann equations for electrons and holes in graphene.

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MS-44
Charge transport in low dimensional structures: Part II

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The minisymposium will be concerned with the mathematical modeling and simulation of charge transport in semiconductors, graphene and other 2D materials and in structures, like double gate MOSFETs, nano-ribbons, nano-wires, where the presence of confinement effects allows for the formal description of the carrier flow as that of a two dimensional or one dimensional electron gas [1]. Graphene, thanks to its peculiar electrical and mechanical properties, is considered as one of the most promising materials for future electron devices. Lately, it has also been realized that, by increasing the miniaturization of devices, hot-spots are observed, that is zones with very high crystal temperature due to the release of energy by high energetic electrons. The effect is particularly relevant in materials with reduced dimensionality and confined structures. For these reasons, the mini symposium will foresee the discussion of the following arguments: ab initio calculations

to furnish the correct band structures for the materials, e.g. doped graphene or graphene nanoribons; thermal effects in the crystal lattice; rippling in suspended graphene as result of coupling between elasticity and Dirac fermions; analytical properties of the Schrödinger equation; Monte Carlo simulations; Wigner transport equation; nonlinear dynamics in charge transport; numerical schemes for the charge carrier transport equation; fluid models deduced from the kinetic transport equations.

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Correlated electron interferometers for quantum computing

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Single-electron and two-electron interference have been realized in a large variety of devices operating in the Integer quantum Hall regime, making them possible candidates for a flying-qubit implementation of quantum computing architectures[3]. In Ref.[1], we demonstrated the viability of coherent electron transport in a scalable design of the Mach-Zehnder interferometer and proposed its integration in a Conditional Phase Shifter, a two-qubit logic gate able to perform the entangling transformation for a universal set of quantum gates.

To this aim, we numerically setup the 2D potential landscape reproducing modulation gates on top of an Hall Conditional Phase Shifter at bulk filling factor 2, and investigate two-electron scattering driven by Coulomb repulsion in its active region. The dynamics of quasiparticles injected by single-electron sources in Hall interferometers is reproduced by describing charge carriers with localized wavepackets of edge states, and the exact two-fermion wavefunction is evolved with a parallel version of the Split-Step Fourier method[2]. In this approach, electron-electron interaction is introduced exactly in the two-particle Hamiltonian with a long-range Coulomb potential in 2D.

We measure the spatial shift induced by Coulomb repulsion in the final two-electron wavefunction, and prove that electron-electron interaction generates a consistent phase shift in one of the four configurations of possible Landau levels occupancy at bulk filling factor 2. We further demonstrate that the conditional phase can be, in our design, as large as π and that it can be controlled by the static confinement potential.

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A Hydrodynamical Model for Charge Transport in 2D Transition Metal Dichalgenides

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We derive a hydrodynamic model for charge transport in a 2D layer of MoS_2, based on the 6-moment equations of the electron distribution function in conduction band, using the parabolic band approximation, with the maximum entropy principle closure. We take into account the scattering of electrons with intravalley transverse and longitudinal acoustic phonons, with intervalley transverse and longitudinal acoustic phonons, with intravalley transverse optical phonons, with intervalley transverse optical phonons, with intervalley longitudinal optical phonons, with intervalley homopolar optical phonons, and the Fröhlich interaction with longitudinal optical phonons. All the closure relations for the spurious moments and the collision terms are explicitly evaluated. The proposed model is integrated numerically in the space-homogeneous case, with application to the computation of mobility.

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Numerical Modeling of Currents in Polymeric Semiconductors and Insulators

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Polymeric materials find multiple applications in Electrical Engineering, either as (semi-)conductors or as insulators. Such application range from nanoscale thin film transistors to insulation in High Voltage Direct Current cables. Modelling electrical currents in such a wide range of devices requires accounting for many different physical phenomena such as charge hopping, polarization relaxation charge injection and extraction. In this talk we review matemathical models and numerical methods for simulating electrical currents in polymeric materials and various approaches for the extraction of the parameters of such models from experimantal measurement data.

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Structure, electronic properties and charge transport of 2D planar structures embedded in 3C-SiC from first principles calculations

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Since the early days of research on silicon carbide, stacking faults (SFs) have monopolized the interest of the SiC community due to their extremely low formation energies and recurrent presence in the various SiC polytypes. The corresponding defect-induced states within the band gaps of the hexagonal polytypes have delayed the development of reliable SiC devices for a long time. Unlike the hexagonal polytypes, SFs do not introduce states within the cubic SiC polytype, making their presence less critical for the operation of 3C-SiC devices. Here we show that a different type of two-dimensional SiC defect, i.e. the antiphase boundary (APB), can introduce both shallow and deep level states within the 3C-SiC bandgap. Our study is based on the density functional theory, whereas results are compared with the structural and electrical characterization of 3C-SiC samples. We show that antiphase boundaries towards the <110> and <111> directions give rise to a local structural perturbation and introduce defect resonances that span from the vicinity of the valence band up to mid-gap positions. Moreover, using Kinetic Monte Carlo simulations we will discuss how APBs generate and interact with SFs during the 3C-SiC material synthesis. Finally, by means of non-equilibrium Green function approach we demonstrate that such defects can have an important role in the electrical properties of 3C-SiC devices structures. Comparisons with experimental characterizations indicate the reliability of the overall scenario.

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Gradient structure, existence of solution and decay time estimates for the kinetic model of scintillating crystals

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Scintillation in inorganic materials is a phenomena related to the electronic band structure of crystals and its detailed description can be found in [3]. For our purposes, it suffices to say that an incoming ionizing radiation excite an electron from the valence band to either the conduction band or the exciton band leaving an associated hole behind, in the valence band. These pairs electron-hole can travel independently or by means of excitons (loosely bound electron-hole pairs) within the crystal lattice. We refer to electrons, holes, and excitons collectively as *excitation carriers*: these carriers can either recombine radioactively by emitting photons in the visible range or by quenching without generation photons. The radiative and non-radiative processes are strongly nonlinear and competitive, their complete understanding is still missing as underlined into the most recent researches [4],[7],[9],[10].

Scintillation is a multi-scale phenomena and a complete and detailed analysis of the various time and length scales is given in [10] where seven length scales related at the various aspects of scintillation within a bulk crystal were described. In our approach, we shall lump these scales into three: the *microscopic scale* which is the atomic scale of the energy conversion of the ionizing radiation into excitation carriers within the activator nucleus, the *mesoscopic scale* which is the scale of the track along which the excitons carriers decays after generating a photon population and the *macroscopic scale* which is the scale of the light propagation within the bulk crystal.

When we turn our attention to the mesoscopic scale, we find that the phenomena of carriers recombination and photon generation can be described by a Reaction-Diffusion-Drift equation which closely reminds those proposed for semiconductors and is coupled with the heat equation and the Poisson equation of electrostatics. However, in scintillators the number of charge carriers is greater than two and the recombination term is more complex. It was shown that such an equation admits three main regimes which are driven by three parameters related to diffusion, mobility and recombination velocity and which originate various approximated models, described in details into [1] and [2].

Here we consider the isothermal case, on one of these approximated models, namely the so-called *kinetic model*:

$$\dot{n}(x\,,t) = r(n(x\,,t))\,, \qquad \text{in } \Omega \times [0\,,\tau)\,, \tag{1}$$

where n is the k-dimensional array of charge carrier descriptors and the recombination term $r(n)$ is a cubic function of n. Such a model is very popular within the experimental physicists (*vid. e.g.* [4]-[7]) and was used to obtain an experimental evaluation of parameters of the recombination term. Equation (1) is coupled with the Poisson equation for the electric potential $\varphi = \varphi(x\,,t)$:

$$\epsilon\Delta\varphi = e\,q\cdot n\,, \qquad \text{in } \Omega \times [0\,,\tau)\,, \quad \nabla\varphi\cdot\mathbf{m} = 0\,, \qquad \text{on } \partial\Omega \times [0\,,\tau), \tag{2}$$

e is the elementary charge, ϵ is the permittivity and $q \in \mathbb{Z}^k$ is the charge vector.

Following [8], we show that the boundary value problem (1)-(2) admits a gradient structure. Moreover, by using the entropy methods as in [8] we also investigate existence results and asymptotic decay estimates. This latter result is of extreme importance in experimental physics since is directly related to the decay time, which is a good performance indicator for a scintillator.

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MS-45
Charge transport in low dimensional structures: Part III

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The minisymposium will be concerned with the mathematical modeling and simulation of charge transport in semiconductors, graphene and other 2D materials and in structures, like double gate MOSFETs, nano-ribbons, nano-wires, where the presence of confinement effects allows for the formal description of the carrier flow as that of a two dimensional or one dimensional electron gas [1]. Graphene, thanks to its peculiar electrical and mechanical properties, is considered as one of the most promising materials for future electron devices. Lately, it has also been realized that, by increasing the miniaturization of devices, hot-spots are observed, that is zones with very high crystal temperature due to the release of energy by high energetic electrons. The effect is particularly relevant in

materials with reduced dimensionality and confined structures. For these reasons, the mini symposium will foresee the discussion of the following arguments: ab initio calculations to furnish the correct band structures for the materials, e.g. doped graphene or graphene nanoribons; thermal effects in the crystal lattice; rippling in suspended graphene as result of coupling between elasticity and Dirac fermions; in analytical properties of the Schrödinger equation; Monte Carlo simulations; Wigner transport equation; nonlinear dynamics in charge transport; numerical schemes for the charge carrier transport equation; fluid models deduced from the kinetic transport equations.

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On ensemble optimal control problems with kinetic models in deterministic and stochastic frameworks

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Kinetic equations are fundamental tools for modelling multi-particle systems with a wide range of applications from the design of nano devices to nuclear fusion. Further, they provide the mesoscopic link between microscopic and macroscopic models. The basic kinetic model is the Liouville (or continuity) equation, which is also the building block of many important evolution equations as the Boltzmann and the Fokker-Planck equations.

In application, it is essential to develop accurate models for simulation and to design control mechanisms acting on these systems in order to achieve given goals. For this purpose, ensemble optimal control problems governed by kinetic equations provide a powerful framework that allows to accommodate different models, control mechanisms, and objective functionals.

In this talk, some recent advances in this field are reviewed focusing on results obtained with the Liouville equation [4], the Fokker-Planck equation [1, 6], and the Keilson-Storer master equation [2, 3]. Moreover, an outlook of ongoing development of the ensemble optimal control strategy with nonlinear kinetic models is given [5]. In all cases, theoretical results concerning existence and regularity of optimal controls are discussed, and deterministic and probabilistic approximation and optimization methods for their determination are presented.

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A greedy algorithm for the Hamiltonian inhomogeneity distributions identification

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The identification of Hamiltonian operators, including the distribution of possible inhomogeneity parameters, plays a fundamental role in fields like quantum physics, quantum chemistry and nuclear magnetic resonance. The term Hamiltonian identification often refers to two distinct problems. On the one hand, it can indicate the inverse problem associated with the identification of a Hamiltonian operator obtained by a numerical fitting of simulated and given experimental data. On the other hand, it can refer to both the problem of designing experimental parameters (allowing an optimized production of experimental data) and the subsequent inverse identification problem. In general, the design of experimental parameters includes the computation of control functions allowing an efficient numerical solving of the inverse problem.

A novel computational greedy-type approach for design of control functions has been introduced in [1]. This strategy is based on an offline/online decomposition of the reconstruction process. In the offline phase, a family of control functions is built iteratively in a greedy manner in order to maximize the distinguishability of the system. This phase exploits only the quantum model, without any use of laboratory information. The computed control functions are experimentally implemented in the online phase to produce laboratory data, which are in turn used to define and solve an identification inverse problem. The offline/online decomposition results particularly efficient if one needs to reduce the number of laboratory experiments.

In this talk, we introduce an extension of the original strategy of [1] to the case of the identification of the inhomogeneity distribution characterizing spin systems [3] and present a novel convergence analysis [2]. The analysis reveals the strong dependence of the performance of the greedy strategy on the observability and controllability properties of the system and allows us to introduce a new and more robust optimized greedy reconstruction strategy whose efficiency is demonstrated by numerical experiments.

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Classical localization in a two-spin tracking chamber: a phase-space perspective

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The problem of track formation in a cloud chamber was first addressed by Mott in Ref. [6]: he studied a model where a central emitter injects a particle with perfectly spherical symmetry (the particle wave function being therefore a spherical wave) and the cloud chamber is represented by a an environment made by only two atoms in fixed (but generic) positions. The detection of the particle in a certain position corresponds to the ionization of the atom that occupies that position. Mott showed that the probability of *both* atoms being ionized is nearly zero unless ta two atoms are aligned with the emitter. The interpretation of this fact is that the particle manifests itself only along one radial, straight, trajectory. Hence, the phenomenon of localization a classical trajectory emerges naturally form the laws of quantum mechanics.

Since then, the model has bee refined in several ways [4, 5, 7]. In particular, a one dimensional model with N spins in fixed positions at each side of a central emitter has been theoretically and numerically studied in Refs. [2, 3, 8]. In this case the detection of the particle corresponds to the spin flip. These studies have confirmed and reinforced the original Mott's result, to the extent that the configurations with the largest probability turn out to be those where the majority of spins have been flipped flipped on just one side (the probability of such states, however, is of course equally distributed at the two sides, which means that the side where the track is formed is completely random).

In this presentation we consider an oversimplified model with only two spins in symmetrical position $x = \pm r$ with respect to the emitter (placed at $x = 0$) and follow the evolution of the Wigner function [1] of the system. In this way, we have a phase-space representation of the localization dynamics. The simulations confirm that the probability of having the detection at both sides is practically zero, and the phase-space perspective provides a new way of viewing and understanding the phenomenon. We also show that, for the dynamic of localization to take place, it is necessary that the two spins are initially in a non-entangled state.

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Modeling quantum corrections and spill-out effects on gap plasmon resonances

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Gap plasmon resonance indicates a electromagnetic mode that may be excited in nanometric resonators whose active layer is constituted by a dielectric slab with thickness of few nanometers.

Since a relevant part of the electromagnetic wave which characterizes a gap plasmon propagates inside to a metal layer, the velocity of the wave is greatly reduced with respect to the case of the free propagation and the dispersion relation is strongly modified. These properties can be tuned in order to devise efficient nanometric resonators which operate at optical frequencies.

Due to the nonometric confinement of the electron density inside the active layer, quantum effects cannot be neglected. They have a primary influence on the value of the resonance frequency of the device.

In this contribution, I will describe a recent work in which the optical properties of a nanometric resonator are modeled. Our model includes quantum effects due to the electronic confinement in term of the so called spill out phenomena which provides a accurate description of the real electronic density profile. I will focus on the modification of the resonance frequency of the device related to the presence of quantum effects and I will compare our results with what is obtained by first principle DFT calculations. Finally, a simplified effective gap model that predicts the correct gap-plasmon effective index is presented.

Wigner Ensemble Monte Carlo simulation of a Resonant Tunneling Diode

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The Wigner transport equation represents a promising model for the simulation of electronic nanodevices, which allows the comprehension and prediction of quantum mechanical phenomena in terms of quasi distribution functions. During these years, a Monte Carlo technique for the solution of this kinetic equation has been developed, based on the generation and annihilation of signed particles. The development of Monte Carlo algorithms for this quantum kinetic equation have been tackled, using a probabilistic model based on a particle system with the time evolution of a piecewise deterministic Markov process [1]. Each particle is characterized by a real-valued weight, a position, and a wave-vector. The particle position changes continuously, according to the velocity determined by the wave-vector. New particles are created randomly and added to the system. The main result is that appropriate functionals of the process satisfy a weak form of the Wigner equation [2]. Moreover, a stochastic algorithm without time discretization error can be introduced [3]. This is a rather pleasant feature, since the problem of choosing an appropriate time step is avoided and, in many cases the no-splitting algorithm is more efficient compared to time-splitting algorithms. Simulation results shell be presented during the conference, where standard analytical band scattering model used for the simulated RTD, assuming parameter values for Silicon and GaAs.

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MS-46
Optimal control, differential games and applications - Part I

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The aim of this mynisimposium is to present new perspectives and applications in control theory and mathematical modeling. We are interested in the control and optimization of problems arising in soft robotics, traffic flow, differential and mean field games, with connections to machine learning techniques.

We taylored our proposal in order to offer a space of discussion of results ranging from the purely theoretical approach to more applicative frameworks. The scope is indeed to drive the audience from original results in optimal control of differential equations, to their applications in the modeling process and, finally, to numerical simulations.

This first part of the minisymposium includes contributions mainly devoted to theoretical results on the control of nonlinear PDEs and to mathematical modeling.

Mean field games approach to finite mixture models

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Finite mixture models [3, Chap. 9] are powerful tool in the statistical analysis of data with applications to cluster analysis. Given a finite data set, Expectation - Maximization (EM) algorithm is used to compute the optimal parameters of the mixture in order to get a faithfull representation of data and to find groups with shares similar features. In this talk, I will explain how Mean Field Games (MFG), a theory developped by Lasry-Lions [5] and Huang-Caines-Malhamé [4] in the framework of differential games, can be interpret as an alternative tool to the EM algorithm. In particular, I will present a MFG multi population model for mixtures of Gaussian and Bernoulli distributions and I will discuss their theoretical aspects [1, 2]. Lastly, I will show applications to some clustering problems.

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Inverse problems for transport equations

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In this talk we present several inverse problems, introduced in [1] and [2], for transport equations via Carleman estimates. We approach also the general case of first-order hyperbolic equations with time-dependent coefficients.

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Exact Controllability for Some Quasi-linear PDEs

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We prove exact controllability for a class of quasi-linear perturbations of the Korteweg-de-Vries equation and of the nonlinear Schrödinger equation. The proof is based on the application of a sharp Nash-Moser scheme, which produces no loss of regularity of the solution with respect to the initial and final data. To apply the scheme, one needs to prove exact controllability for the linearized operator in a neighborhood of zero. We prove this by Hilbert uniqueness method, i.e. we deduce the controllability of the linearized operator by its observability. Such observability is in turn deduced using the techniques developed by Baldi-Berti-Montalto and Feola-Procesi, which allow us to reduce the linearized operator to constant coefficients up to a bounded remainder and to apply Ingham inequality. This is a joint work with P. Baldi, G. Floridia and R. Montalto.

A PDE approach to a tentacle-like soft manipulator: modeling and reachability

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We present a continuous control model for a tentacle-like soft manipulator, based on an extension of the classical Euler's *dynamic elastica*. The model results in a nonlinear, fourth order, evolutive controlled system of PDEs, describing the evolution of an inextensible string endowed with a bending moment, curvature constraints, and curvature controls. The curvature constraint prevents the manipulator from bending over a fixed threshold; the control term, representing the actuators of the device, forces its curvature in a distributed fashion.

We derive the equations of motion in a variational setting, then we focus on the stationary case: we characterize the equilibria and the reachable set of the system. We finally explore some scenarios of application by further discussing the tuning of parameters.

MS-47
Optimal control, differential games and applications - Part II

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The aim of this mynisimposium is to present new perspectives and applications in control theory and mathematical modeling. We are interested in the control and optimization of problems arising in soft robotics, traffic flow, differential and mean field games, with connections to machine learning techniques.

We taylored our proposal in order to offer a space of discussion of results ranging from the purely theoretical approach to more applicative frameworks. The scope is indeed to drive the audience from original results in optimal control of differential equations, to their applications in the modeling process and, finally, to numerical simulations.

This second part of the minisymposium includes contributions mainly devoted to mathematical modeling and to numerical simulations.

A PDE approach to a tentacle-like soft manipulator: optimal control and numerical approximation

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We present some optimal control problems related to a continuous model for a tentacle-like soft manipulator. We first consider optimal reachability tasks, both in free and constrained environments, also including the case of rigid or broken actuators. Then, we consider optimal grasping problems, in the case of prescribed or unknown contact region between the manipulator and the target object. Finally, we introduce a finite difference discretization of the model, and we numerically solve the related optimization problems via a Newton-like augmented Lagrangian method.

A Generalized Mean Field Game Model for the Dynamics of Pedestrians with Limited Predictive Abilities

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In this talk we investigate the model for pedestrian flow firstly proposed in [1]. The model assumes that each individual in the crowd moves in a known domain, aiming at minimizing a given cost functional. Both the pedestrian dynamics and the cost functional itself depend on the position of the whole crowd. In addition, the model assumes that pedestrians do have predictive abilities, but *limited in time*, extending only up to a time period θ in the future, where $\theta \in [0, \infty)$ is a model parameter. a) For $\theta = 0$ (no prediction ability), we recover the modeling assumptions of the Hughes's model, where people take decisions on the basis of the current position of the crowd only. b) For $\theta \to \infty$, instead, we recover the standard mean field game (MFG) setting, where people are able to forecast the behavior of the others at any future time and take decisions on the basis of the current and future position of the whole crowd. c) For very short values of θ (typically coinciding with a single time step in a discrete-in-time setting), we recover instead the MFG setting joined to the model predictive control technique [2].

As in the Hughes's model, the numerical procedure to solve the problem requires to run an offline procedure at any fixed time t, which returns the current optimal velocity field at time t by solving an associated backward-in-time Hamilton-Jacobi-Bellman equation; but, differently from the Hughes's model, here the procedure involves a prediction of the crowd behavior in the sliding time window $[t, t + \theta)$, therefore the optimal velocity field is given by the solution of a forward-backward system which joins a Fokker-Planck equation with a Hamilton-Jacobi-Bellman equation as in the MFG approach.

The fact that a different forward-backward system must be solved at any time t arises new interesting theoretical questions. Numerical tests will give some clues about the well-posedness of the problem.

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Hybrid control approach for optimal visiting problems

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In an optimal visiting problem, we want to control a trajectory that has to pass as close as possible to a collection of target points or regions. We introduce a hybrid control-based approach for the classic problem where the trajectory can switch between a group of discrete states related to the targets of the problem [1]. The model is shown to be effective to solve the "Orienteering Problem" a framework which originates from the sport of orienteering [3]. The model is subsequently adapted to a mean-field game framework to study viability and crowd fluxes to model a multitude of indistinguishable players [2].

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Stop and Go waves in traffic flow: how to reduce them?

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In this talk I deal with a typical phenomenon of congested traffic: the Stop and Go (S&G) waves, which have negative effects on drivers' safety, fuel consumption and emissions [1]. A S&G wave is detected when vehicles stop and restart without any apparent reason, generating a wave that travels backward with respect to the cars' trajectories. Since modelling properly this phenomenon is crucial for developing techniques aimed at reducing it, I will present three different approaches to reproduce S&G waves: from microscopic description to a macroscopic one [3], passing through a multiscale approach [2].

Moreover, traffic flow is exposed to various sources of uncertainties which affect also the triggering and the evolution of S&G waves. Therefore the influence of the uncertainty will be investigated.

Numerical simulations will be presented in order to exhibit the reliability of these approaches.

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MS-48
Advances in Spline Applications

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It is well known that splines have applications in various fields.

At a first level they are the foundation of theoretical applications, such as numerical quadratures, numerical solution of integral and differential problems, also in the context of Isogeometric Analysis, reconstruction of geometries from sets of discrete data, 2D/3D object representations, image processing, etc. At a second level, methods and techniques arising from their use can be usefully employed in Computer Graphics, Industrial Design, Manufacturing, Electronics, Quality Control, Terrain Modelling, Medical Imaging, Modelling of real life phenomena and physical processes, etc.

This minisymposium is so focused on recent advances that spline theory has in several fields both at the above first and second levels, with the aim of gathering researchers that work on such topics to promote exchanges of ideas in spline applications.

Spline-based approximation of digital elevation models

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A digital elevation model (DEM) is a terrain matrix representation where each element of the matrix has a value corresponding to the altitude [4]. The array elements are regularly separated by a distance that determines the resolution of the DEM and is called the cell size. The applications are numerous and among them are Civil Engineering, Hydrology, Environment and Geology.

Given the diversity of products that can be derived from a DEM, it is necessary to know their quality, not only their altitudes, but also the variables, slope, orientation and curvature for which there are formulas that take into account the DEM discrete nature [1, 5]. The quality evaluation is often performed from a reference DEM of higher resolution (smaller cell size) than the DEM to be evaluated. This implies comparing two DEM of different scales for which a DEM reference resampling is necessary to adapt its resolution (decrease) to the evaluated one [6, 7], and this resampling is done in a matrix environment (discrete). However, it would be interesting to have a continuous DEM by adjusting a surface, which would allow greater freedom when calculating the variables altitude, slope, orientation, and curvature in any position, as well as resampling based on a surface rather than an array. Current standards do not assesses DEM quality based on

mathematical surfaces [2], but if surface-based assessment proves to be useful, it could end up being part of new standard versions.

In our study, a novel adjustment technique has been used. Considering that the problem will involve a large amount of data, it is necessary to construct an approximating spline surface with low computational cost. Usually the DEM data are uniformly spaced, so it is reasonable to adopt a tensor product type construction strategy. In addition, the adjustment must not produce an excessively smooth surface to capture the abrupt changes in the terrain shape, so it will be required to be C^1-continuous. On each sub-rectangle of the partition associated with the DEM the surface will be determined by a certain number of values dependent only on the elevations at the partition vertices, avoiding the use of box splines.

The method proposed here is based on the construction of univariate splines of a real function in such a way that the restriction to any one of the subintervals of a uniform partition is determined directly from its Bernstein-Bézier coefficients relative to that subinterval [3]. These will be linear combinations of the values that the function takes at nodes in a neighbourhood of the interval.

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Rational geometric splines: construction, applications and extensions

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Rational geometric splines (RAGS) are spline spaces that directly generalize the classical theory of bivariate polynomial splines on regular domains. In their original definition [1] the parametric domain is an unstructured triangular mesh that is equipped with a C^∞ -differentiable structure by means of appropriate transition maps, namely rational linear functions used to specify the relationship between adjacent triangular parametric domains. The resulting spaces are suitable for representing surfaces of arbitrary topology by means of piecewise-rational functions consisting of a collection of triangular patches that can have arbitrary degree and order of continuity along their boundaries. Thus, on the one hand, RAGS can be viewed as generalizations of the classical Non Uniform Rational B-Splines (NURBS) to non-tensor product meshes and, on the other, they are generalizations of the classical bivariate splines (i.e., piecewise polynomial finite elements). Moreover, an obvious benefit of the fact that RAGS spline surfaces can be globally parametrized by the mesh is the possibility of adding an extra dimension (or dimensions) to the control points (i.e., considering the control points as being four- and higher dimensional rather than three-dimensional) in such a way that one can represent scalar and vector fields (e.g., flow vector fields) over the geometry. In this talk we will present the RAGS concept and illustrate its effectiveness as a tool for representing surfaces of arbitrary topology and spline spaces on such surfaces. We will review how the construction of functions belonging to the aforementioned rational spline spaces is possible by associating the starting mesh with one of the three standard homogeneous geometries (spherical, affine or hyperbolic), depending on the topological genus [2], and see how existing methods for generating smooth curves and surfaces (see e.g. [4]) can be adapted to work with these spaces. We will also illustrate analogs of RAGS for unstructured quadrilateral meshes (i.e. meshes where the number of quadrilaterals sharing a vertex is not necessarily four) without any restriction on the patch layout. These can be derived in a quite natural way from a proper triangular layout by rational linear or bi-linear reparametrizations [3].

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Penalized hyperbolic-polynomial splines

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The advent of P-splines, first introduced by Eilers and Marx (2010) [5], has led to important developments in data regression through splines. With the aim of generalizing polynomial P-splines, we have defined a model of *penalized* regression spline [1], called HP-spline, in which the polynomial B-spline functions are replaced by Hyperbolic-Polynomial bell-shaped basis functions. The starting idea is the definition of a polynomial-exponential smoothing spline, investigated in the framework of the Laplace transform inversion [2, 3, 4]. The HP-splines are defined as a solution to a minimum problem characterized by a discrete penalty term. They inherit from P-splines the advantages of regression models, like the separation of the data from the spline nodes, so avoiding the problems of *overfitting* and the consequent oscillations at the edges. HP-splines are particularly interesting in different applications that require analysis and forecasting of data with exponential trend. We present some recent results on existence, uniqueness and reproduction properties of HP-splines, also with the aim of extending their usage to data analysis.

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A Collocation Method Combined with Refinable Operators to Solve Fractional Differential Problems

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In the last decades, fractional calculus increased his popularity, due to the awareness that many physical problems, such as viscoelasticity, brownian motions, anomalous diffusion, need fractional derivatives to be modeled [4]. For the theory of fractional calculus see, for instance, [1, 7].
The analytical solution of fractional differential problems can be found only in some special cases. Usually, it is expressed through the Mittag-Leffer function, which is a power series that requires efficient numerical tools to be computed [2]. For this reason, in the literature many methods to numerically solve fractional differential problems were constructed (see, for instance, [5] and references therein).

In this paper, we propose to solve fractional differential problems by a collocation method combined with a linear quasi-interpolatory operator. In particular, we consider the following initial problem having time fractional derivative,

$$\begin{cases} D_t^\gamma y(t) + b\, y(t) = g(t), \quad t > 0, \quad 0 < \gamma < 1, \\ \\ y(0) = y_0, \end{cases} \tag{1}$$

where $b \in \mathbb{R}$ is a parameter and $g(t) \in C[0, +\infty)$ is a known function. As for the fractional derivative, we make use of the Caputo derivative

$$D_t^\gamma\, y(t) := \frac{1}{\Gamma(k-\gamma)} \int_0^\infty \frac{y^{(k)}(\tau)}{(t-\tau)^{\gamma-k+1}} d\tau, \qquad k-1 < \gamma < k\,, \quad k \in \mathbb{C}\,, \qquad t > 0\,,$$

where

$$\Gamma(\alpha) := \int_0^\infty \tau^{\alpha-1}\, \mathrm{e}^{-\tau}\, d\tau$$

is the Euler's gamma function [1, 7].

We approximate the solution with the refinable quasi-interpolatory operator considered in [3, 8] using the refinable B-spline basis $\{B_{ijn}(x) = B_n(2^j x - i), i \geq -n\}$ as basis

functions. Here, $B_n(x)$ denotes the cardinal B-spline of degree n [9]. We prove that, under suitable conditions, these operators reproduce polynomial up to degree n. Then, in order to solve equation (1) we use a collocation method where the collocation points are the dyadic nodes [6]. The method turns out to be easy to implement and convergent. Moreover, the numerical results show that it is efficient and accurate.

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A Spatial PH Spline-Based Path Following Scheme for Autonomous Underwater Vehicles

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In the application framework of path planning for autonomous underwater vehicles (AUVs), the design strategy should provide an optimal trade-off between the accuracy of the prescribed trajectory and the efficiency of the control algorithms. In the construction of efficient techniques, the versatility of the motion is usually penalized by approximation schemes based on simple curve types (e.g., linear or circular segments). This kind of restriction can be overcome by considering Pythagorean-hodograph (PH) curves [1], characterized by the distinctive feature of a polynomial parametric speed. Algorithms based on PH curve constructions allow to consider spline path with different smoothness properties, while simultaneously guaranteeing an accurate and efficient arc length computation needed for a robust and stable real-time computation of arrival time estimations, without involving numerical integration techniques.
In this talk we first present an efficient algorithm for the construction of smooth C^1 spline paths, obtained through local interpolation of Hermite conditions with PH quintic curves [2, 3]. The second part of the talk deals with the path planning and guidance module, responsible for the motion of vehicles along a certain trajectory. By suitably extending the results presented in [4], we introduce a path following guidance law, capable to give a robust response to unknown current disturbances even in the case of under-actuated vehicles.
A selection of numerical experiments, based on different data sets, validates the effectiveness of the guidance strategy, when the target position of the vehicle is computed with the PH spline interpolation algorithm mentioned above.

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A Local Approach for C^2 PH Quintic Spline Interpolation of 3D Data Point Streams

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Approximation/interpolation of data streams is a topic whose appeal is recently increasing, since it is of interest for real-time applications, e.g. trajectory tracking [6] and environmental monitoring [7]. In such context local schemes are necessary, since the data are not all simultaneously available, besides being possibly big. A natural approach for addressing the problem consists in relying on quasi–interpolation or local interpolation schemes formulated in spline spaces, see for example [2, 3].

Within such field, the focus of this talk is on local interpolation of univariate Lagrange and Hermite spatial streams, that is sequences of 3D points with possibly associated directions. For this aim in particular we rely on Pythagorean Hodograph (PH) splines, since the arc–length of any PH spline curve can be computed in analytic form with negligible computational cost, being a n–degree piecewise polynomial if n is the degree of the spline curve [5]. This is a feature of high interest for example when a motion has to be defined on a geometric path separately derived [4].

The basic formulation of the local scheme here introduced produces a C^2 PH spline interpolant just using an input Hermite data point stream, despite other local approaches proposed for the same aim in the literature which require also second derivative information [8]. This result has been obtained by adopting PH quintic biarcs, since they are flexible enough for dealing with the considered problem, preserving at the same time the manageability of PH quintic splines. By deriving a Maple implementation of the scheme, its fourth approximation order has been proved under the assumption of available second order information. On the other hand experiments developed starting from analytic curves confirm that such feature is ensured also removing this assumption. The performances of the scheme have been tested even in connection with local formulas available in the literature for a reasonable definition of the necessary first order information [1, 2]. This is of high interest for some applications, since it allows the usage of the scheme also when the data stream includes points but not associated directions.

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MS-49
Clinical Data Integration in Numerical Models - Part I

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New algorithmic challenges are rapidly arising in healthcare thanks to the growing amount of high-resolution clinical data. Computational and data-science research can support many aspects of the medical practice, ranging from diagnosis to the design and

optimization of treatments. This impact can be achieved by developing and implementing suitable data-model integration strategies, that can be based, for instance, on detailed numerical solvers, uncertainty quantification algorithms and/or artificial intelligence. This mini-symposium aims at gathering researchers focusing on the translation of computational models from research to clinical practice.

Flow reconstruction and fluid-structure interaction calibration from medical imaging

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When dealing with clinical applications involving Data Assimilation, medical imaging is a commonly available, non invasive source of information. In the first part of the talk we will describe several possible strategies to deal with these applications and sketch some ongoing contributions. We will then focus then on two problems: flow reconstruction from ultrasound Doppler and fluid-structure interaction calibration from 4d-flow MRI (as proposed in the contribution [1]). Concerning the first problem, we will adopt a variational approach and describe a reduced-order method based on a piece-wise affine optimal reconstruction, which is similar, in the spirit, to [2]. We will discuss several shortcomings and the ways to overcome them. In the case of the fluid-structure interaction calibration by using MRI data, we will decompose the problem solution into two steps. In the first one, a sequential method combining a Kalman filter and a minimising movement is introduced in order to track the motion of the aortic wall from the 4d-flow MRI data. This makes it possible to convert part of the Eulerian information of the MRI sequences into a Lagrangian information on the wall displacement and velocity. Only one segmentation (or an available atlas) is actually needed in order to obtain the reconstruction of the wall motion. This is used, along with the fluid velocity measurement, in order to calibrate a fluid-structure interaction model of the aortic flow.

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Image-based computational hemodynamics of the left ventricle: from cardiac cine-MRI processing to patient-specific simulations

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Cardiac Magnetic Resonance Imaging (MRI) is one of the most used and reliable medical imaging techniques to asses the left ventricle function. Among the different series acquired in a cardiac MRI exam, cine-MRI allows to accurately capture the motion of the ventricles thanks to the high temporal resolution. Conversely, concerning the spatial resolution, the usually sole 3D data available is the so-called cine short-axis (SA) view, that lacks accuracy along the left ventricle long-axis. Long-axis (LA) views, instead, are usually acquired only for few 2D slices.

In this work, in order to overcome the limitations due to the low spatial accuracy of these data, we first propose a method to generate artificial cine-MRI images of higher resolution by mixing the information of the various cine-MRI views. Starting from these images, we propose a novel pipeline to reconstruct the 3D shape and motion of the

left ventricle. Then, the reconstructed geometry and motion are extended to the left atrium and the ascending aorta of a template geometry by solving a Laplace-Beltrami problem that is able to recover a realistic atrial and aortic motion. Finally, hemodynamics simulations are performed solving with the finite element method the Navier-Stokes equations in an Arbitrary Lagrangian Eulerian (ALE) framework, where the motion of the computational domain is the one recovered from the artificial cine-MRI.

By using the proposed pipeline, we are able to enrich classic clinical outputs with information from an image-based hemodynamics simulation. Indeed, the hemodynamics indicators measurable by this type of simulations are of promising interest to study pathological scenarios such as hypertrophic cardiomyopathy or heart valve diseases.

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Assessment of Cardiac Fluid Dynamics in Patient' specific cases after Mitral Valve Repair by Computational Fluid Dynamics

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Fluid dynamics is considered and important factor that influences the myocardial adaptation during cardiovascular disease and after surgical therapy. Surgical Mitral Valve Repair (MVR) is the gold standard therapeutic procedure for patients with degenerative mitral valve regurgitation and follows two fundamental principles: restore a good surface of leaflet coaptation and correct for annular dilatation [1]. The aim of this study is to analyse the fluid dynamics inside the left ventricle (LV) with healthy, prolapsed and repaired mitral valve (MV). Moreover, it will analyze the LV washout as well as the residence time properties of the blood that could reflect in additional risk factors [2]. Geometries are extracted from 4D-transesophageal echocardiography and fluid dynamics is reproduced by direct numerical simulation (DNS) using the immersed boundary method. The numerical model includes a dedicated, image-based, approach to flow-tissue interaction for the MV leaflet [3]. Results confirm that the regurgitated volume is drastically reduced after repair. The analysis of blood wash-out demonstrates that a successful MV repair also restores a balanced flow transit in terms of physiological sub-volumes. An improvement of LV function after repair is observed in terms of vortex formation time. The assessment of blood flow after MV repair is feasible and can identify subclinical LV dysfunctions that influence the long-term clinical outcome [4]. This study shows that numerical simulation represents an integration to clinical imaging for hemodynamic assessments after MV surgery.

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Hemodynamics obstruction in hypertrophic cardiomyopathy: an image-based computational analysis

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Hypertrophic Cardiomyopathy (HCM) is a pathological condition with a prevalence of the 0.2 div 0.6% in the western world, in which the myocardium is abnormally thick (> 15mm) [1]. When the thickening interests the portion of the interventricular septum adjacent to the Left Ventricle Outflow Tract (LVOT), it may result in an obstruction of the blood flow during the systolic phase, and the pathology takes the name of Hypertrophic Obstructive Cardiomyopathy (HOCM). In severe cases, the condition may be worsened by a concurrent Systolic Anterior Motion (SAM) of the mitral valve, which further narrows the LVOT. In the clinical settings, an accurate assessment of the severity of HOCM is often difficult, resulting in a possible underestimation of the obstruction and an increased risk of cardiac death, thus motivating the interest in a more detailed computational approach.

The aim of the present work is to investigate the hemodynamics of different HCM/HOCM patients, and to provide quantitative indications that can help both diagnosis and the design of septal myectomy, which is the main surgical treatment for HOCM. Our study is based on kinetic magnetic resonance acquisitions (cine-MRI), which are the gold standard for the clinical assessment of the cardiac function, and we developed a novel computational procedure to reconstruct the patient-specific geometry and motion of the domain boundary and valves leaflets. The blood flow in the reconstructed moving domain is modeled by incompressible Navier-Stokes equations in an Arbitrary Lagrangian-Eulerian framework, and the mitral leaflets are immersed in the fluid domain by means of the Resistive Immersed Implicit Surface Method (RIIS) [2, 3]. The problem is numerically approximated by a SUPG-PSPG stabilized finite element space discretization and a first-order semi-implicit time scheme, implemented in life^x [`https://lifex.gitlab.io/lifex`], a multiphysics C++ library based on the `deal.II` core [`https://www.dealii.org`].

In these settings, we assess the severity of the HCM-obstruction of the LVOT and classify patients in terms of their intraventricular pressure gradient and peak velocity in the aorta, as well as investigate the associated wall shear stress in significant regions of the domain boundary and vortex structures in the ascending aorta. A synthetic evaluation of pressure on the septum allows to localize the patient obstruction and to identify the most promising region for surgical intervention by septal myectomy.

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Towards personalisation of three-dimensional electro-mechanical models of cardiac function

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Image-based computational models of cardiac electromechanics (EM) are a powerful tool to understand the mechanisms underlying physiological and pathological conditions in cardiac function and to improve diagnosis and therapy planning. However, in order to enable the clinical translation of such models, it is crucial to develop personalised models that are able to reproduce the physiological reality of a given patient. The last years have witnessed numerous contributions in experimental and computational modelling towards personalisation of computer models of cardiac function, based on anatomical and functional personalisation. In this talk we report on recent advances in EM cardiac model personalisation. In particular, we focus on identification of passive cardiac properties and sensitivity analysis of multiphysics cardiovascular models. First, we present a novel methodology to simultaneous perform an automated identification of *in vivo* passive mechanical properties and an estimation of the unloaded reference configuration of the left ventricle (LV)[3]. The algorithm only requires image or mesh data from one time instance

during diastolic filling and a single measured pressure-volume (PV) data point of the end-diastolic pressure-volume relation (EDPVR) as inputs. The methodology is efficient and versatile and can be applied to reproduce clinically-relevant PV relationships for patient-specific LV anatomical models within clinically feasible time frames. In addition, sensitivity analysis demonstrates robustness of the algorithm with respect to initial input parameters. In the second part of the talk we show the results of a preliminary sensitivity analysis on a novel coupled model based on a 3D EM model of the heart function [1], together with a 1D model of blood flow in the arterial system [2]. 1D arterial models of the circulation can efficiently capture the effects of distributed vascular properties and geometric aspects, and they allow to analyse the impact of pulse wave propagation on the circulation and cardiac function. Thus, it is possible to take into account a more detailed and efficient representation of the influence of normal and disrupted pulse wave transmission on the circulation and heart function with respect to standard 3D-0D coupling strategies, that can be beneficial to understand the impact of haemodynamic mechanisms in a broad spectrum of cardiovascular pathologies. Variance-based sensitivity analysis is performed to characterise the relative importance of model input parameters on the coupled model, in the perspective of model personalisation.

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MS-50
Clinical Data Integration in Numerical Models - Part II

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New algorithmic challenges are rapidly arising in healthcare thanks to the growing amount of high-resolution clinical data. Computational and data-science research can support many aspects of the medical practice, ranging from diagnosis to the design and

optimization of treatments. This impact can be achieved by developing and implementing suitable data-model integration strategies, that can be based, for instance, on detailed numerical solvers, uncertainty quantification algorithms and/or artificial intelligence. This mini-symposium aims at gathering researchers focusing on the translation of computational models from research to clinical practice.

Computational Models to support Cardiac Electrophysiology: a Novel Model of Human Ventricular Action Potential to Investigate Extracellular Calcium Effects

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In the last decades a large amount of mathematical models of cardiomyocyte electrophysiology have been developed, and due to the increase of the available experimental data the complexity of these models has raised progressively.

Sudden cardiac death is one of the main death causes all over the world, and it is correlated with the basic pro-arrhythmic mechanisms at the level of ion currents and single ventricular myocyte action potential (AP). To understand these mechanisms, and taking advantage of the increasing availability of specific data on ionic currents gathered from human cardiomyocytes, several mathematical models were developed to describe the biophysical mechanisms underlying the human ventricular AP. Nowadays, the "gold standard" for *in silico* human ventricular cellular electrophysiology is the O'Hara-Rudy (ORd) model [2], due to its validation against experimental data from over 100 undiseased human hearts. It was used in multiple studies and selected for regulatory purposes. However, since mathematical models are reduced representations of the real biological systems, there is always room for improvements. Recently two new human ventricular AP models have been published (BPS2020 by Bartolucci et. al [1], ToR-ORd by Tomek et al [4] - both based on the ORd model [2]) with two different aims of investigation.

With the development of our new human ventricular model (BPS2020, [1]) we have been able to quantify the contribution of the mechanisms involved in the relationship between extracellular calcium concentration $[Ca^{2+}]_o$ and the AP. The importance of electrolyte concentrations for the cardiac function is well established [3]. Electrolyte variations can lead to arrhythmias onset, due to their important role in the AP genesis and in maintaining cell homeostasis. However, most of the human AP computer models available in the literature were developed with constant electrolyte concentrations, and fail to simulate physiological changes induced by electrolyte variations. This is especially true for Ca^{2+}, even in the most widely used models in cardiac electrophysiology.

From earlier studies, it is well known that the L-type Ca^{2+} current (I_{CaL}) is the ionic current mainly affected by $[Ca^{2+}]_o$ changes. In particular, calcium-dependent inactivation (CDI) seems to play the most significant role. For this reason, the ORd model has been changed with these main modifications: (i) a new mathematical description of I_{CaL} current

with an increased sensitivity of its inactivation to $[Ca^{2+}]_o$; (ii) a single compartment description of the sarcoplasmic reticulum; iii) the replacement of Ca^{2+} release formulation.

BPS2020 can simulate the physiological APD-$[Ca^{2+}]_o$ relationship, while also retaining the well-reproduced properties of ORd (APD rate dependence at $[K^+]_o = 4mM$, restitution, accommodation, and current block effects). We also used BPS2020 to generate an experimentally-calibrated population of models to investigate: (i) the occurrence of repolarization abnormalities in response to hERG current block; (ii) the rate adaptation variability; (iii) the occurrence of alternans and delayed after-depolarizations at fast pacing. Our results indicate that we successfully developed an improved version of ORd, which can be used to investigate electrophysiological changes and pro-arrhythmic abnormalities induced by electrolyte variations and current block at multiple rates and population level.

The other modification of the ORd model has been recently published by Tomek et al. (ToR-ORd, [4]). The main aim driving its development (simulation of the negative inotropic effect of sodium current block) was different from the one of BPS2020 (APD dependence on $[Ca^{2+}]_o$). As a matter of fact, both models have been used to investigate and integrate into the equations additional knowledge of basic cardiac cell electrophysiology (some of them in the form of model-generated hypotheses), e.g., sensitivity of CDI to intracellular $[Ca^{2+}]$, extraction of the activation curve from I–V data, to mention only a couple.

Today, we are still in the process of merge the main innovations and goodness of these two new models (BPS2020 and ToR-ORd), with the scope of having a final version of an AP ventricular model able to reproduce the mechanisms clinically relevant and well established, such as APD-$[Ca^{2+}]_o$ relationship, and inotropic effect of sodium current block.

We hope that a new human ventricular model will enable more basic, translational and clinical research into a range of heart diseases and accelerate the development of new therapies. Plus it could become the standard model used by the Comprehensive in vitro Proarrhythmia Assay (CiPA) initiative for drug testing.

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An Inverse Problem for the Identification of Cardiac Activation from the Standard ECG

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An healthy ventricular activation is triggered by several electrical stimuli evenly distributed across the endocardial layer. In normal conditions, the Purkinje network is the main driver of the electrical activation, but under pathological conditions the so-called earliest activation sites (EASs) are possibly sparser and more localized. The number and location of these EASs, however, may not be easily inferred from surface recordings, such as the 12-lead electrocardiogram (ECG), due to the underlying complexity of the model. Nonetheless, finding these EASs would offer a powerful tool to clinicians for planning of therapeutic intervention such cardiac rhythm management (CMR) and ablation.

In the eikonal formulation, the EASs are conveniently modeled as point-wise boundary conditions, making on the geometrical interpretation of their influence on the global activation pattern straightforward. Computing descent directions of a functional depending on EASs location and number is however a challenging task, potentially hindering the application of gradient-based optimization algorithms. Recently, we proposed a simple

derivative-free approach to solve the identification problem from the 12-lead ECG, which also allowed for a variable number of EASs, identified through a two-step procedure [1].

Inspired by the promising results of the method, in this talk we present an alternative formulation of the problem which enables a gradient-based optimization [2]. By reinterpreting the problem in terms of geodesic paths, we expose the location of the EAS in a computationally convenient way. In particular, we discuss the gradient computation at continuous level and in the discretized setting. Moreover, we account for topological changes, that is a change in the number of EASs. We further extend the framework to more general objective functions, e.g., those based on the surface ECG. We show the performance of the method in several numerical tests and patient-specific settings.

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A Computational Analysis of the Electrophysiological Substrate Sustaining Arrhythmias

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Numerical simulations of cardiac electrophysiology based on high-resolution clinical data are progressively becoming a complementary tool to predict and explore the mechanisms of initiation, maintenance, and progression over time of electrical disturbance phenomena [1]. In this talk, we present a new computational approach built upon high-density electroanatomical maps to simulate the mechanisms of reentrant circuits' induction and sustainment in patients affected by atrial fibrillation or ventricular tachycardia.

In particular, we develop a new parametrization of the mathematical models for electrophysiology based on conduction velocities. These latter are numerically approximated with a least-squares approach from high-density electroanatomical activation maps, providing a quantitative description of the patient's electrophysiological substrate [2]. The computed velocity field is then adopted to characterize the heterogeneous electrical and structural properties within the mathematical model for electrophysiology [3]. We specifically consider a parametrized coupled system of equations formed by the monodomain equation and a model describing the dynamics of the ionic species. The parametrized model is finally adopted to numerically predict reentrant circuits, whose dynamics and sustainment are strongly influenced by the local electrophysiological properties of the tissue. Numerical results underline how functional lines of block, resulting from heterogeneity in conduction, and structural slow conduction corridors contribute to the induction and sustainment of reentrant circuits.

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Integration of maps of activation times in computational cardiac electrophysiology

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In this work we firstly address the issue of validating the monodomain equation used in combination with the Bueno-Orovio ionic model for the prediction of the activation times in cardiac electrophysiology of the left ventricle (LV). To this aim, we consider four patients who suffered from Left Bundle Branch Block (LBBB). We developed a geometrical tool able to merge the patient-specific LV geometry and the corresponding electrical data. We use activation maps acquired at the septum as input data for the model and maps at the epicardial veins for the validation. In particular, a first set (half) of the latter are used to estimate the conductivities of the patient and a second set (the remaining half) to compute the errors of the numerical simulations. We find an excellent agreement between measures and numerical results [1]. We then extend the computational tool including six more patients who suffered from LBBB with also a fibrosis distribution following the bullseye plot subdivision. In view of clinical practice, we considered the Eikonal-diffusion model to recover the activation map. We are able to accurately reproduce the epicardial activation maps in absence or in presence of fibrosis, calibrating the model with the coronary sinus (CS) electrical mapping data. In particular, we are able to accurately capture the late electrically activated segment in the CS branches with an almost real-time computational effort [2]. Our computational tool could be used to accurately predict activation times at the epicardial veins with a short mapping procedure in cardiac resynchronization therapy (CRT), i.e. by using only a part (the most proximal) of the standard acquisition points, thus reducing the invasive procedure and exposure to radiation.

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A Computational Framework For Electromechanics Simulations On A Four-chamber Heart

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Cardiac resynchronisation therapy (CRT) is one of the most effective treatments for heart failure. Despite the progress that has been made in recent years in patient selection and therapy optimisation and delivery, still between 30% and 50% of patients do not respond to therapy.

Computational models have the potential to help improve the response rate by providing useful insight in patient's response. Recently, cardiac electromechanics models have been moving from ventricular to four-chamber models, which offer a wider spectrum of simulated dynamics. Previous four-chamber heart studies showed the importance of the pericardium to reproduce physiological atrioventricular (AV) plane displacement and therefore to capture interaction mechanisms between the atria and the ventricles [1, 2]. Additional interaction mechanisms between the four chambers are also mediated by the circulatory system, which connects the atria to the ventricles through blood flow. Therefore, a four-chamber heart model needs to account for both the pericardium and the coupling with the circulatory system represented as a closed loop to simulate complex interaction mechanisms within the heart.

We present our four-chamber electromechanics heart model coupled with a zero-dimensional representation of the circulatory system. Atrial and ventricular electrical activation times were computed with an eikonal model, while mechanical active contraction was simulated with a phenomenological model. The effect of the pericardium was accounted for by applying normal springs on the epicardium of the atria and ventricles [2]. A map to scale spring stiffness was derived from clinical multi-frame ECG-gated

computed tomography acquired from twenty-three heart failure patients [3]. This allowed to account for the local forces that the heart experiences due to the pericardium and the surrounding tissues. The mechanical contraction was coupled with a closed-loop model for the circulatory system based on CircAdapt [4], without adaptation rules.

Our model allows to simulate physiological mechanical interaction between atria and ventricles thanks to the presence of the pericardium. The model predicts a physiological downward AV plane displacement of 9.1 mm and a peak in left ventricular pressure of 100.0 mmHg, consistently with pressure measurements in heart failure patients. The atrial pressure-volume loops present a physiological figure-of-eight shape, with an a-loop and a v-loop arising from atrial contraction and venous return, respectively. The comprehensive set of dynamics that our four-chamber electromechanics framework is able to simulate makes our model suitable to simulate response to CRT, and help optimising response.

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MS-51
Mathematics of inferring, computing and learning from data

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A high descriptive and predictive value of the mathematical models we use to analyze complex phenomena connected with human life is crucial for the technological development of nowadays' society.

Machine learning and data science are fields that are developing at an unprecedented fast pace and data-driven mathematical models, which aim at unveiling hidden structures and learning from data, are nowadays increasingly supporting our daily routines.

Mathematics of data science is, for these reasons, a very attractive and developing research area. A major and exciting challenge is connected with the fact that mathematics of data science relies on a tight interaction between mathematical modeling, data-driven inference and computational techniques.

The main objective of this minisymposium is indeed to bring together researchers from different mathematical communities—from network science, to statistics, optimization and numerical analysis—to discuss and overview novel approaches to a range of problems

connected with the analysis of large data and the development of efficient computational methods.

Training large scale SVMs using structured kernel approximations and ADMM

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Despite their simplicity, non-linear Support Vector Machines (SVMs), are still recognised by practitioners of Machine Learning and Data Science as the preferred choice for classification tasks in certain situations.

On the other hand, the computational complexity of solving non-linear SVMs is prohibitive on large-scale datasets: the use of the Kernel Trick requires the storage of a value for the kernelized distance between any two pairs of points leading to a storage complexity of $O(d^2)$ where d is the dimension of the training set.

In this talk we will demonstrate how to efficiently merge a Hierarchically Semi-Separable [2] approximation of the kernel matrix with the Alternating Direction Method of Multipliers (ADMM) [1] for the solution of the underlying convex optimization problem. The proposed merger delivers a computational framework able to out-perform the state of the art training algorithms for large scale SVMs [3].

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Low rank approaches for the analysis of real data from pre to post processing

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Inspecting data for searching valuable information embedded in them represents a key aspect in several fields, becoming even more challenging because of the continual improvement of technologies which are able to furnish a very large amount of informative data. Fortunately, most of the available data presents an embedded mathematical structure that can be profitably exploited to better investigate latent patterns hidden in them.
Analyzing real data covers a biggest set of approaches ranging from pre-processing to the actual discovery of information. In the first context, one of the main problems with real data is often related to the presence of anomalies that may spoil the resulting analysis as well as contain valuable information. In both cases, the ability to detect these occurrences is very important. Particularly, in the biomedical field, proper identification of outliers allows to develop of novel biological hypotheses not taken into consideration when experimental biological data are considered. On the other hand, the actual process of information discovery can be formulated with an optimization task underlying a matrix structure inside. This can be done with the help of Dimensionality Reduction (DR) that represents one of the most suitable instruments to untangle latent information at different levels. In particular, these methods aim to describe data under analysis onto a low-dimensional space allowing to consider most of all of the intrinsic knowledge as ideal sources (namely basis) of the process under consideration [3]. Often these approaches are also enriched by penalization terms can be added to enforce particular constraints able to emphasize useful properties. In this context, the tune of the hyperparameters controlling the weight of the additional constraints represents a problematic issue.
In this talk, we focus on Linear DR methods for the analysis of data from the pre to the post processing, to untangle latent information at different levels representing data onto a low-dimensional space. In particular, the contribution of this talk will be twofold. We will first address the problem of detecting outlier samples with application to biomedical data, proposing an ensemble approach for anomalies detection in gene expression matrices based on the use of Hierarchical Clustering and Robust Principal Component Analysis,

that allows deriving a novel pseudo-mathematical classification of anomalies [2]. Then, we will focus on Nonnegative Matrix Factorizations (NMFs), which prove to be the most effective among Linear DR methods in analyzing real-life nonnegative data [1]. Some variants of NMF will be also presented as minimization tasks to which penalization terms can be added in accordance with some additional characteristics. In particular, we regard the hyperparameters selection from an optimization point of view, incorporating their choice directly in the unsupervised algorithm as a part of the updating process in a bilevel formulation, providing theoretical and computational results to solve this problem. We will finally sketch future research directions.

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Dual Structure-preserving Tensor Train Kernel for Support Tensor Machine

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Deploying complex relationships between tensor input data into a high dimensional feature space based on structured tensor decomposition models can improve the performance of tensorial machine learning algorithms. In contrast, working directly with vectorized inputs in Support Vector Machines (*SVM*) discards the structure within the data and may lead to poor classification accuracy. Moreover, tensorial data may suffer from the *curse of dimensionality*, that is the exponential dependence of the computational complexity on the dimension of the input data. To overcome this complexity barrier and to fully utilize the nonlinear embedding of the data via a kernel function in SVM, we propose the *Tensor Train Multi-way Multi-level Kernel (TT-MMK)*[1]. This technique combines kernel filtering of the initial input data (*Kernelized Tensor Train (KTT)*), stable reparametrization of the KTT in the CP format, and the Dual Structure-preserving SVM Kernel for revealing nonlinear relationships. We demonstrate numerically that the TT-MMK method is more reliable computationally, is less sensitive to tuning parameters, and gives higher prediction accuracy in the SVM classification compared to similar tensorised SVM methods.

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Blind Identification of Stochastic Block Models from Dynamical Observations

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We consider a blind identification problem in which we aim to recover a statistical model of a network without knowledge of the network's edges, but based solely on nodal observations of a certain process (see Figure 1 for an illustration). More concretely, we focus on observations that consist of single snapshots taken from multiple trajectories of a diffusive process that evolves over the unknown network. We model the network as generated from an independent draw from a latent stochastic block model (SBM), and our goal is to infer both the partition of the nodes into blocks, as well as the parameters of this SBM. We discuss some non-identifiability issues related to this problem and present simple spectral algorithms that provably solve the partition recovery and parameter estimation problems with high accuracy. Our analysis relies on recent results in random matrix theory and covariance estimation, and associated concentration inequalities. We illustrate our results with several numerical experiments.

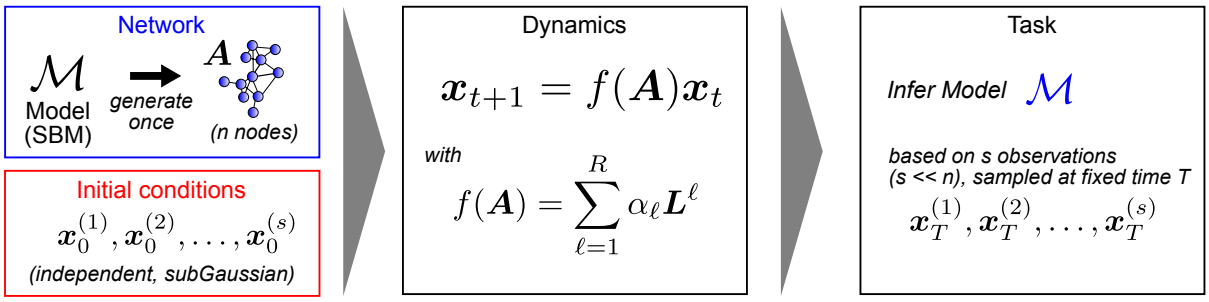

Figure 1: Schematic of the problem setup considered in this work.

Fast cluster detection in networks by first-order optimization

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Cluster detection plays a fundamental role in the analysis of data. In this talk, I will focus on the use of s-defective clique models for network-based cluster detection and show a nonlinear optimization approach that efficiently handles those models in practice. In particular, I will describe an equivalent continuous formulation for the problem under analysis, and some tailored variants of the Frank-Wolfe algorithm that quickly find maximal s-defective cliques. The good practical behavior of those algorithmic tools, which is closely connected to their support identification properties, makes them very appealing in practical applications. Finally, I will show numerical results proving the effectiveness of the proposed approach.

MS-52
Large-scale Optimization and Applications - PART I

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Numerical Optimization is a very active research field with countless applications in all areas of science and technology. Many real-life problems can indeed be modeled as the minimization (or maximization) of functionals over given sets (see for example [1, 2]). The incredible technological development of the last decades determined an increase in the amount, the size and the complexity of data which are collected everyday and need to be analyzed. Moreover, the availability of more powerful computational environments allowed scientists to increase the size and the precision of the numerical simulations of physical, mechanical and natural phenomena. All this generates a need for solving problems that are larger and larger which pushes researchers in the field of numerical optimization to study how to improve onto existing methodologies and how to introduce newer and more efficient ones. This minisymposium brings together researchers in this field to present recent advances and open problems on both theoretical and practical

aspects. Great relevance will be given to large-scale data analysis and machine learning problems which are of great interest for the scientific community.

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Line-search second-order stochastic optimization methods for nonconvex finite sums

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We present a line-search second-order algorithmic framework for minimizing finite sums. We do not make any convexity assumptions, but require the terms of the sum to be continuously differentiable and have Lipschitz-continuous gradients. The methods fitting into this framework combine line searches and suitably decaying step lengths. A key issue is a two-step sampling at each iteration, which allows us to control the error present in the line-search procedure. Stationarity of limit points is proved in the almost-sure sense, while almost-sure convergence of the sequence of approximations to the solution holds with the additional hypothesis that the functions are strongly convex. Numerical experiments, including comparisons with state-of-the art stochastic optimization methods, show the efficiency of our approach. More details are given in [1].

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Barzilai-Borwein and Ritz-like values in steplength selections strategies for stochastic gradient methods

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The steplength selection is a crucial issue for the effectiveness of the stochastic gradient methods for large-scale optimization problems arising in machine learning. In a recent paper, Franchini et al. [1] propose to include an adaptive steplength selection derived by tailoring a limited memory steplength rule, recently developed in the deterministic context [3], to the stochastic gradient approach. The proposed steplength rule provides values within an interval, whose bounds need to be prefixed by the user. On the other hand Tan et al. [2] propose to use Barzilai-Borwein-like (BB) strategies to automatically compute the steplength parameter in stochastic gradient methods. The authors suggest to calculate the BB each m iterates, with $m \in \mathbb{C}$, using a stochastic approximation of the gradient retrieved from a weighted average of all the stochastic gradients employed in the last m iterates. In this contributed talk we generalize the idea suggested in [2] for computing the BB-like steplengths to the strategy for estimating the values of the steplength proposed in [1]. By combining these two techniques, it is not necessary to find a range of values in which the steplengths must be chosen, making the method fully automatic.

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Deterministic, Probabilistic and Stochastic Complexity Analysis of Adaptive Regularisation Methods under Inexact Evaluations

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Within the context of nonconvex unconstrained optimisation, an adaptive cubic regularisation method under inexact derivatives evaluations is presented [1]. Introducing inexactness in the function computations, we then move onto a more general framework, allowing for the use of potentially higher degrees to search for arbitrary order optimality points [2]. At each iteration, it features an adaptive mechanism for determining the inexactness which is needed to compute objective function values and derivatives, in order to preserve the complexity results of its counterpart with exact evaluations. Sharp global evaluation complexity bounds, assuming that the prescribed accuracy requirements for function and derivatives approximation are deterministically fulfilled, hold for any model degree and any order of optimality, thereby generalising known results for first and second-order versions of the method. Such a deterministic complexity analysis is finally extended to the more practical case in which estimates of the function and the derivatives can be obtained only within a certain probability, or are even random, thus showing high probabilistic and stochastic complexity bounds.

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A Two-Level Decomposition Framework Exploiting First and Second Order Information for SVM Training Problems

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We present a novel way to solve the sub-problems that originate when using decomposition algorithms to train Support Vector Machines (SVMs). State-of-the-art Sequential Minimization Optimization (SMO) solvers reduce the original problem to a sequence of sub-problems of two variables for which the solution is analytical [1].

Although considering more than two variables at a time usually results in a lower number of iterations needed to train an SVM model, solving the sub-problem becomes much harder and the overall computational gains are limited, if any.

We propose to apply the two-variables decomposition method [3] to solve the sub-problems themselves and experimentally show that this is a viable and efficient way to deal with sub-problems of up to 50 variables.

As a second contribution, we explore different ways to select the working set and its size, combining first-order and second-order working set selection rules [2] together with a strategy for exploiting cached elements of the Hessian matrix [4].

An extensive numerical comparison shows that the method performs considerably better than state-of-the-art software.

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Exploiting Negative Curvature Directions in Large Scale Optimization to Escape from Nonconvex Regions

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The truncated newton method is a powerful tool to tackle large scale problems since it merges the speed of convergence of the Newton method with the computational efficiency of the truncated scheme. However, in recent years an increasing interest is arising for optimization algorithms that are able to escape from nonconvex regions of the objective function. This feature is extremely relevant especially for large scale problems (e.g. deep neural networks training). In this framework, the definition of strategies for the efficient use of negative curvature directions has been studied for instance in [1, 2, 3]. In this paper, we propose an algorithmic scheme along the following lines. First, we exploit negative curvature directions in a way that draws inspiration from [3]. Second, we employ approximating models of the objective functions to evaluate the relative performances of the truncated Newton direction with respect to the negative curvature one. We also propose preliminary numerical results that show the viability of the proposed approach.

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Iterative regularization for convex regularization

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I will present iterative regularization for linear inverse problems, when the regularizer is convex but not necessarily strongly convex. I will describe the stability properties of a primal-dual gradient based approach, analyzing its convergence in the presence of worst case deterministic noise. As a main example, we specialize and illustrate the results for the problem of robust sparse recovery. Key to our analysis is a combination of ideas from regularization theory and optimization in the presence of errors. Theoretical results are complemented by experiments showing that state-of-the-art performances can be achieved with considerable computational speed-ups.

MS-53
Large-scale Optimization and Applications - PART II

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Numerical Optimization is a very active research field with countless applications in all areas of science and technology. Many real-life problems can indeed be modeled as the minimization (or maximization) of functionals over given sets (see for example [1, 2]). The incredible technological development of the last decades determined an increase in the amount, the size and the complexity of data which are collected everyday and need to be analyzed. Moreover, the availability of more powerful computational environments allowed scientists to increase the size and the precision of the numerical simulations of physical, mechanical and natural phenomena. All this generates a need for solving problems that are larger and larger which pushes researchers in the field of numerical optimization to study how to improve onto existing methodologies and how to introduce newer and more efficient ones. This minisymposium brings together researchers in this field to present recent advances and open problems on both theoretical and practical

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Efficient ℓ^0 gradient-based super-resolution for simplified image segmentation

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Single-Image Super-Resolution (SISR) and Image Partitioning (IP) are two very popular tasks for the image processing community. The former enhances the spatial resolution of an acquired Low-Resolution (LR) data so as to reconstruct a High-Resolution (HR) image overcoming the physical limitations of the optical system involved in the acquisition process. The latter aims at reducing a digital image into homogeneous regions serving as a basis for subsequent analysis. In particular, segmentation, classification and labelling analysis have been shown to benefit of partitioned high resolution images [1]. We consider two constrained and unconstrained variational models for single-image super-resolution based on the assumption that the gradient of the target image is sparse. This assumption is enforced by considering an ℓ^0 regularisation on the image gradient combined with a quadratic data fidelity, similarly as studied in [2] for signal recovery problems. For the numerical realisation of the models, we propose a novel efficient ADMM splitting algorithm whose substeps admit closed-form solutions. We test our models on highly-degraded synthetic and real-world data and quantitatively compare our results with several sparsity-promoting variational approaches as well as with state-of-the-art deep-learning techniques. Our experiments show that thanks to the ℓ^0 smoothing on the gradient, the super-resolved images can be used to improve the accuracy of standard segmentation algorithms for applications like QR codes reconstructions, cell detection and land-cover classification problems.

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Ritz-like values in gradient projection methods for box-constrained optimization problems

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Many important real-world applications (e.g., imaging, signal processing, machine learning) require the solution of large-scale optimization problems subject to simple constraints. Gradient Projection (GP) methods are considered a very effective tool to address this type of problems, due to their simple implementation and low computational cost per iteration. The well-known efficiency of GP schemes strongly relies on suitable choices of the steplength parameter that controls the decrease along the negative gradient direction. Many popular steplength selection strategies, designed at first for the unconstrained case, exploit spectral properties of the Hessian matrix of the objective function involving low cost approximations of second-order information, which do not require the explicit computation of the Hessian. Indeed, their effectiveness is strictly related to the ability of *sweeping* the spectrum of the Hessian matrix. When dealing with constrained problems, however, the spectral properties are influenced by the presence of the constraints, according to the analyses in [1, 2] on Barzilai-Borwein-based rules [5, 4] for special constrained quadratic programs; in particular, practical improvement of GP schemes can be obtained by using selection rules that provide steplengths whose reciprocals tend to approximate the eigenvalues of Hessian submatrices related to the inactive constraints at the solution.

In this talk we will show how to employ the limited memory steplength selection approach developed by Fletcher [3, 6], in the framework of box-constrained optimization. Starting from a spectral analysis aimed at clarifying the relation between subsequent gradients in a sweep, we propose different ideas to generalize the standard limited memory procedure to GP algorithms, taking into account the lower and the upper bounds in

the steplength definition. Finally, we provide numerical evaluations of the proposed approaches.

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Improving the Bunch and Kaufman Decomposition for Large Scale Nonconvex Optimization

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In this work, we deal with Truncated Newton methods for solving large scale (possibly nonconvex) unconstrained optimization problems. In particular, we consider the use of a modified Bunch and Kaufman factorization for solving the Newton equation, at each (outer) iteration of the method. The Bunch and Kaufman factorization of a tridiagonal matrix is an effective and stable matrix decomposition, which is well exploited in the widely adopted SYMMBK routine (see [1, 3, 4, 6, 7]). It can be used to provide conjugate directions, both in the case of 1×1 and 2×2 pivoting steps. The main drawback is that the resulting solution of Newton's equation might not be gradient–related, in the case the objective function is nonconvex (see also [2]). Here we first focus on some theoretical properties, in order to ensure that at each iteration of the Truncated Newton method, the search direction obtained by using an adapted Bunch and Kaufman factorization is gradient–related. This allows to perform a standard Armijo–type linesearch procedure, using a bounded descent direction. Furthermore, the results of an extended numerical experience using large scale CUTEst problems is reported, showing the reliability and the efficiency of the proposed approach, both on convex and nonconvex problems.

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Solving Systems of Nonlinear Equations via Spectral Residual Methods: Stepsize Selection and Applications

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Spectral residual methods are derivative-free and low-cost per iteration procedures for solving systems of nonlinear equations [1]. They are generally coupled with a nonmonotone linesearch strategy and compare well with Newton-based methods for large nonlinear systems and sequences of nonlinear systems. The residual vector is used as the search direction and the steplength is inspired by the Barzilai Borwein method [2]. Analogously to spectral gradient methods for minimization, choosing the steplength has a crucial impact on the performance of the procedure. In this talk we address, both theoretically and experimentally, the steplength selection and provide results on a real application such as a rolling contact problem.

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Local Tuning Techniques for Lipschitz Global Optimization

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In this work we consider two Lipschitz Global Optimization Problems. In the first problem the objective function satisfies the Lipschitz condition while, in the second one, the first derivative of the objective function satisfies the Lipschitz condition. In both cases it is assumed that the function to be optimized is multiextremal over the search domain, its analytical representation is unknown and each evaluation can be an expensive operation.
For this reasons developing acceleration techniques is of great interest. We will describe several Local Tuning techniques which are able to estimate local Lipschitz constants in different areas of the search region allowing to accelerate the search.
The Local Tuning techniques are applied to geometric and information statistical methods. Convergence conditions of the methods are established. Finally, we discuss numerical experiments presenting advantages of these techniques.

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A spectral proximal alternating linearized minimization algorithm for tensor-train based dictionary learning

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The interest around a sparse representation of data has been growing in the past years due to its applicability in a variety of contexts such as image classification and compression, observation denoising and equation solving. Dictionary Learning (DL) is among the leading sparsity promoting techniques in image classification. Given a set of data Y, DL aims to find a matrix D with more columns than rows (the dictionary) and a sparse matrix X to represent Y by minimizing $\|Y - DX\|_F$ subject to structure constraints. The sparsity in X is generally induced by the l_0-norm functional, which however makes the problem non-smooth. Further complexity stems from the bi-linearity between the two unknown matrices D and X. As a result, the standard formulation of the DL minimization problem is NP-hard, see, e.g., [3].

Due to the increased need to analyze multidimensional data, various tensor formulations of the DL problem have been introduced with the aim of preserving data structure and feature heterogeneity, see e.g. [2]. In this case, the problem is numerically attacked by tensor-based minimization algorithms, usually without a supporting convergence analysis.

We propose a new tensor formulation of the DL problem using a Tensor-Train (TT) decomposition of the multi-dimensional dictionary, called TT-DL, together with a new theoretically founded alternating algorithm for its solution. The use of the (truncated) TT decomposition also allows us to limit memory requirements in the construction of D.

To cope with non-smoothness and non-convexity, we develop a new algorithm in the class of proximal alternating linearized minimization (PALM) algorithms [1], which are specifically designed to treat these properties. The new approach, called Spectral PALM (sPALM), alternates a *spectral* gradient step in the smooth part of the objective, while maintaining a proximal step for the nonsmooth part. We prove that sPALM converges to critical points of the proposed TT-DL formulation. Numerical experiments on various benchmark datasets illustrate that the use of second-order information in sPALM allows better performance than standard "Lipschitz constant"- based PALM

algorithms in the solution of DL image classification problems, both in terms of rate of successful classification and CPU time.

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MS-54
Mathematics of Machine Learning - Part 1

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As data become readily available in an ever increasing number of applications, machine learning is becoming the key towards data driven models and decision support systems. While largely driven by applied and algorithmic aspects, progress in machine learning also poses a number of mathematical questions and challenges. Understanding machine learning algorithms, as well as designing new ones, requires a blend of mathematical tools, from functional and numerical analysis to high dimensional probability and statistics. This workshop will overview some of the current mathematical challenges in machine learning with an emphasis on the diverse nature of the mathematical questions involved.

Computational Hardness of Hypothesis Testing and Quiet Plantings

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When faced with a data analysis, learning, or statistical inference problem, the amount and quality of data available fundamentally determines whether such tasks can be performed with certain levels of accuracy. With the growing size of datasets however, it is crucial not only that the underlying statistical task is possible, but also that it is doable by means of efficient algorithms. In this talk we will discuss methods aiming to establish limits of when statistical tasks are possible with computationally efficient methods or when there is a fundamental "Statistical-to-Computational gap" in which an inference task is statistically possible but inherently computationally hard. We will focus on Hypothesis Testing and the "Low Degree Method" and also address hardness of certification via "quiet plantings". Guiding examples will include Sparse PCA, bounds on the Sherrington-Kirkpatrick Hamiltonian, and lower bounds on Chromatic Numbers of random graphs.

On the Sample Complexity of Learning under Invariance and Geometric Stability

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Learning from high-dimensional data is known to be statistically intractable without strong assumptions on the problem. A canonical example is learning Lipschitz functions, which generally requires a number of samples exponential in the dimension due to the curse of dimensionality. Many high-dimensional machine learning problems involve highly structured data such as images, text, or graphs, and may exhibit invariance to certain transformations of the input data, such as permutations, translations or rotations, and near invariance to small deformations. More precisely, if $\mathcal{X}$ is the high-dimensional data domain, and G is a set of transformations $\sigma : \mathcal{X} \to \mathcal{X}$, the learning task can be alleviated if one knows in advance that the target function f varies smoothly under transformations in G: $|f(\sigma \cdot x) - f(x)|$ is uniformly small over $x \in \mathcal{X}$ for $\sigma \in G$.

To further motivate this property, it is useful to view the data domain $\mathcal{X}$ as a space of signals $\mathcal{X} = L^2(\Omega; \mathbb{R})$ defined over a geometric domain Ω, such as a 2d grid. The set of transformations G can then be articulated in terms of Ω rather than $\mathcal{X}$, a much simpler geometric object, and then *lifted* into $\mathcal{X}$ by composition: if $\sigma : \Omega \to \Omega$, and $x \in \mathcal{X}$ then $(\sigma \cdot x)(u) := x(\sigma^{-1}(u))$ for every $u \in \Omega$. The smoothness to transformations can thus be interpreted as a form of *geometric stability*.

In this work, we quantify the sample complexity gains brought by geometric stability. Concretely, we consider target functions f defined on the sphere $\mathcal{X} = \mathbb{S}^{d-1}$ in d dimensions with finite $L^2(\mathbb{S}^{d-1})$ norm. In this case, we view the geometric domain as a discrete s-dimensional grid $\Omega = [1, \dots, d^{1/s}]^s$, and consider geometric transformations G as subsets of the symmetric group of permutations of d elements. Given a set G (not necessarily a group), we consider the *smoothing* operator given by $S_G f(x) = \frac{1}{|G|} \sum_{\sigma \in G} f(\sigma \cdot x)$ for $f \in L^2(\mathbb{S}^{d-1})$, and assume that our target function f is geometrically stable, in the sense that $f = S_G g$ for some $g \in L^2(\mathbb{S}^{d-1})$. In words, the smoothing operator S_G replaces the prediction $f(x)$ by the average over transformations of x. In particular, functions which are invariant under the action of $\sigma \in G$, namely

$$f(\sigma \cdot x) = f(x), \quad \sigma \in G, x \in \mathbb{S}^{d-1}, \tag{1}$$

are also stable, with $f = S_G f$.

Building on the recent work [1], we proceed by studying harmonic decompositions of such functions using spherical harmonics, which generalize Fourier series on the circle to higher dimensions. This allows us to obtain rates of approximation for invariant and geometrically stable functions with varying levels of smoothness, and to study the generalization properties of invariant kernel methods using kernels defined on the sphere. Specifically, our main contributions are:

- By comparing spectral properties of usual kernels on the sphere with invariant ones, we find that the latter provide improvements in sample complexity by a factor of the order of the size of the group when the sample size is large enough.
- We study how this improvement factor varies with sample size, in terms of the structure of the group and on spectral properties of the permutation matrices it contains.
- We extend the invariance analysis to geometrically stable functions, establishing similar gains in sample complexity that depend on the size of the transformation subset.

Our proofs rely on comparing the dimension of invariant and non-invariant spherical harmonics at a given degree, and showing that their ratio decays to the inverse group size as the degree tends to infinity. In contrast to [1], we consider the dimension to be fixed and study non-parametric rates of convergence for potentially non-smooth target functions and general groups of permutations, while they consider high-dimensional limits where only polynomials can be learned, and focus on invariance to translation groups.

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Scalable Gaussian process optimization on continuous domain by adaptive discretization

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Gaussian process optimization is a successful class of algorithms (e.g. GP-UCB) to optimize a black-box function through sequential evaluations. However, when the domain of the function is continuous, Gaussian process optimization has to either rely on a fixed discretization of the space, or solve a non-convex optimization subproblem at each evaluation. The first approach can negatively affect performance, while the second one puts a heavy computational burden on the algorithm. A third option, that only recently has been theoretically studied, is to adaptively discretize the function domain. Even though this approach avoids the extra non-convex optimization costs, the overall computational complexity is still prohibitive. An algorithm such as GP-UCB has a runtime of $O(T^4)$, where T is the number of iterations. In this paper, we introduce Ada-BKB (Adaptive Budgeted Kernelized Bandit), a no-regret Gaussian process optimization algorithm for functions on continuous domains, that provably runs in $O(T^2 d_{\text{eff}}^2)$, where d_{eff} is the effective dimension of the explored space, and which is typically much smaller than T. We corroborate our findings with experiments on synthetic non-convex functions and on the real-world problem of hyper-parameter optimization.

A Measure Theoretical Approach to the Mean-Field Maximum Principle for Training NeurODEs

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In this talk we consider a measure-theoretical formulation of the training of NeurODEs in the form of a mean-field optimal control with L^2-regularization of the control [3]. We present first an informal derivation of first order optimality conditions for the NeurODE training problem in the form of a mean-field maximum principle, and show that it admits unique control solutions, which are Lipschitz continuous in time. As a consequence of this uniqueness property, the mean-field maximum principle also provides a stronger generalization error for finite sample approximations. Adapting arguments in [1], we additionally present a rigorous Lagrangian derivation of the mean-field maximum principle based on a generalized Lagrange multiplier theorem on convex sets of spaces of measures. We also show that the same mean-field maximum principle is equivalent to the one derived via the Hamiltonian approach in [2].

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MS-55
Mathematics of Machine Learning - Part 2

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As data become readily available in an ever increasing number of applications, machine learning is becoming the key towards data driven models and decision support systems. While largely driven by applied and algorithmic aspects, progress in machine learning also poses a number of mathematical questions and challenges. Understanding machine learning algorithms, as well as designing new ones, requires a blend of mathematical tools, from functional and numerical analysis to high dimensional probability and statistics. This workshop will overview some of the current mathematical challenges in machine learning with an emphasis on the diverse nature of the mathematical questions involved.

Convergence analysis of a randomized zero-order algorithm

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In this talk I will present the convergence analysis of a method where each step is given by finite difference approximation of the projection of the gradient on a low-dimensional random subspace. The approximation is two-fold, one coming from the projection onto a random subspace and the other from the use of finite-differences to calculate the directional derivatives. The analysis include as special cases spherical smoothing, coordinate descent, and even discretized gradient descent. I will provide convergence analysis and rates under varying assumptions on the objective function, the step-size, and the discretization mesh.

Scaled and adaptive FISTA algorithm for signal-dependent sparse image super-resolution problems

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We consider a convex optimisation problem written in the form:

$$\arg\min_{x\in\mathbb{R}^n} f(x) + g(x)$$

where $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ is a convex, continuously differentiable function with $\mathcal{L}-$Lipschitz continuous gradient and $g : \mathbb{R}^N \to \bar{\mathbb{R}}$ is convex and possibly non-smooth.

Among the plethora of first-order convex optimization schemes, forward-backward (FB) algorithms have attracted a significant attention due to their easy applicability in many scenarios and their fast convergence properties when endowed with appropriate inertial updates, as in the case of the FISTA algorithm [1]. Their successful application relies, in practice, on the accurate estimation of the Lipschitz constant $\mathcal{L}$, so that if such estimate is coarse, the practical effectiveness of FB methods may be limited. One remedy to solve this issue consists in the adoption of adaptive backtracking procedures, see e.g. [3]. In addition, FB algorithms can also benefit from suitable scaling approaches aimed at capturing some second-order information of the smooth component f, which is particularly effective in the context of signal-dependent image reconstruction problems.

Recently, in [6] the authors proposed SAGE-FISTA, a general FISTA-type algorithm designed for (possibly strongly) convex composite problems where a suitable scaling strategy is combined with an adaptive backtracking technique. In this work we present a scaled adaptive version of the Fast Iterative Soft-Thresholding Algorithm, named S-FISTA, for the efficient solution of convex optimization problems with non-smooth regularization

penalty terms. S-FISTA couples a non-monotone backtracking procedure with a scaling strategy for speading up the proximal-gradient step.

We test the proposed algorithm on some image super-resolution problems in microscopy, where in general a sparsity-promoting regularization term is coupled with a weighted-ℓ_2 data fidelity. The aim is to reconstruct sparse images of molecules (their positions and intensities) from blurred, under-sampled and noisy data. In this scenario, the acquisitions are corrupted by signal-dependent noise, that can be modelled as Poisson noise. In [4], the authors proposed the Weighted Continuous Exact ℓ_0 (WCEL0) model to solve the super-resolution problem in the Poisson noise scenario, where the sparsity promoting regularisation term is non-convex and non-smooth. The optimisation problem in [4] is solved with the iterative reweighted ℓ_1 algorithm [5] using FISTA as inner routine; however, the numerical efficiency of standard FISTA-type algorithms is often reduced by the use of, sometimes excessively, small step-sizes. The data term explicitly incorporates the noise signal-dependence in the ℓ_2 norm of the residuum, weighted by the acquisition. This characteristic encourage the use of a scaling algorithm, hence WCEL0 is particularly suitable for testing S-FISTA.

Our numerical experiments show that S-FISTA significantly improves the convergence speed with respect to standard FISTA when used both as global solver in convex optimization regimes and as inner solver for iterative non-convex optimization schemes such as iteratively reweighted ℓ_1 algorithm [5], reducing the overall computational times. The main contribution of this work is the use of a tailored efficient algorithm for improving overall computational efficiency. We observe that the use of adaptive S-FISTA favors a much faster decreasing of the cost functional without undermining the molecule localisation precision, making its use amenable for the time-consuming processing of the large stacks of images, as required in Single Molecule Localisation Microscopy.

Lastly, sparse reconstruction problems can be formulated in L^p spaces with $p > 1$ and in variable exponents Lebesgue spaces $L^{p(\cdot)}$, whose geometrical properties encourage sparsity in the reconstruction. It is currently domain of research the generalisation of forward-backward algorithms to this Banach spaces scenario that makes the convergence analysis more challenging.

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The Influence of Overparameterization on Distributed Learning

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While large training datasets generally offer improvement in model performance, the training process becomes computationally expensive and time consuming. Distributed learning (DL) is a common strategy to reduce the overall training time by exploiting multiple computing devices. Recently it has been observed in the single machine setting that overparameterization is essential for benign overfitting. However, little is known about the influence of overparameterization on the efficiency of DL.

We analyze distributed ridge(less) linear regression and show that overparameterization is essential for benign overfitting also in the distributed setting. Moreover, we show that the covariance structure determines the efficiency of DL in the presence of overparameterization and amplify this in two complementary cases: For a spiked covariance structure, vanishing regularization is beneficial but DL suffers from a loss in efficiency that is superlinear. In a second case (such that large regularization helps), choosing the amount of regularization dependent on the number of local devices allows to maintain the efficiency compared to the single machine approach.

We illustrate our findings with numerical experiments on both artificial and real data.

Neural network representer theorems by Banach feature maps

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We prove a representer theorem for the regularized empirical risk minimization

$$\min_{f\in\mathcal{B}} \frac{1}{N}\sum_{i=1}^{N} L(y_i, f(x_i)) + \|f\|_{\mathcal{B}}, \tag{1}$$

where $(x_i, y_i) \in \mathcal{X}\times\mathcal{Y}$, $i = 1,\dots,N$, are random samples drawn from an unknown probability distribution, L is a loss function, and $\mathcal{B}$ is a suitable reproducing kernel Banach space. More precisely, we prove that (1) admits a solution

$$\tilde{f} \in \operatorname{span}\{\phi(\cdot,\theta_i) : i = 1,...,N\},$$

where $\phi\colon \mathcal{X}\times\Theta\to\mathbb{R}$ is a feature map defining the reproducing kernel Banach space $\mathcal{B}$, with Θ a Hausdorff locally compact topological space. We apply our representer theorem to the case when ϕ is a continuous cut-off of a bounded or unbounded activation function $\rho\colon \mathcal{X}\times\Theta\to\mathbb{R}$, and we prove that there exists a minimizer represented as a single-hidden layer neural network with activation function ρ. In particular, in the case when ρ is a truncated power activation function, we characterize the regularization term in (1) in terms of the Radon transform adapting ideas from [1].

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MS-56
Mathematical Models and Methods in Biology and Biomedicine

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The application of mathematical ideas and tools to the study of biology and medicine, and in general of life sciences, has recently opened new pathways of interactions, cross links, interdisciplinary collaborations, giving rise to a very large number of new problems and challenges for applied mathematicians and leading reciprocal benefits for both disciplines.

The recent and rapid growth of systems biology has highlighted the central and crucial role of mathematics for a scientific approach of complex biomedical systems, at several scales. The increased computational capabilities allow long simulation at low cost in controlled conditions. The field of application ranges from theoretical analysis of physiological processes to numerical simulations of intracellular processes, from computational hemodynamics to simulation of cell structures and functions, from drug delivery systems to image analysis and geometrical reconstruction algorithms.

The mini-symposium focuses on recent advances in the application of mathematics to biology and medicine, from both theoretical and computational points of view: it offers an overview of different models and techniques for biomedical applications and encourages the transfer of information between methodological and applicative fields, bringing together mathematicians, engineers, biologists, bio-informatics scientists. Our goal is to provide a forum for discussion and exchange of ideas in a multi-disciplinary perspective, leading to the development of more realistic models in life sciences.

In Silico Study of Myocardial Regeneration Therapy: a 3D Free Boundary Problem Applied to Stem Cell and Nutrient Dynamics

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Stem cell-based therapy for the treatment of myocardial infarction and heart failure appears to play a significant role in reducing infarct size and improving cardiac function. A comprehensive mathematical description of all the complex mechanisms involved in the treatment is a challenging task. In the literature many models can be found that describe some selected aspects of the therapy. In this work we aim to employ two coupled differential problems for diffusion-reaction-convection equations to provide a qualitative description of the stem cell and nutrients dynamics in a simplified scenario. Migration, proliferation, chemoattraction, tissue regeneration and nutrient consumption are included in the model.

A small portion of inflamed cardiac tissue is represented by an ellipsoid D containing a necrotic core represented by a smaller concentric ellipsoid N. Stem cells are implanted on a portion A of the external boundary ∂D of D (Figure 1). A diffusion-convection-reaction equation governs the stem cell concentration dynamics in the domain: the diffusion term describes the stem cell motility in the tissue; the convection term describes the chemotaxis; the reaction term accounts for stem cell proliferation and death. The free boundary conditions describe the shrinking of the necrotic core due to the concentration gradient on its external surface Γ. Another initial-boundary value problem for a diffusion-reaction equation, coupled with the previous one, governs the nutrients concentration dynamics, accounting for diffusion and consumption.

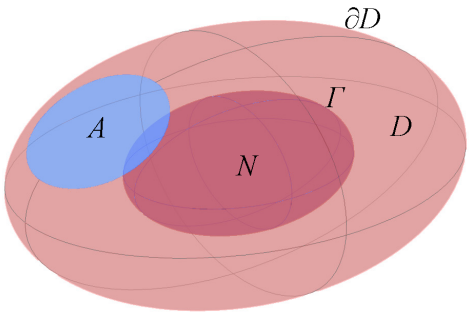

Figure 1: 3D domain

The simulations show the expected qualitative behavior of the system: the stem cells diffuse in the domain starting from the site of implantation, migrate toward the necrotic core due to chemotaxis, and proliferate. The raising concentration gradient on the internal boundary of the inflamed region causes its movement inward and hence the shrinking of the necrotic core. In parallel, nutrients diffuse in the domain and are consumed by the stem cells. A condition on the nutrient flow from outside can also simulate an additional supply of nutrients that promotes cell proliferation causing a greater regeneration of the tissue (Figure 2).

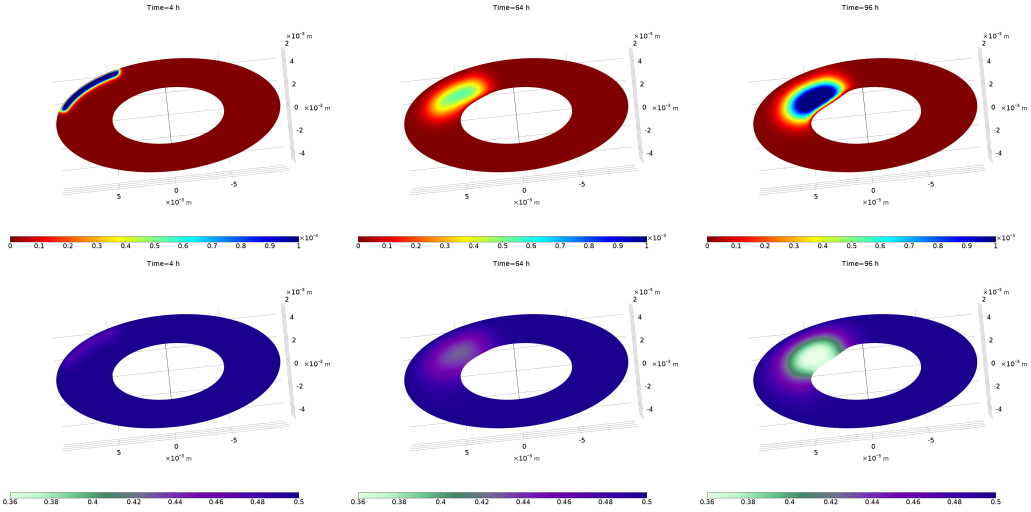

Figure 2: Top: non-dimensionalized stem cell concentration on the xz plane after 4, 64 and 96 hours. Bottom: non-dimensionalized nutrient concentration in the same instants of time

The proposed model is able to capture some main aspects of the stem cells and nutrients dynamics in a heart tissue regenerative therapy under simplified assumptions. Many improvements can be proposed, such as considering a different geometry or coupling the model with a differential problem describing the dynamics of chemokines. In a perspective of a multi-scale approach, we could also distinguish different stages of cell maturation and model cell differentiation.

Study of the Asymptotic Behavior in a Stochastic Framework of Oscillating Biochemical Systems

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The standard and the total Quasi-Steady State Approximations (sQSSA and tQSSA, respectively) are widely used in enzyme kinetics to simplify the equations governing the reactions, to reduce the dimensionality of the system and to fasten numerical simulations.

It is well known that the tQSSA is valid in a much wider range of parameters and initial conditions than the sQSSA, in a deterministic setting, as well as in a stochastic one (see, for example, [4, 1]).

Some enzymatic mechanisms, mainly in presence of feedbacks, undergo oscillations, as in the mitogen-activated protein kinase (MAPK) cascade [4], in the well-known PER-TIM circuit related to circadian rythms [3], in the core network for the interaction among the transcription factors Oct4, Sox2 and Nanog in stem cells [2] and so on.

In this talk we will face some of these mechanisms in a stochastic framework.

It is well known that, in a stochastic scenario, a network of chemical reactions is interpreted in terms of a Continuous-Time Markov Chain (CTMC), whose stochastic behavior is fully characterized by the CTMC initial probability distribution and the propensities or probabilities per unit of time of each reaction.

In order to study the stationary distribution of the CTMC, the stochastic approach is applied to the non-approximated original chemical networks, as well as to the standard and total QSSAs. Simulations confirm the effectiveness and superiority of the latter with respect to the former.

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Mathematical model for gain and loss of function mutations in a chemical reaction network for colorectal cancer.

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Many cancer diseases arises due to the accumulation in the cell of a group of mutations that by inhibiting or enchanting the activity of some proteins alter the functional cell signaling [1]. Chemical reaction networks (CRNs) are a powerful mathematical tool to qualitatively and quantitatively model cell signaling and its alteration. From a mathematical point of view, CRNs are essentially graphs, where the nodes and edges are respectively proteins and reactions involved in the signaling process [2].

By applying mass action kinetics, the dynamic of a CRN comprising n proteins and r reactions can be fully described by the Cauchy problem

$$\begin{cases} \dot{\mathbf{x}}(t) = \mathbf{S}\mathbf{v}(\mathbf{x}(t), \mathbf{k}) \\ \mathbf{x}(0) = \mathbf{x}_0 \end{cases}, \tag{1}$$

where $\mathbf{x}(t) \in \mathbb{R}^n_+$ are the molar (nM) concentrations of the involved proteins at time t; the superimposed dot denotes time derivative; $\mathbf{S} \in \mathbb{R}^{n\times r}$ is the constant stoichiometric matrix; $\mathbf{v}(\mathbf{x}(t), \mathbf{k}) \in \mathbb{R}^r$ denotes the vector of reaction fluxes, $\mathbf{k} \in \mathbb{R}^r$ being the set of the reaction rate constants; and $\mathbf{x}_0$ are proper initial conditions reflecting biological information on the status of the CRN.

In the first part of this talk, I will show how the Cauchy problem (1) can be modified to incorporate in the network two particular class of mutations resulting in the loss or gain of function of one of the involved proteins [3]. In details, the proposed approach makes use of the moiety conservation laws of the system to model gain and loss of function mutations as projections acting respectively on the stoichiometric matrix $\mathbf{S}$ and on the initial condition $\mathbf{x}_0$. Notably, this mathematical model can be easily generalized to mimic the effects of multiple simultaneous mutations.

In the second part of the talk I will demonstrate how the proposed approach have been applied and validated on a CRN specifically devised for modeling the G1-S transition

in colorectal cells [4]. The considered networks comprises $n = 419$ proteins and $r = 850$ reactions involved in 10 interacting pathways downstream the TGFβ, WNT, and EGF families of receptor ligands [5].

Finally I will present some preliminary results on the extension of the proposed model to incorporate the action of targeting drugs.

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MS-57
Novel approaches in the mathematical understanding of COVID-19 epidemic (Part I)

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Innovative mathematical models for epidemic dynamics are now more crucial than ever since their role in describing, inferring, and supporting policy makers had a fundamental role during the whole COVID-19 pandemic. This mini-symposium aims to collect the most recent efforts of the mathematical community to produce reliable models which capture different aspects of the outbreak including social aspects. Several mathematical techniques in connection with epidemiology are included spanning from ODEs to PDEs and network models. Furthermore, both modeling and calibration aspects will be considered with the goal to enhance the comparison of different approaches and techniques. The mini-symposium also promotes the activities of the recently founded UMI Group *Modellistica Socio-Epidemiologica*.

Estimation of epidemiological parameters in SIR models through a Bayesian framework

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The health emergency of international concern due to the epidemic of COVID-19 showed the weaknesses of healthcare systems and political institutions at global, national and sub-governmental level. The need to monitor the ongoing spread of the disease has become more and more fundamental to guide public health awareness and political responses. To provide accurate predictions of the evolution of the epidemic and help institutions to coordinate the health care resources in an efficient way, lots of mathematical models have been proposed and analyzed. SIR models and their extensions are one of the most powerful tools which explain at best the dynamics of the epidemic. A crucial point in the development of these models is the accurate estimation of the epidemiological parameters which best characterize the spread of the disease: on one hand the correct estimation of the transmission rate is a key point to realize successful social distancing measures and lockdown policies, on the other hand, analyses on the total length of hospital stay of COVID-19 patients and the recovery rates are fundamental for an optimal planning in hospitals to satisfy the bed demand. SIR models and their extensions are known to be powerful prediction tools but the non identifiability problem can greatly influences the reliability of these model predictions [1]. The aim of this work is to analyse, using a Bayesian statistical framework, epidemiological parameters related to times which characterize the natural history of COVID-19 disease and understand how different values and distributions of these parameters can affect final predictions of the evolution of the epidemic. A similar study has been proposed in [2] where a Social SIR model has been enriched with some preliminary results on recovery times from a statistical point of view.

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Stochastic hyperbolic transport models for the spatial propagation of infectious diseases on networks

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Standard compartmental epidemiological models represent the spread of viruses only with respect to the temporal evolution of the infection among the population, neglecting spatial effects in favor of an assumption of homogeneity in the population and in the territory [6]. In many cases, the concept of the average behavior of a large population is sufficient to provide useful guidance on the development of an epidemic. However, the importance of the spatial component is being increasingly recognized, especially when there is a need to consider spatially heterogeneous interventions, as it is happening now with SARS-CoV-2 [5, 8].

To permit an effective design of confinement strategies, we propose a hyperbolic transport model for the propagation of an epidemic phenomenon which finds its roots in the discrete-velocity kinetic theory [7]. Thanks to this, instantaneous propagation effects, typical of reaction-diffusion models, are prevented [2]. The model is based on the spatial movement and interaction of a population of commuters moving on an extra-urban scale and of non-commuters acting only over an urban scale, permitting to avoid unrealistic mass migration effects in which the whole population in a compartment moves indiscriminately in the domain [4]. The spatial domain is structured on networks, in which nodes identify cities of interest and arcs represent common mobility paths [3].

Furthermore, since data of the spread of epidemics are generally affected by a great deal of uncertainty [1], we choose to transmit statistical information to the problem, related to random input parameters such as the initial amount of infected people.

The resulting model is solved numerically through a suitable stochastic Asymptotic-Preserving IMEX Finite Volume Collocation method, able to maintain the consistency in diffusive regimes without restrictions due to the scaling parameters.

Several numerical tests confirm the ability of the model to correctly describe the spread of an epidemic, including an application on the emergence of COVID-19 in the Lombardy Region of Italy.

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An epidemic model with age structure and space dependence

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We present a compartment model, inspired by the well known SIR one [3], which is capable of describing some key features of the Covid-19 pandemic. It consists in a system of four hyperbolic renewal equations, which describe the dynamics of Susceptible (S), Infective (I), Hospitalized (H), and Recovered (R) individuals, through their density functions. The four densities S, I, H, and R depend on time $t \geq 0$, on biological age $a \geq 0$, and on a space coordinate $x \in \mathbb{R}^2$. More precisely $S(t, a, x)$ (respectively $I(t, a, x)$, $H(t, a, x)$, and $R(t, a, x)$) quantifies the individuals of type S (respectively I, H, and R) that at time t are of age a and are sited at position x. The key features are:

- Biological age plays a role in the infection and its severity.
- Infection is propagated in space: S individuals can be infected by I individuals of all ages, provided they are at the same time at a distance less than a given threshold.
- S, I, and R individuals move in the space domain with a time, age and space dependent velocity. H individuals are not assumed to move.

While capturing several qualitative properties of the virus spreading, it allows to compute the basic reproduction number, the number of deaths due to the virus and various other statistics; see [2] for more details.

Within this framework, vaccinations can be introduced and different vaccination strategies can be compared and tested. An attempt in this direction is described in [1], which presents an age structured SIR-type model, where various vaccination campaigns are considered.

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Modeling provincial Covid-19 epidemic data using an adjusted time-dependent SIRD model

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In this talk we will present a forecasting model for the spread of Covid-19 infection at a provincial (i.e., EU NUTS-3) level in Italy, by using official data from the Italian Ministry of Health integrated with data extracted from daily official press conferences of regional authorities and local newspaper websites. This data integration is needed as Covid-19 death data are not available at the NUTS-3 level from official open data channels. An adjusted time-dependent SIRD model is used to predict the behavior of the epidemic. Specifically, the number of susceptible, infected, deceased, recovered people and epidemiological parameters are estimated and predicted. The spatial association

between neighbouring provinces has been also considered, using a STARMA (Space-Time Autoregressive Moving Average) model to adjust the predictions. Predictive model performance has been evaluated using comparison with real data, in particular with data of the first two waves of the epidemics which have been observed in Italy.

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Observed patterns in COVID epidemic data and epidemic models

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While most models for describing the dynamics of COVID-19 epidemic in Italy have relied on more or less complex models based on systems of ordinary differential equations [1, 2, 3, 4], some of the observed patterns (the rounded and delayed epidemic peak after lockdown start; the apparent stasis in September) appear difficult to explain with such models.
Beyond possible problems in data collection, memory effects have been proposed as an explanation for the delay and shape of the peaks [5, 6]. While memory effects are definitely present and relevant, we surmise that the subdivision of the population into households and other small groups within which transmission continued normally during lockdown can help understanding the dynamics of the epidemics, and the delayed peaks; preliminary results on the classical household model show a linear increase of delays with group dimension.
Transmission within small groups, together with 'hot zones' in which high viral load transmission occurs, have been suggested in [7] as a possible explanation for periods in which infection rate remains almost constant. We will explore a model of this type under a wider range of assumption, to explore the robustness of the mechanism.

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Spatiotemporal modeling of epidemics: what have we learned?

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In the past year, the COVID-19 epidemic has ravaged humanity in an unprecedented way. The cost to physical and mental health, as well as economic damage, has been tremendous. In order to help better understand the spread of the disease, mathematical models were studied extensively. In particular, models incorporating spatial information using *partial differential equations* were seen as potentially promising, as shown in [6, 7]. In some cases, these showed reasonable predictive accuracy [6]. Extensions of these models have been proposed incorporating other relevant technologies; the use of Bayesian inference to calibrate certain parameters [5], as well as of other compartments and finite element types to increase accuracy [2]. Models incorporating time delays have also been used with success [3].

These models have helped in providing insight to the disease, and have shown to be robust across several different countries with minimal adjustments [4]. Nonetheless, there remain signicant challenges that make their accurate and reliable use in real-world settings difficult.

This talk intends to introduce the framework of the partial differential model for disease contagion and its mechanisms. We will compare agreement of simulation results with measured data in varied areas of the world, with emphasis on certain points of predictive successes. The talk will also discuss currently developing work, particularly those dedicated towards improving short-term predictive power while reducing computational costs [1]. As the ultimate goal is to provide accurate and low-cost tools for public health decision makers, such technologies are essential.

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MS-58
Novel approaches in the mathematical understanding of COVID-19 epidemic (Part II)

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Innovative mathematical models for epidemic dynamics are now more crucial than ever since their role in describing, inferring, and supporting policy makers had a fundamental role during the whole COVID-19 pandemic. This mini-symposium aims to collect the most recent efforts of the mathematical community to produce reliable models which capture different aspects of the outbreak including social aspects. Several mathematical techniques in connection with epidemiology are included spanning from ODEs to PDEs and network models. Furthermore, both modeling and calibration aspects will be considered with the goal to enhance the comparison of different approaches and techniques. The mini-symposium also promotes the activities of the recently founded UMI Group *Modellistica Socio-Epidemiologica*.

Heterogeneity and stochastic sampling effects in manual and digital contact tracing for epidemic mitigation

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The spread of an infectious disease strongly depends on social interactions dynamics and on its adaptation to the pathogen diffusion: isolation of symptomatic individuals, tracing and testing of their non-symptomatic contacts are essential strategies for the control of epidemic spreading [1, 2]. In the last year two complementary protocols for contact tracing (CT) have been proposed: a manual reconstruction of contacts (interview-based) and a digital contact tracing (app-based). The mitigation effects of the CT protocols can be modelled by an epidemic process describing the spread of SARS-CoV-2 upon an adaptive temporal network, which reproduces social interactions and whose dynamics is coupled with manual and digital CT. The epidemic process is described by a compartmental model tailored to COVID-19, with symptomatic and asymptomatic infections: moreover, further compartments are introduced to model the tracing and isolation performed by manual and digital CT. The model features a phase transition between an absorbing and an active phase: within the framework of activity-driven networks [3, 4, 5], a closed analytical relation for the epidemic threshold can be obtained, estimating the effectiveness of CT. The results show that manual tracing is more effective than the digital procedure, even considering the intrinsic delay and limited scalability of the manual protocol. This result is due to the stochastic annealed nature of manual CT, in which each node randomly recalls a fraction of its contacts, in contrast with the quenched nature of digital CT where traceable nodes belong deterministically to the fraction of the population who downloaded the app. The better performance of manual tracing is enhanced by heterogeneity in individual behavior: superspreaders not adopting the app

will never be traced by digital contact tracing, while they can be easily traced manually, due to their high number of contacts. This intrinsic difference in contacts exploration and heterogeneity in agent behavior make the manual procedure dominant also in realistic hybrid protocols [1].

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Assessing the role of information on the adoption of COVID–19–protective tools

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The COVID–19 pandemic that started in China in December 2019 has not only threatened world public health, but severely impacted almost every facet of life, including behavioural and psychological aspects. We focused on the *human element* and proposed Susceptible–Exposed–Infectious–Recovered–like models to investigate the effects of individual opinions and choices in response to disease spread and control. To this aim, we employed the *information index* [3, 4], which mimics the idea that people decide whether to adopt or not adopt a disease–protective tool based not only on the present but also on the past information about the disease status in the community. We considered separately the role of social distancing and quarantine [1], that were the main mitigation strategies enforced in the first phases of the pandemic, and that of vaccination campaign [2], that started in many countries in December 2020. The sensitivity to information–related parameters was determined by evaluating how they affect suitable outbreak–severity indicators. In particular, the hesitancy and refusal of vaccination turned out to be better contained in case of large information coverage and small memory characteristic time.

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Data-driven epidemic models with social structure

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We introduce a mathematical description of the impact of sociality in the spread of infectious diseases by integrating epidemiological dynamics with a kinetic modeling of population-based contacts. The kinetic description leads to study the evolution over time of Boltzmann-type equations describing the number densities of social contacts of susceptible, infected and recovered individuals, whose proportions are driven by a classical SIR-type compartmental model in epidemiology. Explicit calculations show that the spread of the disease is closely related to moments of the contact distribution. Furthermore, the kinetic model allows to clarify how a selective control can be assumed to achieve a minimal lockdown strategy by only reducing individuals undergoing a very large number of daily contacts. In a second part, using a detailed dataset furnished by Italian National Health Authorities, we propose to determine the essential features of the ongoing COVID-19 pandemic in terms of contact dynamics. This combines the mathematical description of the spread of an infectious disease with a detailed analysis of the dataset of all traced infected individuals in an Italian Province. These information are used to develop a data-driven model in which calibration and feeding of the model are extensively used. The results obtained permit, thanks to an uncertainty quantification approach and in the short time horizon, forecasting the average number and the confidence bands of expected hospitalized patients classified by age and to test different options for an effective vaccination campaign with age-decreasing priority.

Behavioural Epidemiology of infectious diseases: going beyond its limits: why not?

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The spread and control of current Covid19 pandemic are much better modellable and understandable by adopting the paradigm of the behavioral epidemiology of infectious diseases (BEID): social distancing; public health authorities interventions, acceptance of the forthcoming vaccines, rational vs irrational behaviors, negationism etc [1, 2, 3, 4, 5, 6]. However, even BEID has learned a lot from what we know of current pandemic [7].
The first and main lesson we have learnt is that we must go well beyond the current limits of BEID. Namely (non exhaustive list!!!):

- We must navigate and exploit the hige sea of behavioral data hidden in Social Networks [8]
- We must start modelling the behavior of policy makers [7, 9]

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Z-controlling with awareness a SEIR model with overexposure. An application to Covid-19 epidemic

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We apply the Z-control approach to a SEIR model including a overexposure mechanism and consider awareness as a time-dependent variable whose dynamics is not assigned a priori. Exploiting the potential of awareness to produce social distancing and self-isolation among susceptibles, we use it as an indirect control on the class of infective individuals and apply the Z-control approach to detect what trend awareness must display over time in order to eradicate the disease. To this aim, we generalize the Z-control procedure to appropriately treat an uncontrolled model with more than two governing equations. Analytical and numerical investigations on the resulting Z-controlled system show its capability in controlling some representative dynamics within both the backward and the forward scenarios. The awareness variable is qualitatively compared to Google Trends data on Covid-19 and qualitative indications are inferred in view of the disease control.

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MS-59
New trends and applications of fractional differential equations

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Fractional partial differential equations (FPDEs) have seen a huge spike of interest from the mathematical community in the recent few years, and have undergone through a great development. The reasons lie on the many applications that involve FPDEs, since several real-world phenomena, like generation and spread of electrical signals across biological excitable tissues or interactions in social networks and human environments, have been showed to be characterized by anomalous diffusion processes and then to be better described by differential equations of fractional order. Such improvement in the physical description however translates in a tougher numerical treatment and asks for specialized strategies, e.g., in terms of discretization methods or linear algebra solvers. The aim of this minisymposium is to promote exchanges between researchers working in the field and to give a little taste of the developments in the area ranging from modelization to numerical solution of FPDEs, from graph theory to numerical linear algebra and numerical analysis.

Space-fractional models of cardiac tissue electrophysiology: characterising structural complexity via fractional exponents

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Fractional-order models have successfully been used in various settings to describe transport phenomena accounting for macroscopic effects of microscopic heterogeneities, without the need to resolve complex spatial structures down to the microscopic level. In this talk, I will present a fractional-order framework to model propagation of electrical signal in cardiac tissue, which is characterised by significant structural complexity already in healthy conditions.

The use of non-local operators in the context of cardiac modelling is a relatively recent approach [1, 2, 3], which presents its own mathematical challenges, and several aspects have yet to be clarified, especially in relation to the formulation of physically meaningful models for a robust and reasonable comparison with experimental data. Here, I will discuss some of the underlying mathematical and computational challenges of the proposed approach, present some simulation results, and outline directions of future research for fractional-order models of complex emerging phenomena in cardiac electrophysiology.

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Multigrids for both isotropic and anisotropic space-fractional diffusion equations

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We are interested in a finite difference discretization of a two-dimensional time-dependent space-fractional diffusion equation (FDE) and in the solution of the related linear systems. Our focus is both on the case where the fractional orders are close to each other (isotropic case), and the one where they are not (anisotropic case). Driven by the fact that the discretization matrices have a block-Toeplitz-Toeplitz-blocks-like structure, and by the well-known negative results on multilevel circulant preconditioning, we opt for a multigrid approach. In this framework, the spectral properties of the matrices and the isotropic/anisotropic nature of the problem guide the selection of both projector and smoother.

In the isotropic case, based on the spectral analysis of the coefficient matrices, we define a multigrid method with classical linear interpolation as grid transfer operator and damped-Jacobi as smoother. In the anisotropic case, inspired by certain multigrid strategies for integer order anisotropic diffusion equations given in literature, we replace the classical linear interpolation with a semi-coarsening technique. Moreover, we estimate the Jacobi relaxation parameter by using an automatic spectral-based procedure. A further improvement in the robustness of the proposed method with respect to the anisotropy of the problem is attained employing the resulting V-cycle with semi-coarsening as smoother inside an outer full-coarsening.

Nonlocal Random Walks on Complex Networks

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There exists several non-equivalent ways of introducing non-local dynamics on complex networks. The two principal approaches have been obtained through variants of the graph Laplacian and has been introduced as instruments for modeling non-local diffusion processes on graphs. These methodologies allow a random walker to "jump" to non-neighborhood nodes and are called the transformed path graph Laplacians [3] and the fractional graph Laplacian for both undirected [4] and directed graphs [1].

In this talk we will briefly introduce these concepts within a unique framework. These new dynamics are made possible by having replaced the original graph G with a weighted complete graph G' on the same node-set, that depends on G and wherein the presence of new edges allows a direct passage between nodes that were not neighbors in G.

We show that, in general, the graph G' is not compatible with the dynamics characterizing the original model graph G [2]: that is the random walks on G' subjected to move on the edges of G are not stochastically equivalent, in the wide sense, to the random walks on G. From a purely analytical point of view, the incompatibility of G' with G means that the normalized graph $\hat{G}$ can not be embedded into the normalized graph $\hat{G}'$. Eventually, we provide a regularization method to guarantee such compatibility and preserving at the same time all the nice properties granted by G'.

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Continuous time random walk with Prabhakar generalized fractional Poisson process

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In this presentation, we consider a generalization of Laskin's fractional Poisson counting process, the 'generalized fractional Poisson process' (GFPP), first introduced by Cahoy and Polito [1]. This process contains two index parameters $0 < \beta \leq 1$, $\alpha > 0$ and a time-scale parameter. We discuss the fat-tailed asymptotic power-law features in the GFPP, the non-Markovian memory effect, and the probabilities of n arrivals ('generalized fractional Poisson distribution'). With these results for the GFPP renewal process, we construct Montroll-Weiss continuous time random walks (CTRWs) on undirected networks. We develop CTRWs subordinated to the GFPP [2, 3] and derive the 'generalized fractional Kolmogorov-Feller (K-F) equation' for this walk and demonstrate that the classical cases are contained (i.e. fractional K-F equation for $0 < \beta < 1$ with $\alpha = 1$ corresponding to Laskin's fractional Poisson, and the standard K-F equation for $\beta = 1$, $\alpha = 1$ of standard Poisson). Then we apply these results to the integer lattice $\mathbb{Z}^d$. For this stochastic motion, we analyze the 'well-scaled diffusion limit' and obtain the same type of fractional diffusion equation as for the fractional Poisson process. This fractional diffusion equation exhibits a subdiffusive t^β-power law ($0 < \beta < 1$) for the mean-square displacement. The occurrence of fractional diffusive features reflects the asymptotic universality of the fractional Poisson process and the corresponding Mittag-Leffler waiting time PDF [4].

The remarkably rich dynamics which is introduced by the GFPP and further generalizations open a wide field of interdisciplinary applications in anomalous transport [5, 6, 7, 8] including new discrete-time versions of Prabhakar generalized fractional Poisson and related discrete-time random walks [9] and generally in the dynamics of complex systems.

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Optimal B-spline bases and the solution of fractional differential problems

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Fractional differential problems having fractional derivative are used to model various physical phenomena, such as the anomalous diffusion, viscoplasticity, population growth. Since their analytical solution is given only for some particular cases, it is of primary importance to construct efficient numerical methods to approximate their solution.
In this talk we present a collocation method based on spline optimal bases that has proved to be easy and accurate when used in the numerical solution of fractional differential problems [2,3]. In particular, we consider the one-dimensional boundary value problem

$$\begin{cases} D_x^\gamma y(x) + f(x)\, y(x) = g(x)\,, & x \in (0, L)\,, \\ \\ \rho_{r0}\, y(0) + \rho_{r1}\, y'(0) + \zeta_{r0}\, y(L) + \zeta_{r1}\, y'(L) = c_r\,, & 1 \le r \le \lceil \gamma \rceil\,, \end{cases} \tag{1}$$

where D_x^γ denotes the Caputo derivative operator and γ is a real positive number such that $0 < \lfloor \gamma \rfloor < \gamma < \lceil \gamma \rceil < 2$. The continuous functions f and g are known terms while ρ_{r0}, ρ_{r1}, ζ_{r0}, ζ_{r1}, c_r are known parameters.
We assume y is a sufficient smooth function and the boundary conditions are linearly independent so that the differential problem has a unique solution [1].
The solution of the fractional boundary value equation (1) is approximated by a spline function that is represented as a linear combination of the optimal basis functions. The unknown coefficients of the linear combination are determined by collocation. At the end, we obtain an overdetermined linear system that can be solved by the least squares method.
We show the performance of the method through some numerical tests.

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Efficient Approximations for Fractional Powers of Operators

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In this talk we consider an efficient numerical approximation of $\mathcal{L}^{-\alpha}, \alpha \in (0,1)$. Here $\mathcal{L}$ is a self-adjoint positive operator acting in an Hilbert space $\mathcal{H}$ in which the eigenfunctions of $\mathcal{L}$ form an orthonormal basis of $\mathcal{H}$, so that $\mathcal{L}^{-\alpha}$ can be written through the spectral decomposition of $\mathcal{L}$. In other words, for a given $g \in \mathcal{H}$, we have

$$\mathcal{L}^{-\alpha} g = \sum_{j=1}^{+\infty} \mu_j^{-\alpha} \langle g, \varphi_j \rangle \varphi_j \tag{1}$$

where μ_j and φ_j are the eigenvalues and the eigenfunctions of $\mathcal{L}$, respectively, and $\langle \cdot, \cdot \rangle$ denotes the $\mathcal{H}$-inner product.

Applications of (1) include the numerical solution of fractional equations involving the anomalous diffusion, in which $\mathcal{L}$ is related to the standard Laplace operator.

In recent years, this problem has been studied by many authors. In the continuous setting of unbounded operators, methods based on the best uniform rational approximation (BURA) of functions closely related to $\lambda^{-\alpha}$ have been considered, for example, in [5, 6, 7, 8] by using a modified version of the Remez algorithm. Another class of methods relies on quadrature rules for the integral representation of $\lambda^{-\alpha}$ [1, 2, 3, 4, 9, 10].

Starting from the integral representation given in [4, Eq. (4)]

$$\mathcal{L}^{-\alpha} = \frac{2\sin(\alpha\pi)}{\pi} \int_0^{+\infty} t^{2\alpha-1} (\mathcal{I} + t^2 \mathcal{L})^{-1} dt, \qquad \alpha \in (0,1), \tag{2}$$

where $\mathcal{I}$ is the identity operator in $\mathcal{H}$, after appropriate changes of variables we consider an alternative approximation based on truncated quadrature rules. We present practical error estimates that can be used to select a priori the number of quadrature points needed to obtain a given accuracy. Some numerical experiments are also shown to demonstrate the reliability of the proposed approach.

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MS-60
Fast Solvers for Large Linear Systems in PDE Discretizations

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The main purpose of the minisymposium is to collect the most recent improvements in iterative methods for matrix sequences stemming from numerical approximations. Indeed, the discretization of partial differential equations (PDE) often requires the efficient solution of linear systems of large size. Consequently, iterative methods play an important role in order to obtain satisfactory approximated solutions. This topic is a dynamic branch of numerical analysis and the application areas include contact mechanics problems [5], linear elasticity, fluid dynamics [4], and many others. Among the discretization techniques, we mention the recent VEM and B-spline IGA approximations [4, 6]. Our proposed solvers are efficient multigrid methods [2], fast preconditioning techniques [6], including space-time block preconditioning [3] and scalable multigrid preconditioning [1, 5].

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Non-overlapping block smoothers for the Stokes equations

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Multigrid methods are efficient iterative solvers for the solution of partial differential equations (PDEs). The efficiency of multigrid methods is due to the combination of suitable smoothers with a coarse grid correction. As one of the two key ingredients smoothers have a significant impact on the performance of multigrid solvers. In many cases, multigrid methods are applied to structured discretizations, allowing for an analysis using Local Fourier Analysis (LFA). LFA is connected to the theory of structured matrices, as it analysis special block-circulant matrices.

For the Stokes equations in most cases an overlapping block smoother is considered. Non-overlapping smoothers can be formulated easily and LFA predict that they work, but they fail in practice. This has been known from the literature for a long time. In [1] we propose another variant that works using different non-overlapping blocks.

In this talk the variant, highlighting the downsides of the analysis of the original smoothers and present the LFA of our approach.

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Scalable multigrid preconditioning for the stabilized contact mechanics problem

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Recently, novel technologies and applications in the subsurface, such as geothermal energy production, hydraulic fracturing, CO_2 sequestration and underground gas storage, have gathered a growing attention. To model these phenomena, one of the key components is the efficient simulation of contact mechanics and fluid flow in faults and fractures. These physical processes are tightly coupled and must be simulated together. Moreover, to achieve the desired accuracy, large domains are usually required, with high resolution representations of geological structures and, specifically, of faults and fracture networks [6]. The increasing demand for better performances is a natural result of these very complex and computationally expensive models. In particular, we focus our attention on the most time-consuming component, i.e., the linear solver. In this work, we present a scalable and efficient preconditioner for the sequence of linear systems arising from the discretization and linearization of the coupled contact mechanics and fluid flow problems.

The Discrete Fracture Model (DFM) [4] is employed as discretization approach, while the Lagrange multiplier method imposes the contact constraints [5]. As proposed in [3], we rely on low order finite elements for the mechanics and a cell-centered finite volume scheme for the fluid flow. This scheme does not require to interpolate between different fields, but does not uniformly satisfy the *inf-sup* condition [7], thus a jump stabilization is introduced. The Jacobian arising from the described problem is a nonsymmetric 3×3 block matrix. With the fields ordered as displacement-traction-pressure, the Jacobian is:

$$\mathcal{J} = \begin{bmatrix} A & C_1 & Q_1 \\ C_2 & H & 0 \\ Q_2 & 0 & T \end{bmatrix},$$

where A is the classical stiffness matrix, C_1 and C_2 are the displacement-traction coupling blocks, Q_1 and Q_2 are the displacement-pressure coupling blocks, H is the stabilization for the displacement-traction pair, and T represents the sum of the mass matrix for the finite volume discretization of the flow problem and the stabilization for the displacement-pressure pair. Please note that H is a singular matrix by design.

Our purpose is to design a scalable preconditioner for this block matrix exploiting the natural block subdivision and an aggregation-based multigrid solver, for instance available

from [1]. According to the unknown orderings, we derive and describe two different approaches, compare the result and find the most promising for complex simulations. We highlight that we do not try to design a novel multigrid preconditioner for block problems, as done in [2], just to provide an example, but focus our attention on coupling a physically-informed block partitioning with a state-of-the-art multigrid preconditioner. Numerical results illustrate the algorithmic scalability, the influence of the relative weight of fracture-based unknowns and the performance on a real-world problem.

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Preconditioners for space-time isogeometric problems

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Isogeometric analysis [1] (IGA) is a method to numerically solve partial differential equations. It is based on the idea of using B-splines (and their generalizations) both for the parametrization of the domain, as it is typically done by computer aided design software, and for the representation of the unknown solution. IGA can also be seen as an extension of the classical finite element method, where the basis functions are allowed to have a higher regularity.

In this talk we discuss preconditioning strategies suited for IGA. It is known that many approaches that are popular in the context of C^0 finite elements, both direct and iterative, tend to perform poorly when applied to IGA linear systems. In particular, their effectiveness deteriorates as the spline degree p is increased.

We address this issue starting from the Poisson problem, and preconditioner that represents the same problem discretized on the reference domain. This preconditioner is robust with respect to h and p and can be applied in a very efficient way thanks to the Fast Diagonalization method, that exploits the tensor structure of the basis functions [4]. We then consider the heat equation, and consider a space-time discretization where smooth splines are used both in space and in time. We develop two numerical formulations for this problem, a symmetric least squares formulation [3], and a nonsymmetric Galerkin formulation [2]. For both approaches, we develop robust preconditioners that can be applied efficiently thanks to a variant to the Fast Diagonalization method. We finally highlight advantages and drawbacks of the two formulations.

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Space-time block preconditioning for incompressible flow

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Parallel-in-time methods have become increasingly popular in the simulation of numerical PDEs evolving in time, allowing for the efficient use of additional MPI processes when spatial parallelism saturates. Most methods treat the solution and parallelism in space and time separately. In contrast, *all-at-once methods* solve the full space-time system directly, largely treating time as simply another spatial dimension. All-at-once methods offer a number of benefits over separate treatment of space and time, most notably significantly increased parallelism and faster time-to-solution (when applicable). However, the development of fast, scalable all-at-once methods has largely been limited to single-variable, time-dependent (advection-) diffusion problems.

In this talk, we introduce the concept of *space-time block preconditioning* for the all-at-once solution of incompressible flow. By extending well-known concepts of spatial block preconditioning to the space-time setting, we develop a block preconditioner whose application requires the solution of a space-time (advection-) diffusion equation in the velocity block, coupled with a pressure Schur complement approximation consisting of independent spatial solves at each time-step, and a space-time matrix-vector multiplication. The new method is tested on classical models in incompressible flow. Results indicate perfect scalability in refinement of spatial and temporal mesh spacing, perfect scalability in nonlinear Picard iterations count when applied to a nonlinear Navier-Stokes problem, and minimal overhead in terms of number of preconditioner applications compared with sequential time-stepping. The findings in this work have been collected in a manuscript currently under review for publication: a preprint version can be found in [1].

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Fast Parallel Solver for the Space-Time IgA-DG Discretization of the Anisotropic Diffusion Equation

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We consider the space-time discretization of the anisotropic diffusion equation, using an isogeometric analysis (IgA) approximation in space and a discontinuous Galerkin (DG) approximation in time. Drawing inspiration from a former spectral analysis of space-time operators in [1], we propose for the resulting space-time linear system a parallel multigrid preconditioned GMRES method, which combines a preconditioned GMRES with a standard multigrid acting only in space. The performance of the proposed parallel solver is illustrated through numerical experiments, showing its competitiveness in terms of iteration count, run-time and parallel scaling. More general parallel space-time multigrid techniques, applied also to non-linear problems, will be also discussed [2], [3].

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Parallel solvers for virtual element discretizations of elliptic equations in mixed form

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In the last decades a large variety of methods for the approximation of partial differential equations on polytopal meshes have been developed. Among them Discontinuos Galerkin (DG), Hybrid High-Order methods (HHO) and the Virtual Element Method (VEM) are the most common ones. Such novel methodologies pose new challenges in the numerical resolution of linear systems arising from the discretization of the partial differential equation at hand.

In this talk we focus on the resolution of the mixed formulation of three-dimensional elliptic equations via VEM. After a first description about the virtual element method itself, we move to the linear algebra. Indeed, we make a deep numerical investigation on the behaviour of both direct and iterative parallel solvers for these type of saddle-point linear systems. Moreover, we analyze the performace of two new kind of block preconditioners: one based on the approximate Schur complement and the other one based on a regularization technique.

MS-61
Trending topics in Uncertainty Quantification - Part III

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In many engineering applications the parameters of the underlying PDE model (e.g., coefficients, forcing terms, boundary and initial conditions, domain shape) are hampered by uncertainty. A very convenient framework is offered by probability theory: the unknown parameters can be effectively described as random variables or random fields with known probability laws. The goal of Uncertainty Quantification (UQ) is to estimate how the randomness in the input parameters affects the outputs of the PDE - typically its solution or related quantities of interest. Other related tasks are (i) to infer the probability density function of the input parameters exploiting measurements of the PDE output

(inverse problems); (ii) to achieve some target by controlling the PDE system subject to uncertainty (optimization problems).

UQ techniques often rely on sampling approaches, i.e. the repeated solution of the PDE at hand for various combinations of the input parameters, thus entailing a significant computational effort. Nowadays, the most promising strategies to reduce the computational complexity are: (i) Reduced Order Modeling, which aims at replacing the original high-dimensional PDE problem with a surrogate model for the sake of UQ analyses; this approach often requires some dimensionality reduction, where the parameters with limited impact on the quantity of interest are identified and neglected; (ii) Multi-fidelity paradigms, where most of the variability is explored by querying cheap computational models, still relying on a moderate use of the computationally intensive models to correct the predictions based on the cheap models. Last, but not least, artificial intelligence and machine learning techniques are also more and more employed in this context.

The aim of this minisymposium is to bring together researchers working at the methodological level to make UQ methods more effective, as well as scientists concerned with the applications of these models to large-scale problems.

A Comparison of Two Multi-Fidelity Computational Approaches for the Uncertainty Quantification of Ship Performance

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In this talk we present a comparison of two methods for the forward Uncertainty Quantification (UQ) analysis of a passengers ferry advancing in calm water and subject to two operational uncertainties, namely the ship speed and payload. Specifically, the performance of Multi-Index Stochastic Collocation (MISC) and multi-fidelity Stochastic Radial Basis Functions (SRBF) surrogates is assessed. The estimation of the expected value of the (model-scale) resistance to advancement, as well as of its higher order moments and probability density function, are presented and discussed. Both methods need to repeatedly solve the free-surface Navier-Stokes equations for different configurations of the operational parameters. The required CFD simulations are obtained by a multi-grid Reynolds Averaged Navier–Stokes (RANS) equations solver. Both MISC and SRBF use as fidelity levels the intermediate grids employed by the RANS solver. A relevant aspect for

the comparison of the two methods is that the CFD simulations are affected by numerical noise, which is due to the iterative algorithm on which the solver is based. In particular, we discuss the impact of the noise on the forward UQ analysis and investigate some strategies to improve the performance of the two methods with respect to this issue.

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Uncertainty quantification and identifiability of SIR-like dynamical systems for epidemiology

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In this talk, we provide an overview of the methods that can be used for prediction under uncertainty and data fitting of dynamical systems, and of the fundamental challenges that arise in this context, see [1]. The focus is on SIR-like models, that are being commonly used when attempting to predict the trend of the COVID-19 pandemic, but most of the points that we touch upon are actually generally valid for inverse problems in more general setups. In particular, we raise a warning flag about identifiability of the parameters of SIR-like models; often, it might be hard to infer the correct values of the parameters from data, even for very simple models, making it non-trivial to use these models for meaningful predictions.

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Rate optimality of an adaptive multilevel stochastic Galerkin finite element method

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We consider an adaptive multilevel stochastic Galerkin finite element method for a class of elliptic boundary value problems with parametric or uncertain coefficients. Stochastic Galerkin approximations are based on a sparse polynomial expansion with spatial coefficients residing in finite element spaces associated with different locally refined meshes. The adaptive algorithm is steered by a reliable and efficient *a posteriori* error estimator, which can be decomposed into a two-level spatial estimator and a hierarchical parametric estimator [1]. We show that, under an appropriate saturation assumption, the proposed adaptive strategy yields convergence of the approximation error to zero with optimal algebraic rates with respect to the overall dimension of the underlying multilevel approximation spaces [2].

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Shape optimization for a noise reduction problem by non-intrusive parametric reduced modeling

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We study a PDE-constrained optimization problem, where the shape and liner material of the nacelle of an aircraft engine are optimized in order to minimize the noise radiated by the engine. More precisely, the acoustic problem is modeled by the Helmholtz equation with varying wavenumber k on an exterior domain. A model reduction strategy is employed to alleviate the cost of the design optimization: the minimal rational interpolation technique is used to construct a surrogate (w.r.t. to the wavenumber k) for the quantity of interest at fixed shape/material parameter values, and a parametric model order reduction approach is employed to combine surrogates at different shape/material designs, resulting in a nonintrusive methodology. Numerical experiments for shape and shape/material optimization are provided, to showcase the effectiveness of the presented methodology. The present talk refers to the publication [1].

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Uncertainty Quantification for Parameter dependent Partial Differential Equations using Deep Neural Networks

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In many fields, such as engineering, healthcare and finance, Uncertainty Quantification (UQ) plays an essential role in the development of robust and reliable models. UQ techniques often involve many-query algorithms, such as those typical of MonteCarlo methods, Frequentist and Bayesian inference. As a consequence, in the case of high-dimensional and complex systems such as those driven by PDE models, UQ becomes extremely challenging and computationally expensive [4]. One possible solution is to reduce the computational cost by introducing a suitable surrogate model, which approximates the underlying Full Order Model at a negligible compromise in accuracy. Here, we consider models described by parameter dependent PDEs and we focus on the use of Deep Neural Networks (DNNs) as model surrogates [2, 3]. In order to fully exploit the nonlinear capabilities of DNNs, we base the construction of the network on the concept of *manifold-width*, as defined in [1]. After discussing the theory and the driving ideas of our approach, such as minimal AutoEncoders and mesh-informed layers, we present some numerical examples with applications to UQ and microcirculation of oxygen.

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Enabling Uncertainty Quantification for PDEs by Reduced Order Modeling & Machine Learning

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Projection-based reduced order models (ROM), built through, e.g., the reduced basis method or proper orthogonal decomposition (POD) provide rapid and reliable approximations to parametrized PDEs. ROMs are nowadays essential to enhance the solution to many-query problems such as, e.g., forward UQ, sensitivity analysis, and inverse UQ (parameter estimation and data assimilation) whenever they involve complex physics-based models described in terms of PDEs. Indeed, employing high-fidelity, full order models (FOMs) would make the solution of the aforementioned problem computationally infeasible. Although typically more intrusive to implement, ROMs often yield more accurate approximations than purely data-driven emulators (built, e.g., through Gaussian Process regressions, polynomial chaos expansion, or artificial neural networks) and usually generate more significant computational gains than lower-fidelity models obtained introducing modeling simplifications (e.g., coarser meshes or simplified physics). Nevertheless, building efficient ROMs for nonlinear time-dependent parametrized PDEs could be a difficult task because of the use of expensive hyper-reduction strategies, or the intrinsic difficulty to handle complexity with linear superimpositions of modes.

To enhance the ROMs' efficiency in order to address variance-based global sensitivity analysis and forward UQ problems, we account for the approximation error with respect to the FOM by means of inexpensive ANN regression models. Compared to purely data-driven approaches such as, e.g., ANN-based models emulating the input-output relationship, the proposed approach provides better results in terms of both accuracy and offline costs [5].

Moreover, we show that combining classical projection-based ROM techniques with artificial neural networks or deep learning (DL) algorithms, proves to be a suitable strategy to make ROMs non-intrusive, ultimately yielding the opportunity to perform numerical simulations in real-time [1, 4]. Indeed, we show that *(i)* performing a prior dimensionality reduction on FOM snapshots through POD, *(ii)* exploiting deep (e.g., feedforward, convolutional, autoencoder) neural networks and *(iii)* relying on a multi-

fidelity pretraining stage, the resulting POD-DL-ROMs are extremely efficient at both the testing stage, when evaluating the PDE solution for any new testing-parameter instance in a non-intrusive way, and the training stage, when the ROM is built [2, 3].

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MS-62
ACRI YITP Minisymposium - Part I

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The Department of Mathematical, Physical and Computer Sciences (DSMFI) of the University of Parma, together with SIMAI 2020+21 Congress, is one of the winners of the competition for the Young Investigator Training Program (YITP) 2019 promoted by ACRI, the Italian organization representing Foundations of banking origin and Savings Banks.

The YITP supports the participation of young researchers, working abroad, to international conferences held in Italy, delivering research prizes which are meant to finance a visiting period of at least one month in one of the Italian research institutions of YITP-Conference network.

Twelve young researcher have applied to the competitive call issued by DSMFI in 2021 and ten of them have been declared, by the evaluation panel, winners of YITP 2019 Research Prizes granted by ACRI in the framework of SIMAI 2020+21 Congress.

The ACRI YITP Minisymposium - Part I and Part II - collects the scientific contributions of the YITP 2019 prize winners.

Discovery mathematical models from experimental data

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In this talk, I will present two techniques to discover mathematical models from data using machine learning. In the first part of the talk, we advocate the use of Dynamic Mode Decomposition (DMD), an equation-free method, to approximate the data with a linear model. DMD is a spatio-temporal matrix decomposition of a data matrix that correlates spatial features while simultaneously associating the activity with periodic temporal behavior. With this decomposition, one can obtain a reduced dimensional surrogate model and use for future state predictions or extrapolate missing information from the data. I will show applications to fire data and human mobility using data provided by TIM ([1]).

In the second part of the talk, we address the problem of discovering nonlinear ODEs and PDEs from data. We will show that we can recover the mathematical problem by means of sparse optimization methods such as LASSO and RIDGE regression. Examples and applications of the methods will be showed during the talk ([2]).

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On and beyond Total Variation regularisation in imaging: the role of space variance.

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The use of space-variant regularisation models for inverse imaging problems have become very popular over the last years to improve upon the inability of standard image regularisers to adapt to local features, such as regularisation strength, sharpness and directionality. In this talk we focus on the case of standard Total Variation (TV) regularisation and discuss on how an adaptive mathematical modelling accommodating local regularisation weighting, variable smoothness and anisotropy can improve upon well-known reconstruction drawbacks, being it more tailored to describe local image structures. We further show how these models can be interpreted within the flexible Bayesian framework of Generalised Gaussian Distributions and further combined with maximum likelihood and hierarchical optimisation approaches for efficient hyper-parameter estimation. Our combined modelling is then validated on some standard image restoration problems.

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Data-driven rate-dependent fracture mechanics

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We extend the model-free data-driven approach to quasi-static fracture mechanics presented in [1] to rate-dependent and fatigue crack propagation. In our formulation, the fracture-related material modeling assumptions are removed and the fracture constitutive behavior is encoded in a discrete set of material observations, termed *material data set*. In the case of monotonic loading, this relates the critical energy release rate with the crack tip velocity and, eventually, with the crack size. For the sub-critical fatigue crack growth, the material data set is composed of points associating the crack growth rate to the nominal range of energy release rate spanned during a cycle. Also, the epistemic laws of fracture stemming from the variational principle of local energy minimization are retained and encoded in a set of Kuhn-Tucker conditions that define the *set of allowed material states* [1].

The data-driven approach to fracture mechanics relies on the definition of a discrete quantity, generally termed distance between the material data points and the set of allowed material states. At each load step, this distance attains its minimum in correspondence of the solution of the crack propagation problem, namely at the point in the material data set that best fulfills the conditions imposed by local minimization [1, 2]. In this non-conservative framework, irreversibility is naturally introduced as non-negativity of the crack tip velocity or growth rate. Also, the crack extension plays the role of a measurable history variable and the proposed approach belongs to the class of differential materials [3].

The proposed approach is tested on double-cantilever-beam examples with different geometries, using artificially generated material data sets, with or without random noise and reproducing different rate-dependent and fatigue fracture behaviors. The results demonstrate that the proposed approach is able to correctly reproduce reference solutions obtained adopting analytical constitutive models. Also, we show that the monotonic rate-independent evolution can be reproduced as special case when adopting data sets relating critical energy release rate, crack tip velocity and crack size, while it can be

obtained in the limit for slow loading rates in case of data sets dependent on the crack tip velocity only.

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Bayesian operator inference for the reduced order modeling of time-dependent problems

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Operator inference [1] is a non-intrusive approach to the reduced order modeling of time-dependent PDEs. In this projection-based scheme, the snapshot data of full-order state variables are projected onto a low-dimensional POD basis, and the reduced-order operators are then recovered from the projection data through least squares. In this talk, we present a probabilistic formulation of operator inference, in which linear Bayesian inference with Gaussian priors is employed to recover the reduced operators. Compared to the deterministic operator inference, the proposed Bayesian formulation can quantify modeling uncertainties in the recovered reduced-order model, and posterior distributions are also given for the predictions of future states. When ill-conditioned issues are encountered, recommended penalty coefficients of L_2 regularization can be obtained with the aid of maximum marginal likelihood. The proposed Bayesian formulation of reduced operator recovery provides new perspectives of regularized operator inference [2, 3] and its uncertainty quantification. Such a method of reduced order modeling works as a 'grey-box' scheme, which inherits the basic physics but does not require access to the full-order solvers. The proposed method's effectiveness will be demonstrated by a 2D single-injector combustion problem [2, 3] in this talk.

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Collocation IGABEM for 3D potential problems using Quasi-interpolation quadrature schemes

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In recent years, isogeometric paradigm has gained a lot of attention in Boundary Element Method (BEM) research community. The paradigm's main idea is to represent the geometry exactly with CAD standard objects and to use the same type of functions also in the discretization space. In many cases the isogeometric BEM (IGA-BEM) offers better "accuracy versus number of degrees of freedom" ratio and better convergence orders than its more common non-isogeometric counterpart. To fully exploit these advantages in practice, one of the crucial steps is to develop novel accurate and efficient high order quadrature rules.

In this talk we present a new class of quadrature rules to integrate weakly singular integrals. The focus is on the governing integrals of Boundary Integral Equations for 3D Laplace boundary value problems, using a collocation method within the isogeometric paradigm.

The rules lean on two important ingredients. The first one is a novel higher order isoparametric singularity extraction technique. With this approach we can remove the singular contribution of the integral and evaluate it analytically. For the remaining part

of the integral, which is regular, we apply a recently developed integration scheme that is based on spline quasi-interpolation technique. The scheme has high order converge rates and since it is tailored for spline integrands, it perfectly fits in the isogeometric framework.

A selection of numerical examples confirms that when utilizing the above-mentioned quadrature rules, the expected convergence orders of the approximate solutions are obtained.

MS-63
ACRI YITP Minisymposium - Part II

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Studying the effects of pulse wave propagation on cardiac function using a novel 3D model of cardiac electromechanics coupled to a 1D model of the circulatory system

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The influence of increased vessel wall stiffness and pulsatile load on the circulation and the heart function is documented not only for cardiovascular events but also for ventricular dysfunctions. Thus, computer models of cardiac electromechanics (EM) shall integrate effects of the circulatory system on heart performance for clinical applications. In order to ensure a satisfactory trade-off between accuracy and computational cost, simplified representations of the circulation shall be adopted. To date, most three-dimensional (3D) computational models of the heart function proposed in the literature consider lumped 0D models as boundary conditions to model the circulation [1]. However, when local vascular changes or distributed properties and their impact on central pressure waveforms and cardiac function are studied, 1D circulatory models may be preferred over 0D models.
In this talk, we describe a novel strategy for a coupled model based on a 3D EM model of the heart function [1], together with a 1D model of blood flow in the arterial system. The coupling approach is based on the resolution of a saddle-point problem for the volume and pressure in the cavity. As a first illustration, we show the effects of vessel stiffening in a configuration composed by a 3D model of the left ventricle (LV) coupled to an arterial outflow consisting of a 1D viscoelastic tube with stenosis [3] and lumped terminal boundary conditions. As a second example, we analyse the results for a coupled system consisting of the LV and an aortic vessel network with 116 vessels [2] in two physiological configurations, corresponding to a healthy younger and a healthy older individual, in order to explore the effects of ageing on cardiac function. Finally, from the perspective of model personalisation, we show the results of a preliminary sensitivity analysis on the model. The use of 1D arterial models enables to efficiently capture the effects of vascular changes and distributed properties, since they allow for a more accurate representation of

the impact of pulse wave propagation on the circulation and cardiac function. Therefore, the use of our 3D-1D coupled model has great potential in understanding the impact of haemodynamic mechanisms in a broad spectrum of cardiovascular pathologies.

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Symbol Based Convergence Analysis in Multigrid Methods for Block Structured Matrices

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The first aim of the talk is to provide the generalization of the convergence results of multigrid algorithms [1, 6] applied on linear systems where the coefficient matrix sequence is a block circulant or a block Toeplitz-like matrix sequence. That is, they can be associated with matrix-valued symbols $\mathbf{f}$ [3] instead of scalar-valued symbols. In particular, we focus on the crucial choice of conditions that should be fulfilled by the trigonometric polynomial $\mathbf{p}$, used to construct the grid transfer operator, in order to ensure the optimality of the two-grid and v-cycle methods [2, 3]. The latter are expressed in terms of eigenvectors associated with the ill-conditioned subspace and this permits to extend the class of suitable trigonometric polynomials that can be chosen to construct the operators.

Furthermore, we test the efficiency of some standard projectors [4, 5] whose associated polynomial, indeed, fulfills our derived conditions.

Finally, we conclude with an outlook on possible applications stemming from linear elasticity problems which present a challenging block structure nature.

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From low to high order hybrid discretisation methods for flow problems

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In recent years, hybrid discretisation methods have gained increasing attention due to their flexibility to devise robust and accurate numerical approximations of partial differential equations, both in low and high order settings, making them suitable to treat complex problems of engineering interest. This talk will present some recent advances in the development of robust face-centred finite volume (FCFV) [6] and high-fidelity hybridisable discontinuous Galerkin (HDG) [1, 4] methods for the simulation of compressible and incompressible flows. On the one hand, for the simulation of flow problems involving large-scale domains, industry still requires the employment of fast and robust techniques capable of providing overnight results. In this context, FCFV represents a competitive paradigm to handle general unstructured meshes, achieving first-order convergence of the stress tensor without requiring flux reconstruction strategies. Hence, the results are insensitive to cell distortion and stretching [6]. In addition, FCFV provides non-oscillatory approximations of sharp discontinuities without the need for any shock capturing or limiting technique [8]. Finally, the method is robust in the incompressible limit and provides stable approximations without the necessity of a specific treatment of the velocity-pressure coupling [2]. On the other hand, when high-fidelity simulations are required, high order methods are the preferred choice due to their low diffusion and dispersion errors. Nonetheless, this additional accuracy often comes with a reduced robustness. To remedy this issue, the development of positivity-preserving and shear-preserving approximate flux Riemann solvers will be discussed in the context of high order HDG discretisations of compressible flows. The resulting HDG strategy with HLL and HLLEM Riemann solvers outperforms traditional Lax-Friedrichs and Roe fluxes in the approximation of shock waves, especially in supersonic cases where physically admissible solutions are obtained without requiring user-defined corrections [7]. In addition, the presented high order HDG

paradigm is also robust in the incompressible limit [3] and for weakly compressible flows, in the context of fluid-structure interaction problems [5].

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Convergent finite element methods for the Ericksen model of nematic liquid crystals

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Liquid crystals (LCs) are materials which exhibit properties intermediate between isotropic liquids and crystalline solids. The Ericksen model [1] describes nematic LCs in terms of a unit-length vector field $\boldsymbol{n}$ and a scalar function s. Equilibrium states of the LC are given by admissible pairs $(s, \boldsymbol{n})$ that minimize the energy functional

$$E[s, \boldsymbol{n}] = \frac{1}{2} \int_\Omega \left(\kappa |\nabla s|^2 + s^2 |\boldsymbol{\nabla n}|^2 \right) + \int_\Omega \psi(s),$$

where $\kappa > 0$ is constant and ψ denotes the double well potential. We propose a simple but novel finite element approximation of the problem that can be implemented easily within standard finite element packages [2]. The scheme does not employ a projection to impose the unit-length constraint on $\boldsymbol{n}$ and thus circumvents the use of weakly acute meshes, which are quite restrictive in 3D but are required by recent algorithms for convergence. We show stability and Γ-convergence properties of the new method in the presence of defects. We also discuss an effective nested gradient flow algorithm for computing minimizers that controls the violation of the unit-length constraint of $\boldsymbol{n}$. We present several simulations in 2D and 3D that document the performance of the proposed scheme and its ability to capture quite intriguing defects.

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Numerical continuation for fractional PDEs within `pde2path`

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Partial differential equations (PDEs) involving fractional Laplace operators have been used increasingly to model non-local diffusion processes and are actively investigated using both analytical and numerical approaches. In order to study the effects of the spectral fractional Laplacian on the bifurcation structure of reaction–diffusion systems on bounded domains, we need advanced numerical continuation techniques to compute the solution branches. Since currently available continuation packages only support systems involving the standard Laplacian, we extend the `pde2path` software to treat fractional PDEs (in the spectral definition). The numerical approximation is based on a sinc quadrature approximation of the Balakrishnan representation formula. The new capabilities are then applied to the study of the Allen–Cahn equation, the Swift–Hohenberg equation and the Schnakenberg system (in which the standard Laplacian is replaced by the spectral fractional Laplacian). In particular, we investigate the changes in snaking bifurcation diagrams and in the spatial structure of non-trivial steady states upon variation of the fractional order.

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Individual contributions

Simulating the COVID-19 epidemic and vaccination campaign in Italy with the SUIHTER model

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We present the epidemiological model SUIHTER for the simulation and (short term) forecast of the COVID-19 epidemics in Italy. The model is named after the seven compartments that is made of: Susceptible (S), Undetected (U), Isolated (I), Hospitalized (H), Threatened (T), Extinct(E), and Recovered (R). The compartments have been chosen to reflect the data supplied daily by the Italian Civil Protection Department. The model, that was originally proposed in [1] and later extended in [2], can account for different variants of the virus, each characterized by a different transmission rate. In this talk, we further extend the model to account for the vaccination campaign. Two additional compartments are introduced, counting the individuals who have received only the first vaccine dose (V1) and both doses (V2). In our model, vaccinated individuals can still be infected with a lower probability than susceptibles and are less prone to develop severe symptoms. The SUIHTER model has been used to perform scenario analyses to estimate the impact of different Non-Pharmaceutical interventions (NPIs), both for predictions and what-if analyses to quantify the effect on past epidemic trends in case different NPIs had been implemented. We also developed a mathematical dashboard, described in [2] and publicly accessible at www.epimox.polimi.it, for the analysis of the Italian COVID-19 epidemic. The dashboard allows visualizing the data supplied by the Italian Authorities and some critical indicators, together with the forecasts and scenario analyses provided by the SUIHTER model.

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The IMFogram
An alternative view to time-frequency representation of nonstationary signals

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The time-frequency analysis of nonlinear and nonstationary processes is, in general, a challenging task. Standard techniques, like short time fourier transform, and wavelet transform are limited in addressing the problem. An alternative way to tackle the problem is to first decompose the signal into simpler components and then analyze them separately. This is the idea behind what is called the Hilbert Huang Transform (HHT), published originally in 1998. HHT had and is still having a big impact in many filed of research as testified by the more than 15300 citations (based on Scopus). HHT is made of two stages: the decomposition of the signal into simple oscillatory components, called Intrinsic Mode Functions (IMFs), obtained via the Empirical Mode Decomposition (EMD) method, and the time-frequency representation of these components obtained via the Hilbert Transform.

However, the mathematical properties of EMD and its generalizations, like the Ensemble EMD, are still under investigation. For this reason an alternative technique, called Iterative Filtering (IF), was proposed recently.

In this talk we review the mathematical properties of IF and its fast implementation via FFT called Fast Iterative Filtering (FIF) [1], and we introduce an alternative method for the time-frequency representation of the IMFs called IMFogram [2, 3].

We show the IMFogram robustness to noise, its locality and ability to produce, in a fast manner, crisp and artifact-free time-frequency plots. We conclude presenting applications of this approach to real life signals and future directions of research.

This is a joint work with H. Zhou (Georgia Tech), W. S. Li (Georgia Tech), and P. Barbe (CNRS)

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Mechanical Circulatory Support Systems For Cardiogenic Shock Conditions: Towards An In Silico-Based Clinical Decision Support System

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Computational models (CM) are being used more frequently to support R&D processes and clinical research due to their capability of inspecting a high variability of scenarios at a moderate cost in terms of time, money and lives. Moreover, as time passes by, efficiency of CMs grows along with their capability of simulating and providing insights on extremely complex scenarios, opening the doors to new contexts of use.
In this study, we present a multi-scale, closed loop mathematical model of the whole human cardiovascular system that extends previously validated models [2] and show multiple use cases in which we simulated the activity of four mechanical circulatory support (MCS) devices (VA-ECMO, LVAD, pVAD and IABP) in cardiogenic shock (CS) condition.
Numerical results for CS condition are being validated by comparison with experimental measurements taken on a mock circulatory loop developed by FDA [1]. Lumped-parameter models of each MCS device are coupled to the cardiovascular model to simulate their activity and inspect their performance in such a complex pathological scenario.
The obtained numerical predictions of hemodynamic-related vital signs as well as blood pressure and flow waveforms for CS condition are coherent with literature values. Effects of MCS are well caught and outcomes are comparable to available clinical data. Furthermore the versatility of this model allows testing peculiar scenarios such as use of Ecpella (VA-ECMO+Impella) and obtaining insights on crucial dynamics such as ventricular unloading and organs perfusion.
The effectiveness and versatility of this simulation tool make it a reliable basis to develop a comprehensive clinical decision support system that will endow clinicians with the possibility to test several therapies identifying the most effective alternative to improve patients' health.

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Two FEM-BEM methods for 2D transient elastodynamics problems in unbounded domains

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We consider transient 3D elastic wave propagation problems in unbounded isotropic homogeneous media, which can be reduced to corresponding 2D ones. This is the case, for example, of problems defined on the exterior of a bounded rigid domain, which are invariant in one of the cartesian directions. For their solution, we propose and compare two alternative numerical methods, both based on the coupling of a (vector) PDE, representing the given 2D elastodynamics problem, with the associated space-time Boundary Integral Equation (BIE). The BIE is prescribed on an artificial boundary, chosen to determine a bounded computational domain of interest, and defines a condition which is non reflecting for both incoming and outgoing waves. In the first approach the differential equation is the classical one of elastodynamics while, in the second one, the latter is replaced by a corresponding couple of scalar wave equations, obtained after performing the displacement Helmholtz decomposition. By this decomposition, the elastic equation is split into two equations, describing the propagation of P-waves and S-waves, which are coupled by the Dirichlet boundary condition of the original problem. The latter approach has been used in [1] to solve an interior problem by a finite element method, and in [2] to solve an exterior problem by means of the associated space-time BIE representations. Here, in both coupling approaches, the differential equation is discretized by applying a finite element method in space and the time marching Crank Nicolson scheme, while for the discretization of the BIE we apply a time convolution quadrature and a space collocation boundary element method. To compare the performances of the two approaches, some numerical test are also presented.

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On the coupling of Curvilinear Virtual Element and Boundary Element Methods for 2D exterior Helmholtz problems

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We consider the Helmholtz equation defined in unbounded domains, external to 2D bounded ones, endowed with a Dirichlet condition on the boundary and a radiation condition at infinity. We propose a numerical method that approximates the solution using computations only in an interior finite domain. This is obtained by introducing a curved smooth artificial boundary on which a non-reflecting boundary condition, defined by a boundary integral equation, is imposed. For the numerical discretization, we propose a Galerkin approach based on the curvilinear virtual element method in the interior of the computational domain. This choice is based on the fact that the virtual element method allows to broaden the classical family of the finite element method for the discretization of partial differential equations for what concerns both the decomposition of domains with complex geometry and the definition of local high order discrete spaces. Moreover, the use of curvilinear elements instead of polygonal ones allows to avoid the sub-optimal rate of convergence for degrees of accuracy higher than 2. The main challenge in the theoretical analysis, based on the pioneering Johnson-Nédélec paper in which the coupling approach is proposed for the Laplace equation (see [1]) , is the lack of ellipticity of the associated bilinear form. However, using the Fredholm theory for integral operators, it is possible to prove the well-posedness of the problem in case of computational domains with smooth artificial boundaries. We present the theoretical analysis of the method in a quite general framework, and we provide an optimal error estimate in the energy norm. The numerical tests we present confirm the theoretical results and show the effectiveness of the new proposed approach.

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Decentralized dynamic pricing of transportation networks

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Over the past years dynamics and control of traffic flows over networks have received a great deal of research attention, motivated by applications both to communication networks and to road transportation systems. A central aspect, as it is well known, of dynamical flow networks is related to the routing decisions. In this paper, we consider, as in [2], a multiscale dynamical model of the transportation network whereby the traffic dynamics describing the real time evolution of the local traffic level are coupled with those of routing choices. We assume that the latter evolve following a perturbed best response to global information about the traffic status of the whole network and to decentralized flow-dependent tolls. We prove that by using a class of decentralized monotone flow-dependent tolls [3] and in the limit of small update rate of the aggregate routing choices, the transportation network globally stabilizes around a generalized Wardrop equilibrium. In particular, this result implies that using decentralized marginal cost tolls, stability of the dynamic transportation network is guaranteed around the social optimum traffic assignment. Then we present numerical simulations comparing the asymptotic and transient performance of the system with dynamic decentralized feedback marginal cost tolls and constant marginal cost tolls. While it is known that the latter can be computed to enforce the social optimum equilibrium, we show that not only do the former achieve the same optimal asymptotic performance but they also guarantee faster convergence and are strongly robust to variation of network topology and exogenous traffic load. Finally, we study the effect of time-delays in the global information of the routing decision dynamics and analyse their influence on the evolution of the multi-scale dynamical system.

All the above results can be found in [1].

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Detailed hydropower production modelling over large-scale domains: the HYPERstreamHS framework

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Climate change impact assessment on hydrological cycle often requires the aid of large-scale hydrological modelling to understand the interactions between the projected variations of meteorological forcing and the processes occurring in the watershed under investigation. However, the natural variability of hydrological cycle is nowadays strongly altered by the presence of anthropogenic water uses, which modify timing and magnitude of streamflows. Furthermore, hydropower production involves the largest share of water volume among all water uses in the Italian Alps: therefore, a detailed modelling of such renewable energy production is crucial for a reliable assessment of water resources evolution under a changing climate. The implementation of hydropower system models over large-scale domains represents however an open challenge in the hydrological science due to the unavailability of sufficient information concerning the hydropower systems themselves; furthermore, these simulations often require considerable computational effort due to the simultaneous handling of large datasets and to the structure of model calibration algorithms. In an attempt to fill these gaps we developed HYPERstreamHS, a hydrological modelling framework [1] tailored to make use of high performance computing tools and capable of simulating explicitly the presence of human infrastructures associated to hydropower production. The modeling framework was validated in several meso-scale

catchments in the Italian Alpine Region by successfully comparing observed and simulated time series of daily streamflow and monthly hydropower production [2].

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Machine learning based decision support system in oncology

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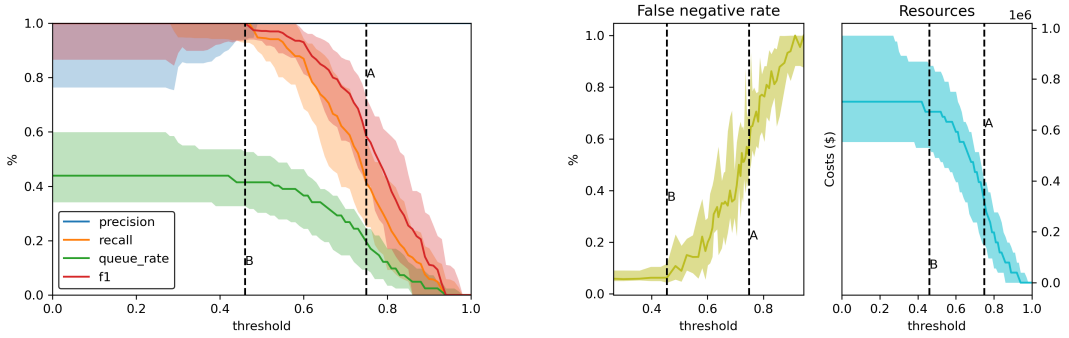
Machine learning allows automatic feature learning from patterns encountered in the input data: applied to genetics could fill the gap between a fast accumulation of data and a slower, time-demanding interpretation. However, communicating how prediction models can impact decisions can be challenging. In binary classification problems, a way to address interpretability is to identify a decision threshold linked to the outcomes of the confusion matrix. Here, we built a theoretical cost-benefit simulation exploitable by healthcare managers or private insurance companies developed from a previous investigation related to bladder cancer survival [1]. Interpretation of this graphical simulation could provide a tool for deriving solutions to bridge between developers and healthcare managers by combining ML outcomes with real-world decision-making scenarios and communicating ML more effectively to non-experts, offering them a perspective closer to their background.



(a) ML model behavior and patient "queue" rate (b) forecasted type II errors and operating costs

Figure 1: Cost-Benefit simulation

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An OpenFOAM-7 implementation of the Immersed Boundary Method applied to polymer processing problems

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Mixing of polymeric materials is performed with the aid of machines characterized by very complex geometries in which body-fitted simulations can hardly be applied. Immersed Boundary Methods (IBM) represent the best alternative to simulate such processes with complex kinematics (mixers, extruders etc.). The basic procedure consists in generating an extremely simple computational mesh that entirely contains the object in motion. Then, the motion has to be imposed in a nonconforming way using a certain strategy. We have first explored a diffuse interface method to impose Dirichlet conditions in [2], loosing however an order of convergence, unless a certain level of local refinement is achieved. To recover the second order of convergence, typical of OpenFOAM's Finite Volume Method (FVM), we revisited the IBM's implementation present in the OpenFOAM's fork *foam-extend-4.0* [1]. We first migrate the code to a newer version of OpenFOAM (the 7th) and then we aim to characterise its numerical properties and limits, making improvements in terms of robustness and accuracy.

In this talk we apply our IBM to problems involving laminar flows of non-Newtonian fluids with temperature dependent viscosity, developing an ad hoc solution algorithm. We then investigate its main properties in terms of accuracy and robustness. A comparison with basic diffuse interface method is performed showing that second order of convergence is recovered. Finally we quantify the ability of the IBM in approximating solutions of problems characterised by dominant transport (that is the case of energy conservation), boundary layers and very small geometric gaps.

This work has been supported by Pirelli and Fondazione Politecnico in the framework of the Joint Research Lab Politecnico di Milano/Pirelli.

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Forecasting *M&A* deals with MIDAS count model

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We propose a new model to improve forecasting properties of count models by taking into account past trends in high-frequency data and the disclosure of the conditional overdispersion into short-term and long-term components. Our model relies in the dynamics in the first two moments of the distribution to allow for the evolution over time of both parameters in the Negative Binomial distribution. We employ this model in several dataset of *M&A* count models where we obtain forecast improvements compared to benchmark INGARCH models.

An accurate and efficient implicit Discontinuous Galerkin solver for the incompressible Navier-Stokes equations

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We propose an accurate, efficient and robust implicit solver for the Navier-Stokes equations, based on a low order DG spatial discretization and on the TR-BDF2 method for time discretization [1] in order to combine both accurate and flexible discontinuous finite element discretizations and efficient and unconditionally stable time discretizations [2]. The parallel implementation in the framework of the *deal.II* utility, with a matrix-free approach, allows for accurate and efficient adaptive simulations in complex geometries and makes the proposed solver attractive also for industrial applications. Time discretizations based on implicit solvers have already been proposed; however, we claim that the combination employed is optimal for a low order h-adaptive solver. The superior efficiency and accuracy with respect to some widely used alternative schemes on a number of classical benchmarks has been established. Possible extensions to compressible flows will be also discussed.

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Matrix Equation Techniques for Certain Evolutionary Partial Differential Equations

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In this talk we illustrate how the discrete operator stemming from time-space discretization of evolutionary partial differential equations can be represented in terms of a single Sylvester matrix equation. A novel solution strategy that combines projection techniques with the full exploitation of the entry-wise structure of the involved coefficient matrices is proposed. The resulting scheme is able to efficiently solve problems with a tremendous number of degrees of freedom while maintaining a low storage demand as illustrated in several numerical examples.

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Obstruction to extension of Wasserstein distances for variable masses

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Wasserstein distances are powerful tools to study both mathematical modeling problems, with applications ranging from large-scale systems, to economy, imaging, and control engineering, and theoretical problems, concerning, e.g., gradient flows and geometric evolution equations. Despite their great usefulness, Wasserstein distances have several drawbacks, the most apparent being the fact that they are defined only between measures having the same mass. In order to overcome this limitation, there have been several attempts at defining generalized Wasserstein-like distances—we mention, e.g., [1, 2, 3].

In this talk we consider the possibility of extending the p-Wasserstein distance to a metric d, defined on the whole space $\mathcal{M}(\mathbb{R}^n)$ of non-negative measures on $\mathbb{R}^n$, such that

$$d(\mu,\nu) = f(|\mu|)W_p\left(\frac{\mu}{|\mu|},\frac{\nu}{|\nu|}\right), \tag{1}$$

for some $f : (0,+\infty) \to (0,+\infty)$, whenever $|\mu| = |\nu| > 0$. The main result consists in proving that no such distance exists, under the additional assumption that the isometries of $\mathbb{R}^n$ induce isometries for d, via the push-forward of measures.

Moreover, we prove that no distance satisfying (1) exists, if we also assume that the "cost" of "creating" or "destroying" mass is (locally) uniformly bounded with respect to the distribution of the mass. Remark that the main obstruction is given by the presence of the zero measure. Indeed, one can define such a distance on the space of strictly positive measures, but only with f constant. This represents a big limitation to the usefulness of this metric in applications.

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Proper Orthogonal Decomposition Strategy for Edge Finite Elements

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One of the main practical difficulties concerning the solution of parametrized problems derived from Maxwell's equations is the required running time. These problems often use edge finite elements for the approximation of the main unknown that belongs to the space $H(\text{curl}, \Omega)$. Our studies are focused on applying Reduced Basis (RB) methods to Edge finite elements and verifying their effectiveness. In particular, we use Proper Orthogonal Decomposition (POD) as strategy to generate the RB space. The aim of this work is to study the performance of this approach when the first family of Nédélec finite elements, see [2], is used. For all the tests we employ the RBniCS software [3].

We use an abstract parametrized model problem of the form

$$\text{curl}(\alpha \text{ curl } \mathbf{u}) + \beta \ \mathbf{u} \ = \mathbf{f}$$

with Dirichlet or parametrized Robin boundary conditions. The results have been the expected ones, since they were perfectly comparable with the ones produced by an analogous problem in $H^1(\Omega)$ using Lagrange finite elements. We observed that the speedup numbers for the electromagnetic problem are very significant.

These results are preliminary to the study of time harmonic Maxwell's equations with impedance boundary conditions parametrized in terms of the frequency, see [1].

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A novel multi-age/multi-group SEHIRDV model for the COVID-19 epidemics

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In this talk, we present a novel epidemiological model for the simulation of the COVID-19 epidemics in Italy, named SEIHRDV, which accounts for the following compartments: Susceptible (S), Exposed (E), Infectious (I), Healing (H), Recovered (R), Deceased (D) and Vaccinated (V). Our model is multi-age, as it considers the population split into 15 age groups and it is multi-groups as it considers 7 different contexts of exposition to the infection. Thanks to this structure, our model can help investigating the epidemics dynamics across different ages and different contexts of exposition. In addition, the model can better address the efficacy of non pharmaceutical interventions, as well as possible vaccination strategies. We specialize the model to the COVID-19 epidemics in Italy and we use it to analyse past epidemic trends, to realize what-if studies and scenario analysis, other than to forecast future evolution.

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Elastic-plastic dynamic drill-string simulation based on Cosserat rods

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In this talk, we present the application of the theory of Cosserat rods to the geometrically nonlinear dynamics of a drill-string for oil and gas applications. The underlying model, based on strains and generalized velocities of the cross sections and their dual generalized stresses and momenta as variables, is presented. In this approach, an important role is played by the special Euclidean group and algebra [1–4]. The traditional plasticity laws were adapted to this model and redefined in order to properly operate in this strain-stress framework. Benchmark solutions are compared with other numerical results available, to validate the model. The proposed method is able to provide elastic-plastic response applied to a nonlinear dynamic model, with competitive simulation times. Results of the model, applied to real oil and gas wells, are presented.

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Industrial Session

IS-1
Solution methodologies of inverse problems: application to engineering issues

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Normally the standard physical problems, usually known as direct problems, concern the determination of the effect starting from the causes. Otherwise it is possible to say that inverse problems involve the estimation of the causes from the measurement of the effect [1]. The word "estimation" is used talking about inverse problems because in measurements, errors are always present, and they affect the accuracy of the calculation [2]. A general direct problem can be formalised as the determination of the effect y of a given cause x when a definite mathematical model M is postulated: Mx = y. The operator M is assumed to be well-posed and continuous: it results in a unique effect y for each cause x and small variations in x outcome in small changes in y. But this direct problem is only part of the issue since, once the discussed direct problem is assumed,

two inverse problems may be instantly set. These are the inverse problems of causation (given M and y, determine x) and model identification (given x and y, determine M) [3]. The inverse heat transfer problems are much more difficult to solve analytically than the direct problems but in the direct problem many experimental impediments could be present in measuring or producing given boundary conditions. The major difficulties in the solution of inverse heat transfer problems are connected to the fact that from the mathematical point of view they are classified as ill-posed while the direct problems are usually well-posed [2, 4]. In order to bypass the ill-posedness of inverse problems, many techniques based on the processing of the experimental data have been suggested and validated in literature [2]. Among these methods, regularization techniques, methods based on filtering proprieties, the function specification methods, probabilistic methods and iterative methods could be found. The area of application for the theory of inverse problems regards almost all fields of science that use mathematical methods [5]. The major goal of this minisymposium is to present real application examples of such problems in the wide field of engineering and, consider the challenges they present, discuss methods designed to meet those challenges.

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Optimum Experiment Design for Simultaneous Estimation of Thermal Properties of High-Conductivity Materials

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The optimal experiment for the thermal properties (thermal conductivity k and volumetric heat capacity C) estimation of high-conductivity materials using the plane source method [1] is designed. The experimental apparatus here investigated consists of a thin layer heater sandwiched between two identical samples of the same material and thickness. To design the optimal experiment for the simultaneous estimation of k and C, a complex model accounting for both thermal inertia of the heat source (thin heater) and imperfect thermal contact occurring at the heater-sample interface is suggested. In particular, the former is considered through the volumetric heat capacity of the heater modelled as a lumped body, while the latter through a surface contact resistance Rc, which represents another parameter to estimate.
Once the temperature field within the sample for an unlimited heating period is known [2], a finite heating period can be considered by applying the superposition principle. Also, to make a comparison available, other models commonly used in the specialized literature to describe the thermal behaviour of the specimen (neglecting the disturbances related to the heater thermal inertia and imperfect contact) are discussed.
Also, a sensitivity analysis requiring the computation of the scaled sensitivity coefficients of temperature is performed. Then, the optimal experiment for the simultaneous estimation of k, C and Rc can be designed using a D-optimum criterion [3]. In particular, three experimental variables are investigated: the optimal heating duration, the optimal experiment duration and the optimal temperature sensors locations. The expected standard deviations of the estimates when performing the optimal experiment are also computed. Finally, ordinary least square estimation procedure is used for several numerical simulations of the optimal experiments (under different models) involving a specimen made of Armco iron. It is shown that the optimal heating duration and the optimal experiment duration increase with the thermal inertia of the heater and the contact resistance. The complex model accounting for both the heater thermal inertia and the contact resistance allows k, C and Rc to be estimated accurately.

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Optimizing an optimization method: an application to image deblurring

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In this talk we propose a novel neural network to approach the image restoration problem [1]. This architecture is inspired from an interior point proximal optimization algorithm, capable of imposing useful constraints on the sought solution [2]. In particular, the network is composed of proximal steps alternated with convolutional structures that are able to estimate in an automatic manner the involved parameters, such as the regularization parameter, the steplength and the barrier parameter. This is one of the advantages offered by the proposed network with respect to variational methods traditionally employed in image restoration, for which the choice of parameters is performed either empirically or with suboptimal techniques. Also, numerical experiments for image deblurring/denoising show that our network trained in a supervised fashion is much faster and leads to a better restoration quality than standard optimization methods.

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An Ensemble Kalman Filter-based methodology to estimate the inflow to an ungauged river section

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Despite the great importance of knowing the discharge time series along an open channel course, frequently very few stations are equipped to measure water levels over time and have a reliable stage-discharge relationship useful for obtaining the corresponding flowrate. If the discharge hydrograph is required in an ungauged section downstream of a gauged site, well known forward routing techniques can be applied. On the contrary, when the only available information is collected downstream of the ungauged site of interest, a reverse flow routing procedure is a valid alternative. We applied an Ensemble Kalman Filter based method, namely the Ensemble Smoother with Multiple Data Assimilation (ES-MDA) to solve the reverse flow routing problem. ES-MDA[1] is an iterative data assimilation method that updates the unknown parameters (time-discretized upstream hydrograph in this study), based on the knowledge of observed data (downstream hydrograph or water levels observed at specific times) and a given forward model that relates parameters and observations. We coupled ES-MDA with a one-dimensional forward hydrodynamic model able to accurately describe the flow propagation in a river reach. The procedure is tested by means of a synthetic example, since it allows the comparison between the results of the inverse algorithm and the reference solution [2], and then we applied the methodology to a real case study. Different settings of the inverse algorithm have been investigated and the covariance localization and inflation techniques have been implemented to reduce the ensemble size and to better address the nonlinearity of the forward problem. The results of the synthetic case show that the proposed procedure can accurately reproduces the inflow hydrographs (the Nash-Sutcliffe efficiency criterion is 99.98%) with errors in the estimation of the inflow peaks less than 0.3%. Moreover, the modifications introduced to the original ES-MDA method allow a substantial reduction of the total number of forward model runs and therefore of the total computational cost. In the real case study, we obtained results fully consistent with the available observations and the considered

river reach.In summary, the modified ES-MDA method is able to solve the reverse flow routing problems with performances comparable to those of other optimization techniques available in the literature [3] but with a substantial reduction of the total computational cost.

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Image processing with neural networks

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Traditional methods for image processing (i.e. image denoising, deconvolution, segmentation, or image reconstruction from projections) are nowadays improved or substituted by neural networks, which exploit large data sets for learning image features. In this talk we will consider the particular task of X-rays Computerized Tomography (CT) image reconstruction from projections and we will present some recent techniques using neural networks. CT images are widespread not only in medicine, but also in industry and cultural heritages to visualize the internal structure of organs or objects.

Thermographic evaluation of surface fractures in concrete

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The presence of cracks is a determining factor for the deterioration of reinforced concrete structures. Laser Spot Thermography (LST) is a fast and contactless technique which allows cracks classification according to depth. A survey of recent computational procedures in LST is presented here: 1. Beta-tool: an analytical relation between the thermal gap across the crack and the unknown depth of the defect is derived from a heuristic form of the temperature at the concrete slab surface.
2. Decomposition: the temperature of the damaged specimen is represented as the sum of a term (with known analytical form) due to an infinite virtual fracture and the solution of an initial boundary value problem for the heat equation on one side of the fracture (i.e. on a rectangular domain). The depth of the fracture is a variable parameter in the boundary conditions that can be estimated from additional data.
3. Reciprocity Gap: this method, based on the mathematical theory of differential operators, leads to the construction of a very "smart" inversion algorithm whose attitude to be used in applicative context is still to be explored.
4. More "standard" methods based on optimization, genetic algorithms and Tikonov regalarization. Whatever method we use, we are able to study shallow fractures only (no more than 15 mm deep). Fractures identified as deeper than 15 mm require further specific analysis.

Inverse heat transfer analysis of pulsating heat pipes for space applications

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In the last 20 years, the industry has become more and more severe with regards to thermal management. Specifically, the cooling of electronic components is nowadays considered a technological challenge due to the continuous miniaturization of chips, coupled with ever-increasing amount of power generated during their operations. This is valid not only on ground, but also for space applications, where the design of thermal systems is even more challenging due to the number of constrains in terms of compactness, durability and the need to dissipate efficiently heat in microgravity conditions too.
Pulsating Heat Pipes (PHPs) are relatively new two-phase passive heat transfer devices that aims at meeting all these requirements. Their advantages, such as compactness, flexibility, the ability to work without an electrical energy input and the versatility to work in weightlessness are promising. Despite of such significant advantages, the PHPs' governing phenomena are not yet completely fully understood. To analyze and deeply understand the fundamental principles of their thermal behavior, many studies have been carried out in the last years.
However, almost all the tests performed with the purpose of studying the thermal working principles of PHPs, concerned the analysis of the heat transfer rate averaged over the whole heat exchange area (evaporator or condenser) or the study of the overall thermal resistance of the system. This simplified approach, comes from practical difficulties of local measurement of the heat flux through the internal wall surfaces. For instance, the sensor implementation is difficult due to the size of the probes and the poor accessibility. Nevertheless, the understanding of local thermal characteristics is of primary importance for the PHP design. Hence, data about the local convective heat flux over the heat transfer surface could provide a deeper insight into the heat transfer augmentation mechanisms and the causal relationship between the induced pulsating field and the convection enhancement effect.
The present work aims to start filling this gap by presenting a procedure[**?**] to estimate the local heat flux inside pulsating heat pipes from the infrared images, acquired on the external wall surface of the pipe; these images become the input data for the inverse heat conduction problem in the solid domain.

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Recovering the contaminant source location and its release in a water distribution network

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Water distribution systems are a core infrastructure in people lives. Intentional or accidental contaminations can threaten their health and have to be detected in the shortest possible period to reduce damages. Early warning systems should be put in place to detect both the source location and the release intensity.
How to identify a contaminant source from concentration observations at monitoring locations can be cast as an inverse problem for which different approaches are available, e.g.[1]. In this work, the ensemble Kalman filter (EnKF) is chosen, e.g. [2].
The EnKF is demonstrated in the Anytown network, which is a benchmark in water supply system analysis. The network is subject to a time variable demand in which a contaminant is introduced. The contaminant source is determined from concentration observations made in time at different frequencies. Measurement errors on concentration and estimation errors on the base demand are included to make the test case more realistic.
The case study deals with a release with uniform intensity that is originated from a source located in a node of the network. The sensors of the network register concentration values in time with a certain frequency. The scheme adopted for concentration sampling considers a malfunctioning of the sensor network, which introduces observation errors, and it is also assumed that sampling starts sometime after the release has occurred and the contaminant has already spread through the pipeline systems.
Different locations of the source, frequency sampling and acquisition data period have been considered. The results of the tests are very satisfactory for all the examined cases, in spite of the limited number of the ensemble members (48 realizations) and the non-stationarity of the concentration field, due to the intrinsic functioning of the network.
Results show that for the Anytown network, an early detection of solute concentration (within 60 minutes from the release beginning) together with a sampling frequency of 30 minutes is sufficient to accurately detect the source parameters in a short time. If the monitoring starts later, e.g. 3 hours after the beginning, the identification takes a longer time.

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IS-2
Mathematical problems in automation and robotics

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The minisymposium aims to illustrate some mathematical problems arising from industrial applications. The first three talks are related to motion planning for automated vehicles. In particular, the first talk considers the numerical solution of the HJB-equation for path planning. The second one discusses speed planning for mobile vehicles along prescribed paths. The third talk presents problems of path and trajectory planning in industrial AGVs. The fourth talk is related to sensor calibration in industrial AGVs. The last two talks are related to optimization problems of industrial relevance. Note that all problems discussed in this section have emerged from industrial collaborations.

Fast numerical solution of optimal control problems for switched systems: an application to path planning

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We consider a finite element approximation of the Hamilton-Jacobi-Bellman equation for the optimal control of switched systems in which the switchings from one system to another are governed by a finite state machine. In particular, we show that the obtained finite dimensional problem belongs to a special class of problems that we already studied in a previous work. This reformulation allows to exploit the iterative algorithm introduced in [1], and further studied in [2], for efficiently solving the problem. As an application, we present the problem of generating parking maneuvers for self-driving vehicles. We model the vehicle as a switched system in which each switching represents a change to a different type of motion. For instance, each change between forward and backward motion is associated to a switching cost. In this way, this added cost penalizes the maneuvers with a larger number of direction changes allowing us to obtain maneuvers that are simpler, more human-like and with a limited number motion switchings. Note that a similar problem is solved in [3]. Here, we generalize the contribution of [3] by using four different models for the finite state machines associated to the vehicle and by placing the specific application of the parking maneuver into a more general framework. Finally, we present the parking maneuvers generated using the aforementioned models for two typical urban parking scenarios.

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An online jerk-bounded velocity planner: a trade-off between safety and efficiency

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In recent years, the number of collaborative applications in industrial contexts involving robots and humans is growing. The robotic systems, which were originally confined in specified compartments of the warehouses, are currently free to move around the whole plant. Collaborative environments give rise to several issues concerning safety aspects. The safeness of coworkers and of the overall plant must be assured, despite it is antithetic with respect to efficiency. The target of the work presented in this talk is to propose a planning strategy which assures that both objectives are simultaneously satisfied, i.e. the plant productivity is maintained and improved through a smart trajectory planner which also guarantees safe working conditions. In the considered industrial framework, the velocity planning problem covers an important role since, for efficiency reasons, traveling times should be minimized, while the coworkers safeness must be always guaranteed; hence, the velocity function must be obtained by solving online an optimization problem, in order to promptly react to unforeseen situations. Autonomous vehicles are equipped with certified laser sensors, which are used to guarantee the safeness of the human workers and of the plant. The information provided by such laser sensors is used to obtain an analytical representation of a safety constraint, which then becomes part of the optimization problem. Generated trajectories must also comply with the kinematic limits of mechatronic systems, so that additional constraints must be accounted for in the optimization process. For example, the longitudinal velocity and the norm of the lateral acceleration must be bounded. The velocity planner proposed, which was developed in the framework of the SAFERUN European project [1, 2], is conceived to satisfy the above mentioned requirements. In fact, it is able to compute a velocity reference which satisfies the safety and kinematic constraints. Furthermore, it also limits the longitudinal jerk, in order to reduce vehicle solicitations and load stresses. In addition, the velocity reference is always computed in real-time, while the vehicle is moving. Finally, the proposed velocity planner has been tested in a real plant, under actual operative conditions [3]. The planner proved its reliability and it is still used in the industrial plant which was selected for the experimental validation.

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Faster than a Forklift, Safer than a Car

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Robotics and controllers have been greatly improved in recent years and the industry is fol- lowing these developments. As Elettric80, a main protagonist in the automation of industrial plants and warehouses, many of our efforts are spent in obtaining the best performances from our automated plants and, as the R&D department, we have been tasked with the mathematical formulation of optimization problems and their solution. During the

rst part of this talk, we will discuss the steps taken to de

ne optimal and sub-optimal trajectories for our vehicles, using non-linear problems with mixed target func- tions and we will show the results achieved. This process, carried out with the cooperation of the University of Parma, started from the geometric line to be followed [3] and the ve- locity planner [4] to obtain the best feasible traveling time. Then it moved to the safety of these paths, with respect to static obstacles [6] and with respect to unforeseen objects detected by on-vehicle safety devices. In the second part, we will introduce our next goals for path-planning in industrial plants. The

rst goal is to continue using the mixed target approach, applying it in the reduction of energy consumption, as it was done in [7] and [5]: this would improve the general efficiency of our vehicles, the functioning costs of plants and the mechanical stress on the vehicle components. The second goal is to design a new and faster path-planning tool to be used in active plants, so that a vehicle can travel around an obstacle if it is in its way. Another goal is focused on the coverage of a portion of the warehouse area, as in [1] and [2], and combine it with our optimization problems, so to move a vehicle in all points of an assigned area.

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Simultaneous Calibration of Odometry and Sensor parameters for Industrial AGV

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Automated Guided Vehicles (AGVs) are commonly used to transport goods and to efficiently handle logistics of industrial warehouses. Accurate localization and navigation of AGVs depend on the correct assessment of their odometric or intrinsic parameters and of the position and orientation (or extrinsic parameters) of the exteroceptive sensors used for localization. Incorrect calibration causes systematic error and displacement of the AGV when reaching operation points. This work presents calibration problem in a mathematical perspective and illustrates a method for the estimation of both intrinsic and extrinsic parameters. The proposed approach follows the principle presented in [1] for differential drive kinematic model and that have been applied to three and four wheel models [2, 3] commonly adopted for industrial AGVs. This approach compares the trajectory measured by the on-board sensor and the expected trajectory. To observe trajectories, the robot must be equipped with on-board sensors enabling egomotion estimation like laser scanners. These different measurements are encoded by a set of constraints among intrinsic and extrinsic parameters, which are exploited to perform least-square estimation. The kinematic models addressed in this work include Tricycle, Ackermann and Dual Drive. Tricycle AGVs have three wheels with the front one actuated, whereas Ackermann and Dual Drive have both four wheels, but different con

guration of actuacted and steering wheels. Due to modelling differences, the procedures for their intrinsic calibration are slightly differents, which mostly result in linear relations except for the asymmetric model of Tricyle. The four wheels models present observability issues, which require preliminar manual alignment of the front wheels of the robot. Closed-form solutions have been derived for all the for- mulations. The intrinsic calibration equations accurately describe the real motion of AGVs under the assumption of wheel alignment and negligible wheel slipping. The presented extrinsic calibration algorithm estimates the pose of the sensor once the kinematic parameters have been obtained. The proposed closed-form solutions are suitable for implementation on PLCs (Programmable Logic Controllers) used for industrial AGVs. The methods have been tested in real plants and enable full estimation of calibration parameters in about 10 -15 minutes. Repeated calibration trials have exhibited numerical stability and precision in the values of computed parameters. Positioning tests on actual AGVs have also demonstrated the higher accuracy of the proposed calibration algorithm w.r.t. manual calibration.

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A task and crew scheduling problem to optimize distributed services in hospitals: a case study at Coopservice

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One of the key operational processes in hospitals concerns the organization of the cleaning tasks that need to be performed by workers regularly, to maintain the necessary level of cleanliness and sanitary security. Scheduling cleaning tasks is a complex problem [1] that belongs to the general field of personnel scheduling [2]. Our interest originates from the activity of Coopservice, a large third-party service provider. However, the problem can be generalized to a large variety of services that need to be performed in a distributed manner across large facilities. To solve the problem, we need to create groups of cleaning tasks, assign them to different days and hours in the considered planning period (e.g., a month), and then allocate them to the available workers to minimize costs while satisfying given services requirements. To this aim, we propose a hybrid three-step approach based on the combined use of heuristics and mathematical models. As input, we are given a set of rooms, each with an associated set of cleaning tasks and a level of sanitary risk, and a set of workers. First of all, to allocate the cleaning tasks for the rooms to the days of the period, we invoke a generalized assignment problem and solve it as a mixed-integer linear program (MILP). Second, for each day, we create a sequence of cleaning tasks across the rooms by solving a Vehicle Routing Problem with Time Windows (VRPTW). Due to its NP-Hardness, we solve the VRPTW with a heuristic, obtained by invoking a savings-based algorithm [3, 4]. Third, the task sequences we created are assigned, in a crew rostering problem, to the available workers while satisfying several constraints. For this step, we use another MILP embedded into a rolling horizon procedure. This defines which worker will execute which sequence in which day, and how much this will cost. The three-step approach has been tested on a real-world hospital operated by Coopservice, and the results that it obtained have been positively validated. The approach can help the organization in generating and testing a large variety of solutions in a fast way. It allows obtaining solutions that not only have low cost but also better reflect the workers' needs. Furthermore, we obtain full coverage of the cleanliness requirements of the hospital, reducing the level of sanitary risks.

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A Decision Support System for Attended Home Services

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This Talk presents a decision support system (DSS) developed to solve a practical attended home services problem faced by Iren Group, an Italian multiutility company operating in the distribution of electricity, gas, and water. The company operates in several regions across Italy and aims to optimize the organizational system appointed to dispatch technicians to customer locations, where they perform installations, closures, or maintenance activities within time slots chosen by the customers. Indeed, attended home services (AHS) are service delivery systems in which a supplying company and a customer agree on a time window during which the customer will be home and the service will be performed [1]. Typically, the optimization of AHS requires solving a two-stage problem, combining appointment scheduling and vehicle routing [2]. The DSS uses historical data and helps operations managers in performing a number of strategic decisions: grouping municipalities into clusters; designing sets of model-weeks (i.e., matrices of resources distributed among five working days and eight daily time slots of one hour, that define the capacity allocated to a given cluster); evaluating the obtained solutions by means of a dynamic rolling horizon simulator; and providing as output several key performance indicators, as well as visual optimized technician routing plans used to analyze different scenarios [3]. The system integrates simple machine learning techniques, mathematical models, heuristic algorithms and simulation methods that have been specifically developed to take into account different quality of service levels, in accordance with the directives imposed by the authority that regulates the Italian market. Computational experiments carried out on data provided by the company confirm the efficiency of the proposed methods, both in terms of effort reduction and routing costs saving (10% on average) [4].

Additionally, the DSS constitutes a powerful tool that can support the company in the strategical evaluation of existing and potential market opportunities.

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IS-3
Mathematical approaches for Civil Engineering

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Over the last few decades, computational methods in civil engineering have grown to become an essential tool for engineers. As a consequence, nowadays most of the engineering problems can be solved with computational methods based on mathematical models.
The present mini-symposium aims at providing a forum for an in-depth discussion of mathematical and numerical methods for solving problems in civil engineering (both for modeling and experimental work).

Second-kind self-similar solutions for power-law fluids gravity currents in converging channels

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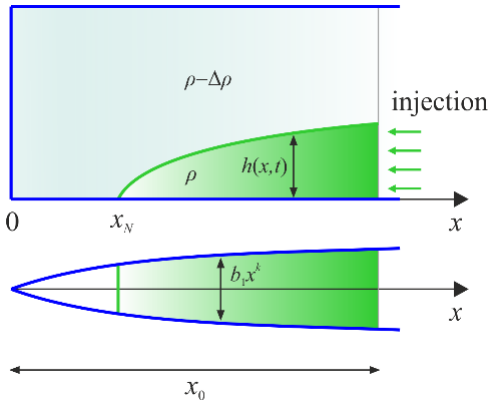
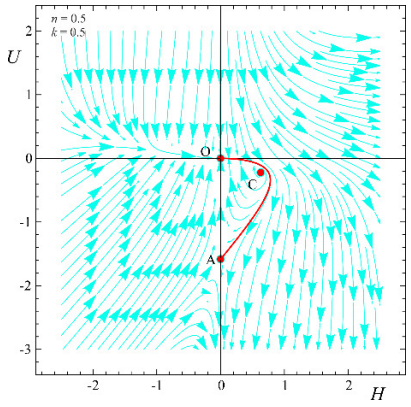
We report the theoretical and experimental results on converging gravity currents (GC) of a Ostwald-deWaele fluid in homogeneous porous media, that may be described by self-similar solutions of the second-kind. Dimensional analysis is not sufficient to describe the problem in terms of the classical self-similarity of the first kind (see [2]) since a new length scale is introduced, rendering the general problem subject to partial similarity ([1]). The second-kind self-similar solution is found with a phase-plane analysis, and then compared to experiments conducted in a wedge filled with homogeneous glass ballotini. The talk will focus on (i) an overview of the general problem of self-similarity; (ii) the description of the methodology as applied to the specific problem of converging GC; (iii) the description of the experiments and the comparison between theory and experiments. Perspectives and future activities are described for Herschel-Bulkley fluids.



Schematic of a converging gravity current in a channel with varying gap thickness $b_1 x^k$.



Phase portrait of the differential problem for a shear-thinning fluid with fluid behaviour index $n = 0.5$ and $k = 0.5$.

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Constitutive Model for Bituminous Stabilized Materials and Modelling of Cold Recycled Pavement Layers

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Cold recycling techniques are becoming more and more popular everywhere in the world, as it is well proven that bituminous stabilized mixtures (BSM) are sustainable both from an environmental and economical point of view [1, 2, 3]. There have been limited studies focusing on mechanical properties of those mixtures and on their performance with respect to the service lives of pavement structures with in-place recycled layers. For this reason, this research focuses on the design of a constitutive model for different types of BSMs and on the modeling of flexible pavement structures with BSMs as base layers. A 3D Elasto-Plastic model was created using ABAQUS software in order to calibrate and validate the constitutive mechanical properties of the different cold mixtures, the outputs obtained were then used in a multilayer axisymmetric 2D model for traffic simulation. The modelled structures were subjected to a cyclic loading of 0.1 second with 0.9 second of rest period. The load applied on the structures has been calibrated in order to have a comparable effect to the real tire pressure experienced by the structures under traffic. Rutting evolution curves until a failure threshold value of 20 mm have been developed and the results have clearly shown how the BSM as a base layer can provide superior or comparable performance in terms of rutting as compared to granular virgin material.

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An ADER DOT solver for augmented Shallow Water Equations and its application to urban flooding

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In the framework of flood risk management, the development of fast, stable and accurate numerical models for flood simulation represents a crucial task to increase the resilience against those natural disasters [1]. Focusing on urban flooding, the Shallow Water Equations (SWEs) with porosity can describe in a synthetic way the effects exerted by buildings using relatively coarse grids (with limited need of computational resources), thus avoiding the use of high-resolution meshes otherwise needed to resolve the flow in urban areas. This work presents a novel high-order approximate Riemann solver capable of treating discontinuities in the porous and terrain fields, in the framework of the 1D SWEs with porosity. To achieve this goal, a new set of augmented well-balanced governing equations, which allow treating the effects of the source terms as additional non-conservative fluxes, is derived. Following the path-conservative DOT scheme [2], a novel numerical approximate Riemann solver is developed. The implementation in the ADER framework, together with a Total Variation Diminishing reconstruction, allows achieving a non-oscillatory second order accurate scheme in both space and time. The proposed numerical solver is intrinsically entropy-satisfactory and it preserves the quiescent flow condition over a non-flat bottom and with a non-uniform porous field (C-property). Finally, the numerical model is validated against a selection of Riemann problems (e.g. the dam-break case shown in Fig. 1), which develop across porosity discontinuities and bed steps, including shocks and transonic rarefactions.

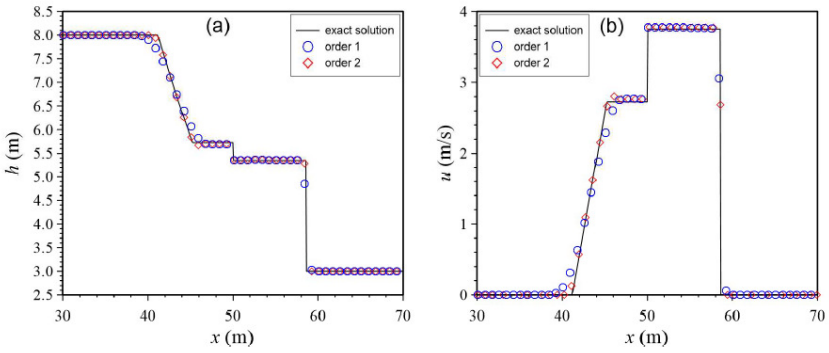

Figure. Dam-break test over a flat bottom. At time $t = 0$ water is at rest with different depths at the left (8 m) and right side (3 m) of $x = 50m$, where a jump in porosity is present (0.9 at left, 0.7 at right). The figure compares the exact and numerical solutions at $t = 1$ s for water depth (a) and velocity (b).

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Optimal Solution in the Shakedown of Frictional Contact Problems

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During their lifetime, structural components are often subjected to a combination of loads of various nature, including thermal actions and vibrations which result in time variable stresses. When components that are in mutual contact are subjected to cyclic loading, they are exposed to the detrimental effect of frictional slips, but they might also develop a favorable occurrence, where slips cease after a few cycles. Due to the similarity with an analogous phenomenon observed in the theory of plasticity, this event is commonly known as frictional shakedown [1]. Methods are sought to provide a reliable and efficient assessment of systems under variable loads, primarily with the aim of finding the load limit below which the shakedown is guaranteed. Employing the so-called direct methods derived from the theorems of limit analysis, we consider a specific class of linear programming problems formulated for the shakedown of elastoplastic systems with non-associated flow rule [2]. Indeed, Coulomb's frictional law does not obey the normality rule, save for the specific case when normal and tangential reactions along the contact interface are uncoupled [3]. In this work, we illustrate the linear programming algorithm which enabled us to derive the shakedown limit load from the solution of a constrained optimization problem [4, 5, 6]. Specifically, we have considered two- and three-dimensional elastic systems, containing a single conforming contact interface, and subjected to static and cyclic loading. The full loading history is replaced by a convex load domain, so that the solution consists in finding an optimal distribution of frictional slips which maximizes a positive multiplier of the load domain. Moreover, the three-dimensional solution is based on an approximation of the frictional law by means of a piecewise linearization of Coulomb's cone. The obtained shakedown loads compare favorably with those derived from traditional, more cumbersome, step-by-step simulations.

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Cover cracking in carbonated RC elements: a phase field approach

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Corrosion of steel reinforcement bars (rebar) has always been an important issue for the reinforced concrete (RC) structures. Being one of the most common deterioration mechanisms, corrosion severely affects the serviceability and durability of the structure as the steel reinforcement suffers from a reduction of the cross section and mechanical properties. Additionally, due to the steel oxidation process, residual material is formed and the volume occupied by the reinforcement increases, leading to cracking and spalling of the concrete cover.

Concrete carbonation process is coupled with the phase-field approach to brittle fracture to simulate the corrosion of rebar and the subsequent cracking phenomenon. First, a Fickian law is used to describe the carbon dioxide (CO_2) diffusion within the concrete which leads to a generalized corrosion process. Eventually, the volume expansion which affects the portion of rebars subject to corrosion is considered, and the cracking phenomena induced by the stress state within the surrounding concrete are captured via the phase-field approach to brittle fracture. Numerical simulations are performed and validated against experimental examples from literature, presenting a phase-field strategy capable to describe the cover cracking of corroded RC beams.

IS-4
New Trends in Finance Industry

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The financial sector is continuously changing and heavily influenced by the global financial markets. The latest financial crisis has highlighted the need for a more scientific and rigorous approach to the problem of pricing and risk control. Now more than ever, financial institutions need to perform under strict regulation and evolving market conditions. The requirements for companies operating in the financial sector are increasingly sophisticated and complex.

This minisymposium combines multi-disciplinary and specialist knowledge of the financial sector with experience in the industry's most significant cases, taking advantage of advanced statistical, mathematical and numerical techniques and fast computer systems nowadays available.

Non-parametric risk management using conditional GANs

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A key problem in financial time-series modelling is that we can only observe one realization of the complex stochastic processes governing the market. Modelling such distributions is crucial for many tasks, e.g. to assess the risk of portfolios and investment strategies by computing the Value at Risk (VaR), a common risk measure and often required by regulators. Parametric methods for estimating the VaR rely on simple known distributions such as the Gaussian, however we can overcome the need for assumptions on the distribution functional form through the use of deep generative models, able to exibly learn a generating distributions directly from the data. Generative Adversarial Networks (GANs) have

rst been applied to computer vision tasks[1], typically the generation of realistically-looking images, however in recent years they have been increasingly used in other domains and on non-visual data[2]. In this work, we apply GANs to the problem of modelling

nancial timeseries and estimating the VaR [3] and compare this approach with a traditional GARCH baseline[4]. Our results show that GANs can potentially become a promising candidate for risk management in the future.

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Valuation Adjustments in Practice

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The financial crisis started in 2007 has shown that any pricing framework must include from the very beginning the possibility of default of any market player. Therefore, derivative valuation and risk analysis have moved from exotic derivatives managed on simple single asset classes to simple derivatives embedding credit risk and new, or previously neglected, types of complex and interconnected non-linear effects. The detailed analysis of how a trade is really implemented between two counterparties in the market is a requirement to track all the possible costs and risks. Derivative valuation is adjusted to include counterparty credit risk and contagion effects along with funding costs due to collateral posting, treasury policies, and regulatory constraints. A second level of complexity is produced by moving from a single trade to the whole bank portfolio. Aggregation-dependent valuation processes, and their operational challenges, arising from non-linearities are discussed both from a mathematical and practical point of view. By following the developments of recent literature, an arbitrage-free valuation framework is developed for bilateral counterparty risk adjustments, inclusive of wrong-way and contagion risks, collateralization and funding costs. The resulting valuation equations take the form of semi-linear PDEs, or backward SDEs, depending only on real market rates and processes, and no longer on unobservable risk-free rates. Collateralization is described starting from the day-by-day operations followed by the counterparties to implement the credit support annex. Segregation and re-hypothecation policies are discussed both for bilateral-traded and centrally-cleared deals along with funding implications. Margining and funding costs are included into the derivation of pricing formulae, along with their relationship with hedging strategies and liquidity policies. Fund transfer pricing procedures driving the business strategies of the bank are presented and their impact on funding costs is described.

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RFR Made Easy

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It is a fact that the issue of the new risk free benchmark rates (RFR) is becoming paramount. Besides offering a new full framework on reference rates, such a change is deemed to introduce havoc in software products that deal with the banking book. Moving from forward looking benchmarks to backward looking is carrying lots of consequences. With a well developed derivatives market and a specific regulation establishing how to extract forward rates from discounting curves, it will still be possible to maintain the existing framework. Harder is the situation where optionalities are involved as would be the case for most loans with a cap or floor condition. For example, most of the indications coming from the SONIA (British Pound) market seem to endorse a practice based on flooring the daily rate rather than the final compounded rate. This situation can not be mapped in today's practice. The goal of this work is to device an empirical procedure to minimize the impact of these modifications on the existing software products that deal with the banking book. This is not a trifle issue given that we talk about very complex software systems and major changes in the approach would turn out to be a significant cost.

IS-5
Math 2 Product

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Mathematical modelling and numerical techniques have gained an increasing importance in the simulation of industrial problems. The efficient use of these models and methodologies is strongly transforming the ways of planning and designing research strategies.
The goal pursued by this mini-symposium is twofold. On the one hand, cases of successful interaction between mathematics and industry will be presented in accordance with SIMAI mission and vision.Special emphasis will be devoted to the benefits provided by the transfer of knowledge and technology in different fields of industrial applications. On the other hand,new emerging technologies in computational science and engineering

will be dealt with to foster cross-fertilization of ideas from academic research groups to real-world problems, tackled in research and development industrial centres.

Distortion prediction and compensation of industrial components by Selective Laser Melting

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Additive Manufacturing by Selective Laser Melting is constantly growing as an innovative technology for the production of mechanical, aerospace, automotive, and biomedical components. However, the thermo-mechanical phenomena occurring during the process may lead to severe production issues such as geometrical distortions, cracks, and failures. In the present work, we use Amphyon software to set up a fast, efficient, and complete framework to predict and compensate distortions in components produced with Selective Laser Melting technology. We adopt an easy and manageable experimental test to calibrate inherent strain for the simulation of a geometrically complex industrial component, manufactured with slender support structures. Predicted numerical distortions are used to calculate a compensated model. The computational scheme is validated through comparison between a micro Computed Tomography reconstruction of the additively manufactured compensated component and the nominal geometry counterpart. Particular attention is given to the meshing strategy, focusing on the necessity of a detailed representation of the intersecting zones between component and support structures. Finally, we present a comparison between computational times scored on CPUs and GPUs computing. We prove that GPUs computing gives a consistent advantage in terms of computational times reduction.

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Design of patient-specific orthopedic insoles: a multiscale topology optimization approach

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Additive manufacturing has been innovating the industrial production thanks to new possibilities in terms of achievable designs, production costs and customization. Moreover, the use of lattices, graded metamaterials and specific infill patterns has contributed to optimize the target performances of the final products, independently of the field of application.

We present an efficient coupling of micro- and macroscopic topology optimization in a multiscale framework. The procedure is divided into two steps. First, we employ an adaptive topology optimization algorithm, microSIMPATY, combining the asymptotic homogenization theory with the SIMP method for topology optimization [1]. This method yields a dictionary of microstructures retaining target homogenized mechanical properties. As a second step, we devise the optimal allocation of such microstructures inside a macroscopic domain in order to comply with some given prescriptions on the final mechanical performances [3].

In this presentation, we introduce the multiscale approach in a generic setting and we customize the numerical simulation, verification and validation phases to the design of patient-specific orthopedic insoles [2].

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Adjoint Optimisation Methods for Automotive Applications

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Adjoint optimisation is an exciting and fast-growing field that has many applications in the automotive industry. In this paper we focus on the usage of adjoint for the optimisation of aerodynamic performance in road vehicles and automotive components. While adjoint methods have come to the attention of mainstream Computational Fluid Dynamics (CFD) through inclusion in prominent commercial codes, most of the available tools are severely limited, precluding productive use in this field. In this work we detail a methodology that is based on the continuous adjoint method and is implemented in an Open-source framework. While more mathematically demanding in terms of its derivation, the continuous adjoint method requires fewer resources (memory and computational time) than the alternative discrete approach common to mainstream CFD codes.

In the work detailed here, the continuous adjoint formulation method was successfully applied to various automotive engineering optimization problems, including both internal and external aerodynamics problems. Given the emerging trends in vehicle drive trains, improvement of aerodynamics has become much more important to overall fuel consumption and vehicle efficiency. The continuous adjoint promises an effective and efficient method for tackling this problem.

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Graph convolutional neural networks for fast, accurate prediction of material properties for solid solution alloys using open-source datasets

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We present a deep learning (DL) approach to produce highly accurate predictions of macroscopic physical properties of solid solution binary alloys and magnetic systems. We use graph convolutional neural networks (GCNNs) models to predict the total energy. GCNNs abstract the lattice structure of a solid material as a graph, whereby atoms are modeled as nodes and metallic bonds as edges. This representation allows GCNNs to naturally retain geometrical information about the structure of the material, thereby eliminating the need for computationally expensive data pre-processing required with standard DL approaches. We train GCNNs on open source ab-initio DFT data for iron-platinum (FePt), and silicon-steel (FeSi) that has been generated for varying sizes of the lattice structure by running the LSMS-3 code, which implements a locally self-consistent multiple scattering method on the supercomputer Summit at the Oak Ridge Leadership Computing Facility (OLCF). We find that the final attainable accuracy of GCNNs is an order of magnitude better than that of standard DL approaches.

The application of reduced order models to computational fluid dynamics simulations for ship design

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The present contribution will discuss the application of Reduced Order Models (ROMs) to systems of parameterized Partial Differential Equations (PDEs) arising from Computational Fluid Dynamics (CFD) applications in ship design. Typical virtual prototyping design cycles require that several CFD simulations based on PDE problems are solved, modifying the input parameters until satisfactory or even optimal values of the resulting output parameters are obtained. Despite the last decades remarkable growth in computational power, the many query scenario described might lead to severe computational costs, which can be mitigated through the acceleration of each CFD simulation. Reducing the computational cost of the PDE problem associated with each CFD simulation, ROMs represent an interesting opportunity to speed up the entire ship design cycles, test more configurations, and even consider non conventional and potentially interesting solutions. We will first discuss the application of Dynamic Mode Decomposition (DMD) for the acceleration of ship hydrodynamics simulations based both on fully nonlinear potential flow and Reynolds Averaged Navier–Stokes (RANS) models [1]. Then, we will discuss the effectiveness of non intrusive ROMs in the approximation of both velocity and pressure fields resulting from Large Eddy Simulation (LES) computations for the hydroacoustic design of ship propellers [2]. More specifically, in such case we will consider the application of both DMD with mid cast and Proper Orthogonal Decomposition (POD) with interpolation. We will then present an intrusive POD Galerkin projection scheme and its application to turbulent RANS simulations of the unsteady flow past crossflow cylinders [3]. Finally, we will provide some detail on shape parameterization algorithms.

Such algorithms are a key ingredient in design and optimization cycles, as well as in the development of ROMs. In fact, on one hand they allow for mapping shape modifications to variation of numerical parameters required as input by the PDE systems solved in the design cycles. On the other hand, they are used to retain the mesh topology throughout the parameterized simulations, which is an important requirement of the ROMs development. All the ROMs and shape parameterization applications presented are carried out at mathLab, the applied mathematics laboratory of the International School for Advanced Studies at Trieste, Italy, in the framework of several industrial research projects.

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Reduced order modeling of a packaging system

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The assembling of liquid food packages involves very complex physical phenomena related to the structural response of materials and to the interaction between moving parts and the fluid, so the aid of simulation tools is essential for the design and the control of the filling machines used in the process. When it is necessary to obtain results in a short time, such as in the preliminary phase of a project and in Uncertainty Quantification or parametric studies, state-of-the-art numerical solvers often are not the best choice because, even though they can compute accurate solutions also for strongly coupled problems, on the other hand they are computationally very expensive. In these cases it is better to rely on efficient reduction strategies, which are the topic of the present talk. We successfully applied them in an industrial collaboration with Tetra Pak, that represents one of the major companies in food processing and packaging solutions in the world. We focused on Proper Orthogonal Decomposition and on Reduced Basis Method in particular. Regarding the latter technique, we considered an implementation which is effective to treat highly

nonlinear parameter dependencies and a suitable version where the complete construction of reduced-order operators is not required.

IS-6
Mathematical methods for data science: business case studies

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Data Science is an interdisciplinary field that uses scientific methods, processes, algorithms and systems to generate complex models from data and transform them into information of quality and knowledge, available to politics or private individuals. It brings together researchers in computer science, mathematics, statistics, machine learning, engineering and social sciences. Thanks to new advanced data analysis algorithms, changes in connectivity, increased network computing solutions, increasingly powerful microprocessors and increasingly less expensive data storage, Data Science applications have been exponentially accelerated in the last decade. Data analysis requires transversal skills in which information technology and mathematics play a central role. In particular, the latter provides a universal language to abstractly describe the models and study their statistical properties, providing advanced computational techniques to solve the forecasting algorithms. The aim of this symposium is to collect several case studies from companies in the Emilia-Romagna area in which statistical approaches, machine learning algorithms and numerical optimization methods are exploited to practically solve concrete real-world problems, with the aim of comparing different strategies, sharing common knowledge and presenting open questions and challenges for applied mathematicians devoted to technology transfer activities.

Robust control of a waste-to-energy facility

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Waste-to-energy (WTE) facilities are electrical power plants that use non-reusable, non-recyclable and non-compostable waste as their fuel. WTE plants follow steam-electric power plants design, where fuel combusted in the furnace heats and vaporizes water in the pipes, increasing its enthalpy, which is then converted to energy in a turbine. The sizing of WTE plants is such that they can operate at a reasonably wide range of flow rates, to accommodate for the variability of waste entering the combustion chamber. While supplying enough energy to meet demand in the most efficient way, WTE facilities must also obey many operational and regulatory constraints, such as maintaining state variables within safety ranges of working condition, and limiting the emission of un-combusted and polluting fumes. Controlling WTE facilities can be challenging due to the high number of control and environmental variables which influence the system. While this makes forecasting difficult, experience has shown that proportional-integral-derivative (PID) controllers often struggles to meet the many requirements and constraints characterizing the problem. For this reason we resort to a robust model predictive control (MPC) approach [1], where the relevant physics of the plant have been modeled and the control variables are adjusted to meet requirements and constraints within a predefined time window. While the first step of the standard approach of MPC is to analyze the system using impulse response functions, this is clearly not feasible for an on-line power plant. We instead develop a data-driven model using several months of history for the control and state variables of interest, and concatenating a sequence of models spanning linear regression models and multiscale convolutional neural networks [2]. In this talk we will illustrate the modeling strategy employed in order to address the many challenges posed by this system, including long input-output lags, discontinuous sensor readings, operational

noise in the data, very uncertain inputs (e.g. waste heat capacity). The model will be used within the robust MPC cost, meeting multi-objective and multi-constraint requirements. We will finally showcase the integration of the controller in an real on-line WTE facility.

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Machine Learning for automotive cybersecurity

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In the last years, vehicle connectivity is rapidly increasing and, together with it, the need to design and introduce security solutions able to protect the vehicle and all its communication interfaces with the outside. In this scenario the capability to monitor the traffic transmitted over the network connecting all the vehicle Electronic Control Units, e.g. the CAN bus, highly increases the vehicle protection against potential intrusions. While the syntax correctness of transmitted frames can be ensured by static rules and thus classical programming [1], the monitoring of the data semantics requires machine learning strategies [2]. In particular, anomaly detection techniques [3] can be used to build a "normal" vehicle network behavioral model that will act as a reference model for the detection and isolation of attacks, identifying as potential intrusions any deviation of the system from the normal behaviour. In this work we apply Long-Short Term Memory networks to time series [4] coming from data transmitted over the CAN bus and describing vehicle dynamics. A use case is presented where a network, trained on vehicle dynamics data in ?normal? conditions, i.e. without attacks, is able to identify an anomalous behaviour once inferred on data transmitted when a real attack is occurring.

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On how to develop machine learning algorithms for the control of industrial-grade fruit sorting machines

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Nowadays, applications based on Machine Learning are so pervasive that it seems unusual to have non-ML-based solutions. In fact, the story is a bit different and the industry sees only a few ML-based applications operative in production. This dichotomy between what is perceived and what is in reality is due to intrinsic difficulties in developing industrial-grade solutions. The main, and most misunderstood, concept regards the statistical assessment of a ML algorithm. If in a typical visual task an accuracy greater than 99% is considered an academic success (and indeed it could be a success in real medical scenarios too [1]) for industrial manufacturing (think to automotive) a residual error of 1% is an unacceptable burden to manage. Another well-known issue regards the common request by data scientists of huge dataset labelled by hand. This need, if not properly inserted into a clear and planned workflow, discourages a large part of potential adopters into investing time and money into ML-based applications. In this speech, guided by a well-founded statistical and risk analysis framework, we will present a simple but paradigmatic ML solution that has been implemented by us in recent years to automatically control grading and sorting machines in the agri-food sector [2]. Since fruit is a natural product with low cost and wide availability but without conscience and legal rights, we will be able to focus only on the fundamental aspects that should be taken into consideration when planning to provide industrial-level solutions. Unexpectedly, statistical requirements in industry are more stringent in respect to medical ones since every decimal of accuracy has a direct economic counterpart for the end user. In addition, robustness, maintainability and computational efficiency are taken for granted by the end customer while they are intrinsically difficult to manage due to the black box paradigm. A possible approach to overcome these limitations should come from the eXplainable Artificial Intelligence [3] paradigm which will be briefly explored in the discussion.

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Applied machine learning methods: predicting anomalies in a packaging line

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Nowadays industrial automation is a highly researched topic. Industrial machines are almost everywhere and, with the growth of the IoT, many of them are shipped with several sensors which continuously communicate and check for the machine health and status. Being able to gather information from those sensors to autonomously take decisions can bring a lot of benefits to the companies in terms of, e.g., costs and management.

In this work an example of anomaly detection on a multivariate time series, as an unsupervised and supervised machine learning problem, is proposed. We will analyze a packaging production line equipped with a system composed of sensors and cameras. Our goal is to show that the sensing system alone can provide a prediction of the presence of anomalies in the formed packages (briks), while the camera detections will be used only to retrieve the anomaly information of the briks. Moreover, the identification of the causal factors that produced them from a set of observations is also addressed, in the field of anomaly detections in Packaging engineering [1].

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System identification and machine learning for predictive maintenance in industrial application

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Prognosis and Health Management of machine devices and parts is a hot topic in the Industry 4.0 era. In this fashion, automated procedures to evaluate machinery working conditions are essential to minimize downtime and maintenance costs. In this talk, we illustrate the study on how to monitor the decrease in performance of a paper sheet feeder for the packaging industry under heavy-duty cycle operations. The main measurable outcome of such degradation is the increase in clearance among the device moving components.

The core of the approach to this monitoring problem consists in the use of a simple yet efficient diagnosis methodology that can exploit machinery controllers (i.e., PLCs) edge-computing capabilities. Vibration measurements are known in literature to retain information about the system's mechanics. Model-of-Signals, a data-driven approach based on black box system identification, allows to extract that information reliably during machinery working cycle: Accelerometer signals are modelled as AutoRegressive (AR) processes whose coefficients are then considered as features to feed to machine learning algorithms, which are employed to perform severity evaluation of the ongoing degradation. Estimation and prediction are both implementable on-board the PLC, while the learning task can be carried out remotely, in a cloud computing perspective.

The analysis results in an evident correspondence between the measured clearances and the information provided by the combination of AR models and machine learning algorithms. While the application of health indicators to the AR coefficients depicts a trend comparable to the increase in clearance, the machine learning classification algorithms (e.g., Support Vector Machine) provide a valid strategy to inspect the different measured levels of clearance.

The exploitation of AR modelling gives a simple and inherent methodology for feature selection, serving as a foundation of the machine learning stage. We make use of classification algorithms to analyze how obtained models represent the various levels of clearance in the device and develop a suitable predictor of the degradation severity.

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A *fingerprint* of a heterogeneous data set

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In this talk we will present the fingerprint method, a technique to classify bags of mixed-type measurements. The method was designed to solve a real-world industrial problem: classifying industrial plants (individuals at a higher level of organisation) starting from the measurements collected from their production lines (individuals at a lower level of organisation). In this specific application, the categorical information attached to the numerical measurements induced simple mixture-like structures on the global multivariate distributions associated with different classes. The fingerprint method is designed to compare the mixture components of a given test bag with the corresponding mixture components associated with the different classes, identifying the most similar generating distribution. When compared to other classification algorithms applied to several synthetic data sets and the original industrial data set, the proposed classifier showed remarkable improvements in performance.

IS-7
Advanced CFD and Applications - Part 1

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Numerical simulation based processes are nowadays widespread in many engineering fields, thanks to the capability to study complex phenomena otherwise intractable, e.g. the flow in human body in biomedical context, or save time and resources to measure the performance of products in the industrial sector. Advanced numerical analysis plays a fundamental role to ehnance methods, both in terms of accuracy and performances.

The minisymposium will foster discussion on industrial and medical applications related to computational fluid dynamics (CFD) in automotive, naval, nautical, geophysical, biomedical engineering and cardiovascular surgery as well. Several state-of-the-art techniques, among which advanced reduced order modelling, high performance computing and data management, parameter space reduction, and real time computing and visualization, will be presented.

Talks will present methodological developments in numerical analysis with emphasis on mathematical modelling and applications in a wide range of computational engineering fields, bringing together research centers within industry, university spinoffs, and academia.

Digital Twins and graph theory: a parallel fault-simulation software with naval applications

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The Digital Twin is defined as a virtual representation of a physical counterpart, the real asset. This concept is the climax of continuous improvement in the field of product design in engineering activities [1]. How do we represent a Digital Twin in practice? We are going to provide an example of it, through GRAPE (GRaph PArallel Environment) [4]. It is a powerful tool, based on graph theory, able to model complex interconnected systems like industrial plants, and to simulate a complete risk analysis on it.
We have adopted weighted graphs in our description. Weight is very useful to specify the preferable itineraries for service stream, with respect to areas in which its course can be less favored. It is of immediate integration within the context of graphs, and it allows a very efficient calculation of shortest paths as the paths with the minimum length. All the calculations are carried out in an HPC framework.
Damage within the graphs can be limited with the activation of switches. Their best configuration is identified via a generative approach [2]. The main idea is to generate a population of individuals representing the possible states of the switches, and make it evolve based on the total number of actions (with respect to the initial condition of the switches), the total number of survived nodes after the perturbation and the total final service.
In the end, an example of industrial application is going to be presented. The project in which GRAPE has been employed is called SAFE (Realtime Damage manager and Decision Support), funded by Regione FVG, POR-FESR, Piano Operativo Regionale Fondo Europeo per lo Sviluppo Regionale, involving Cetena S.p.A. as leader, together with Arkitech S.r.l., SISSA, Università degli Studi di Udine and Lloyd's Register EMEA. The aim of SAFE project is to design new tools and methodologies to quantify the damage that can occur on a passenger ship. The scope is the development of a decision support tool to evaluate the damage occurred as a consequence of fire or flooding, and to support the crew in the activities related to ship safety and to residual operational capacity. The main causes of perturbation of passenger ships are usually fire or flooding. If not limited, a damage can quickly propagate with a cascade effect. We define the casualty threshold as the maximum amount of damage a ship is able to withstand, and still safely return to port [3]. If the casualty threshold is not exceeded, we are in a Safe Return to Port

scenario, and the ship can proceed to the next port. If this quantity is exceeded, the directive to leave is given to all people. The main goal is to be able to simulate scenarios on single plants, as well as on the combined overall ship structure.

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Structural optimization of a passenger ship hull using reduced order models for both inputs and outputs

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Nowadays, the shipbuilding industry is moving towards solutions with a reduced environmental impact. We contribute to this aim by presenting advanced numerical techniques to reduce the metal raw materials used during the manufacturing. They ensure an efficient way to approximate of all the quantities of interest during the optimization loop, while saving computational resources.

In this talk we present a modular and efficient structural optimization pipeline applied to modern passenger ship hulls. We exploit several reduced order modeling techniques to fight the curse of dimensionality for both the input parameters [1] and the output fields of interest. We show how to combine a data-fusion nonlinear autoregressive scheme with active subspaces [3] to enhance the prediction accuracy of POD based non-intrusive reduced order methods (ROMs) [2] in the context of linear elasticity.

We employ Bayesian optimization and we exploit the ROMs created in the offline phase to evaluate in real-time both the target function to minimize and the stability constraints. The approximated optimum is then validated with the high-fidelity solver and the solution database is updated to increase the accuracy of the ROMs.

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Mathematical methods for safety assessment of road tunnels

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In order to guarantee the safety of road tunnels, it is crucial to carry out in-depth inspections regularly, so as to be able to early identify possible defects of the structures and provide to their repair. However the inspection process is often quite long and expensive: it is therefore important to develop smart mathematical tools that can help the engineers recognize quickly and with little data which tunnels are more at risk, thus allowing for a more efficient planning of inspections and maintenance.

In this talk we present the results of an initial study, done in collaboration with the Lombardi civil engineering group, about the development and applicability of mathematical methods for supporting decisions regarding the safety of tunnels in Italy's highway system [1]. More in details, we discuss how dimensionality reduction algorithms such as dynamic mode decomposition (DMD) and its variants (implemented numerically in [2]) can be applied to predict the time evolution trend of defects in a tunnel, and how deep learning techniques such as convolutional neural networks are able to speed up the detection and classification of these defects and provide a quick estimate of the level of risk of a tunnel.

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Closure Models for reduced order methods in turbulent flows: a balance between consolidation and innovation

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Dealing with CFD shape optimization problems requires the analysis of a large number of parameterized geometries in order to find the best performing configuration. The computational cost may become unaffordable quite rapidly in case an efficient technique is not employed for this scope [1].

The resolution of turbulent flow problems can be nowadays achieved by the usage of a large variety of turbulence models. The possibility to obtain a reduced efficient method which is not dependent of the selection of the closure model is, of course, very appealing. In this talk we present a general architecture characterized by a data-driven approach for the approximation of turbulence dynamics [2].

Specifically, we combined classical projection-based techniques applied to incompressible Navier-Stokes equations with deep learning methods for turbulence treatment. This choice makes the method very usable and general while preserving reliability and efficiency properties [3].

The work we present has been carried out in the framework of the Aria European project (Accurate ROMs for Industrial Applications) in collaboration with Markus Mrosek and Carsten Othmer from the Volkswagen research center.

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A Virtual Boundary Method for industrial applications in a Finite Volume setting

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Immersed Boundary Methods (IBMs) [3] allow to simulate moving or deforming bodies characterized by complex surface geometries embedded in a fluid region. The main feature that makes IBM an useful and versatile technique is related to the fact that the Navier-Stokes equations are discretized over an orthogonal Cartesian grid and the effect of the no-slip boundary condition at the physical surface of the immersed body is obtained by introducing an additional body force term in the momentum equation.

Depending on whether the force is applied onto the continuous or discretized Navier-Stokes equations, these methods can be categorized into a continuous forcing approach and a discrete forcing approach, respectively [3]. The continuous forcing approach, in addition to the original Peskin method [4], includes also the Virtual Boundary Method (VBM) introduced by [2]. The VBM has been extensively investigated within a Finite Difference framework as well as a Spectral framework, although obiously other space approximations are possible.

In this work, we combine the VBM with a computationally efficient Finite Volume (FV) method. Furthermore, we propose to modify the standard feedback forcing scheme, based on a Proportional-Integral (PI) controller, with the introduction of a derivative action, in order to obtain a Proportial-Integral-Derivative (PID) controller. A stability analysis for the Backward Differentiation Formula of order 1 (BDF1) and 2 (BDF2) time schemes is carried out.

Firstly, our approach is validated against numerical data available in the literature for academic benchmarks involving a stationary/rigidly moving 2D circular cylinder in several configurations. Then a Fluid-Structure Interaction (FSI) benchmark, related to the frequency response of a cantilever beam coupled with a fluid, is presented. Finally, we test the performance of our approach through the application to a realistic industrial problem concerning the simulation of the deformation of steel plates inside pickling tanks [1].

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Boundary Heat Flux Estimation in Continuous Casting Molds Using Data Assimilation

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In continuous casting of steel, the most critical component is the mold. In the mold, the steel begins its solidification, and several complex physical phenomena happen. To ensure a proper control of the process, it is necessary to know how the steel is behaving inside the mold. However, it is not possible to make measurements inside the solidifying steel and the only available data are pointwise temperature measurements in the interior of the mold plates. To provide a tool for the proper control of the process, we developed a methodology for the real-time estimation of the heat flux at the steel-mold interface given the temperature measurements. With this tool, we allow the caster operator to quickly detect any malfunctioning in the casting increasing the safety and the productivity of continuous casters

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IS-8
Advanced CFD and Applications - Part 2

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Numerical simulation based processes are nowadays widespread in many engineering fields, thanks to the capability to study complex phenomena otherwise intractable, e.g. the flow in human body in biomedical context, or save time and resources to measure the performance of products in the industrial sector. Advanced numerical analysis plays a fundamental role to ehnance methods, both in terms of accuracy and performances.

The minisymposium will foster discussion on industrial and medical applications related to computational fluid dynamics (CFD) in automotive, naval, nautical, geophysical, biomedical engineering and cardiovascular surgery as well. Several state-of-the-art techniques, among which advanced reduced order modelling, high performance computing and data management, parameter space reduction, and real time computing and visualization, will be presented.

Talks will present methodological developments in numerical analysis with emphasis on mathematical modelling and applications in a wide range of computational engineering fields, bringing together research centers within industry, university spinoffs, and academia.

Numerical simulations for design, virtual prototyping, procedure planning, and follow-up assessment of endovascular devices

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The present study discusses the use of numerical simulations along the various stages of endovascular devices such endografts or stents along the whole life cycle of the device, from the design to its performance assessment during the clinical follow-up.
In particular, the talk discusses the virtual prototyping of a novel endoprostheses or endovascular strategies such the minimally-invasive repair of aortic root [4] and the assessment of novel embolism prevention [1]. Moreover, the integration of structural finite element analysis (FEA) with computational fluid dynamics (CFD) is presented to support the clinical planning of Thoracic Endovascular Repair (TEVAR) in order to predict post-operative hemodynamics based on pre-operative data and medical images [2]. Finally, how CFD is used to understand failure modes of endovascular devices along the follow-up, such peripheral stenting impaired by thrombosis [3].

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Registration-based model reduction of parameterized advection-dominated PDEs

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We propose a model reduction procedure for rapid and reliable solution of parameterized advection-dominated problems. Accurate approximation of travelling parameter-dependent waves is extremely challenging for traditional model reduction approaches based on linear approximation spaces: to address this issue, we propose an adaptive registration-based data compression procedure to align local features in a fixed reference domain, to ultimately improve the compressibility of the solution manifold. We further develop an hyper-reduced projection-based (Petrov-Galerkin) framework for the computation of the mapped solution. Numerical results for a two-dimensional inviscid flow past a bump (Euler equations) empirically demonstrate the potential of the method.

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Advanced Ship Performance Analysis by High-Fidelity CFD Methods

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In the picture of the worldwide shipbuilding industry the use of advanced computational techniques and approaches is still limited to relatively few large shipyards that build unconventional vessels or very particular vehicles such as Autonomous, Unmanned Surface or Underwater Vehicles. We present some high-fidelity Computational Fluid Dynamics (CFD) techniques that are mature to be transferred to the industry and that can improve the quality of the hydrodynamic analysis needed to design better ships. In particular, the talk will focus on some advanced problems, i.e. ship selfpropulsion [1], manoeuvring [2], propeller-rudder interaction [3], design of wake equalizing ducts [4], super-cavitating hydrofoils [5] and unconventional propellers [6]. These problems have been solved by using a CFD approach relying on a high-fidelity RANSE-based solution, achieved by using the OpenFOAM library, combined to ad-hoc developed methods at different levels of computational fidelity. Results coming from the different approaches are presented and discussed in terms of comparison among the methods. Results are then analysed in terms of global physical characteristics, such as integral quantities of the coupled systems, e.g. ship and propeller or rudder and propeller, and local flow fields. Convergence properties of the methods, possible limitations and the burden of computational resources needed to achieve the solutions are discussed too. At the end of the talk we will demonstrate that advanced and combined CFD techniques can represent a reliable and accurate approach to be massively used by the shipbuilding industry to support the decision-making process to design more efficient ships.

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A computational pipeline exploiting reduced order modeling techniques for industrial shape optimization problems

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Despite the last years advances in technology, simulation–based design and optimization still remains a challenging procedure from the computational point of view. Such problems require indeed to numerical solve complex PDEs in an iterative way, resulting in a huge global computational burden. In this work, we present a numerical pipeline to efficiently treat shape optimization problems, integrating different reduced order modeling (ROM) methods to lighten the computation of solution of time-dependent PDE in a parametric context. In details, dynamic mode decomposition (DMD) and proper orthogonal decomposition with Gaussian process regression (POD-GPR) are employed in a cascade fashion for reducing the dynamical and parametric systems, respectively. Thanks to the equation–free nature of both methods, we can couple these latter to a large variety of numerical solvers, without requiring any knowledge about the original mathematical model but only the discrete solutions computed — for certain time steps and parameters — with traditional methods, e.g. finite volume, finite element.

A big constraint of the aforementioned ROM methods is represented by the space discretization performed in the original model: the numerical solutions are required to have the same number of degrees of freedom, which may result a challenging point dealing with a parametric domain. We present then a possible solution for obtaining a parametric computational grid involving a radial basis function interpolation (RBF). Finally, we show the numerical outcomes of the application of such pipeline to a naval hull, both in terms of ROM accuracy and global speedup.

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Reduced Convolutional Neural Networks for image recognition in professional appliances

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Artificial intelligence is increasingly used in industries in order to introduce innovation in their products and to solve problems coming from different sectors. In the context of industrial applications involving machine learning techniques, a challenging problem is represented by image recognition. A possible approach to deal with image recognition problems is represented by Artificial Neural Networks (ANNs) and in particular by Convolutional Neural Networks (CNNs). Such architectures well performs the classification of objects in pictures, but may require an high number of layers to extract all the features of the problem at hand. This leads to several issues in the case the aforementioned networks have to operate in an embedded system inside a professional appliance. In our case, the space constraints of the latter systems have led to the implementation of a reduced version of the original CNN, in order to minimize the numbers of neurons and layers. We propose an extension of [1] for dimensionality reduction of CNNs, exploring both the active subspace (AS) property and the proper orthogonal decomposition (POD) technique. The reduced network is so constructed by retaining a certain number of layers of the original CNN and replacing the remaining ones — assuming they contain the less important features — with a feed–forward network. In this way, we are splitting our CNN in two different nets connected by the reduction method: the first one that recalls the structure of the starting net and aims to detect the main convolutive features and a second one that deals with the classification part. We finally provide the numerical results obtained by applying such method to a generic images database (CIFAR) and an application-specific one, using as starting point the VGG16 [2] model and presenting the final outcome in terms of final accuracy, memory allocation, speed of the procedure.

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Edu-SIMAI

Edu-SIMAI session

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In continuity with what was already undertaken in previous conferences SIMAI 2018 and SIMAI 2016, the 3rd Edition of Edu-SIMAI will be held on August 31, 2021, both in presence and in online mode, on the occasion of the National Conference of the Italian Society of Applied and Industrial Mathematics (SIMAI).

Edu-SIMAI is an event dedicated by SIMAI to the relationship with secondary schools. It has, as its main objective, the cooperation between the School and the Academy on

the subjects of Applied Mathematics and the relations between the School world and the world of Research and Industry.

The event is sponsored by the Italian project "Piano lauree Scientifiche" and the European project "IDENTITIES".

Questioning interdisciplinarity from society to school: design and analysis of interdisciplinary teaching projects

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This talk focuses on the problem of how to transpose interdisciplinary practices into school and what is the role that the different disciplines can play in school institutions, with special focus on the role of mathematics in relation to other disciplines. We present some results in the line of research of the anthropological theory of the didactic (ATD). In particular, we address the design, implementation and analysis of the so-called study and research paths (SRP) for secondary education, as well as for teacher education. The SRP are proposed as an inquiry-oriented instructional device, based on the inquest into open questions with the aim of making disciplinary and interdisciplinary knowledge emerge to address these questions.

We present the particular case of an SRP about the modelling process of the COVID-19 evolution. The analysis of what has happened outside school during the pandemic in 2020-21 has been the base to detect some questions sensitive to make interdisciplinary knowledge emerge. We analyse two case studies: a teacher education proposal to progress into the necessary tools to bring interdisciplinarity into classrooms and the two-consecutive implementation of the SRP about the evolution of the pandemic in secondary school.

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Dalla realtà ai modelli matematici al calcolo scientifico

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Ho iniziato a rivolgermi al mondo della scuola superiore qualche anno fa quando con Alfio Quarteroni mi sono dedicata alla stesura del libro "I delfini delle Eolie, i battiti del cuore, i motori di ricerca – Modelli matematici per comprendere, simulare, esplorare" pubblicato da Zanichelli nel 2019.

Nello scrivere questo testo ci siamo posti l'obiettivo di aiutare gli studenti degli ultimi tre anni di scuola superiore a comprendere come si deriva un modello matematico, come esso funziona e quale potenziale offre, procedendo sìper esempi legati alla vita reale, all'informatica, alla fisiologia o alla biologia, ma allo stesso tempo con l'ambizione di descrivere i processi che sottendono un modello matematico nella loro generalità. Ci ha guidato l'intento di incoraggiare i ragazzi a modellizzare altri problemi e ad acquisire sempre maggiore consapevolezza della potenza descrittiva della matematica.

In questo percorso non ci siamo fermati alla modellizzazione matematica (teorica), ma abbiamo dato ampio spazio anche ai modelli numerici e al calcolo scientifico, consapevoli che essi costituiscono il ponte ideale fra teoria e computer, rendendo possibile la risoluzione concreta di problemi reali che non sarebbero risolubili con carta e penna.

Il libro è stato utilizzato come filo conduttore per un corso Policollege del Politecnico di Milano rivolto a studenti meritevoli di quarta e quinta superiore, riscuotendo ampio interesse da parte dei ragazzi.

La scienza in azione: Research in Action
Vogliamo che il mondo sia fonte di osservazione, di scoperta, di analisi

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Research in Action è un Percorso per le Competenze Trasversali e per l'Orientamento del liceo scientifico G.B. Grassi di Latina, ideato e coordinato da Gualtiero Grassucci (http://researchinaction.it/).
Si tratta di un tentativo di dare un senso all'insegnamento della matematica nel liceo scientifico, spronando alunni e alunne a fare da soli davanti a un problema, qualunque esso sia, cercando di mettere a frutto le loro conoscenze e (soprattutto) le loro competenze in contesti diversi da quelli usuali.

Insegnare matematica è difficile, nella scuola secondaria di secondo grado forse ancora di più. A ragazzi e ragazze, che iniziano a scontrarsi con i simboli e le rappresentazioni della disciplina, con il suo aspetto astratto e incorporeo viene spesso richiesto un enorme atto di fede nel fatto che la manipolazione di simboli che lì per lì sembra loro del tutto inutile, un giorno sarà loro utile, ma non dovrebbe essere tutto ciò che viene insegnato. Potremmo anche porre delle domande aperte...

Domande e problemi che richiedono di pensare strategie risolutive, di usare gli strumenti conosciuti in modo originale e creativo, di chiedere e cercare nuovi strumenti perché quelli che si possiedono non sono sufficienti o non abbastanza affinati.

In questo percorso a studenti e studentesse sono proposti problemi concertati con alcuni ricercatori e docenti universitari basati su dati ed esperimenti reali, richiedendo la soluzione di questioni anche complesse legate al contesto.

Ecco, è proprio questo uno degli atteggiamenti che il progetto vuole promuovere negli studenti: l'uso della matematica nella sua concezione più alta e generale, un linguaggio per la descrizione e la comprensione della realtà. Una volta raggiunta questa comprensione del pezzetto di realtà oggetto di studio, la matematica diventa lo strumento ideale per concepire e architettare una soluzione del problema.

L'idea di matematica applicata che è alla base del progetto è questa!

A oggi sono stati realizzati 14 laboratori e altri sette sono in via di completamento con il materiale didattico di supporto che spazia dai videotutorial per xMaxima e Blockly fino a un simulatore della macchina Enigma (costruibile con carta, forbici e colla) per il laboratorio di crittografia. Tutto disponibile sul sito del progetto: http://researchinaction.it/.

I percorsi sono stati realizzati in collaborazione con l'Istituto delle Applicazione per il Calcolo (CNR-IAC), l'Istituto di Fotonica e Nanotecnologie di Roma (CNR-IFN), l'Istituto di Ingegneria del Mare (CNR-INM), l'Istituto di Scienze Marine (CNR-ISMAR), il Dipartimento di Matematica e il Dipartimento di Informatica, Elettronica e Telecomunicazioni (DIET) dell'Università La Sapienza di Roma, il Dipartimento di Matematica Pontificia Università Cattolica di Rio de Janeiro (PUC-Rio).

Flipped Classroom ed Educazione Finanziaria: imparare mettendosi in gioco

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La mancanza di educazione finanziaria è un problema che riguarda larga parte della popolazione del nostro paese [2]. Alcuni avvenimenti recenti lo hanno ampiamente dimostrato: i bond argentini, i bond Parmalat, i derivati collocati presso imprese di medie-piccole dimensioni, le perdite legate al titolo Lehman Brothers, le obbligazioni subordinate e il bail-in delle banche in difficoltà negli ultimi anni. Questi episodi, che hanno creato situazioni di disagio sociale localizzate ma rilevanti in quanto alcune persone hanno perso i risparmi di una vita, affondano le loro radici anche nella limitata conoscenza degli strumenti finanziari e delle più elementari nozioni di finanza, quali ad esempio leggi di capitalizzazione, diversificazione degli investimenti, e trade-off rischio-rendimento [1].

L'azione del progetto EDUFIN@POLIMI si inserisce in questo contesto sperimentando modalità innovative di "fare formazione" su temi complessi. Con questo progetto si vuole proporre la realizzazione di un modello formativo innovativo per l'acquisizione di conoscenze finanziarie da parte di studenti e non solo. La peculiarità dell'intervento proposto consiste nell'entrare nelle specificità analitiche di alcuni temi finanziari e nello svilupparne la capacità di calcolo. Si entra quindi nel merito di come si calcolano gli interessi di un mutuo, di come si calcola l'onerosità di un prestito e di come si gestisce effettivamente un portafoglio in un'ottica di ottimizzazione rischio-rendimento. Sono varie le attività attualmente promosse da EDUFIN@POLIMI che sta ottenendo ottimi risultati sia in termini di adesioni che di efficacia.

La prima proposta promossa da EDUFIN@POLIMI riguarda lo svolgimento di un'attività formativa nelle classi delle scuole superiori in modalità "flipped classroom". Lo scopo di questa metodologia didattica, validato anche da ricerche in materia di didattica della

matematica,è quello di promuovere un apprendimento attivo e autonomo da parte dello studente. La lezione è divisa in due parti: la prima svolta autonomamente dallo studente (solitamente a casa e con l'ausilio di materiale multimediale) e la seconda realizzata in classe, sotto la guida dell'insegnante. L'attività di "flipped classroom" è stata divisa in tre diversi percorsi e divisi a loro volta in moduli monotematici per permettere una maggiore flessibilità e organizzazione da parte del docente degli argomenti che desidera affrontare. Tutto il materiale fornito è utilizzabile attraverso moduli online per agevolarne l?utilizzo in DAD. Il progetto EDUFIN@POLIMI offre tutto il materiale necessario sia per lo studente che per guidare il docente nel percorso formativo. Durante i percorsi proposti si affrontano tematiche quali le leggi di capitalizzazione, l'analisi di serie storiche, la creazione di un portafoglio di azioni e la diversificazione.

In parallelo, è stato progettato il gioco "Labirinto delle Finanze", proposto sia a conclusione delle lezioni di educazione finanziaria, sia come attività isolata per avvicinare i ragazzi a questi temi. Questa attività è analoga a una pilota di EDUFIN@POLIMI chiamata "Caccia al Tesoro Finanziaria" che si è svolta negli ultimi anni presso il campus del Politecnico di Milano. Tali proposte prevedono lo svolgimento di una gara a squadre in cui gli studenti vengono coinvolti nella risoluzione di problemi di carattere finanziario. I quesiti sono strutturati in modo che non siano necessari particolari prerequisiti. Il gioco può essere svolto in qualsiasi classe occupando alunni e insegnanti per un paio d'ore. Questa proposta permette di avvicinare gli studenti ai temi dell'Educazione Finanziaria tramite un'attività ludica e informale, introducendo nuove conoscenze e lanciando alcuni spunti che possono poi essere approfonditi durante le ore di lezione.

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Literature as a Support for Learning the Basic Concepts of Symbolical Logic

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The research reported in this talk is part of a wide study which seeks to unravel and manipulate possible interrelationships between mathematics and literature for the construction of non-exclusive or compartmentalized knowledge, taking as reference the discussions of the complexity theory [1] and the transdisciplinarity [2]. The activities described here deal with the construction of elementary notions of symbolical logic and had, as an entry point, the literary opus of Lewis Carroll, from which it is possible to discuss the mutual impregnation of the mother tongue with mathematical language [3] and study how propositional calculus emerges from the literature in well formed formulas. This meeting of mathematics and literature provided the study of the operators of conjunction and negation and cases of conditional and biconditional [4]. When elaborating such activities, Carroll's [5] opinion was considered, for whom the teaching of formal logic could take place through games or fun situations, without relinquishing the rigid structure of discipline. The central idea is to assist in the development of students' logical reasoning, from the first school years, creating recreational learning environments that prepare them to, later on, learn easily the programming languages, which are the support for the study of robotics, among with other points. The partial results of these studies that articulate mathematics and literature have shown the existence of in-between places [6] that enhance the construction of knowledge in an integrated way and help students to realize that the rationality of mathematics does not necessarily exclude other human dimensions, such as fantasy and the illusory [7].

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Esperienze didattiche al Liceo Matematico con il linguaggio Python: concorso AstroPi dell'ESA e analisi di similarità fra testi letterari

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Nella corso della presentazione saranno illustrati due percorsi didattici realizzati in u seconda liceo scientifico ad indirizzo matematico dell'Istituto B. Russell di Roma:

- l'esperimento AstroRussell realizzato a bordo della Stazione Spaziale Internazionale utilizzando il computer a basso costo Raspberry Pi e premiato fra i 10 vincitori della gara "AstroPi" promossa dall'Agenzia Spaziale Europea (ESA).
- il progetto interdisciplinare sull'analisi di similarità fra testi letterari che ha ottenuto una menzione speciale al Concorso Internazionale ISLP per Poster Statistici dell'ISTAT con l'analisi dei discorsi dei presidenti della Repubblica Italiana.

Questi percorsi sono stati realizzati sfruttando una delle due ore aggiuntive di matematica derivanti dalla sperimentazione del liceo matematico. In particolare, queste due esperienze didattiche sono accomunate dall'utilizzo del linguaggio Python che è stato introdotto agli studenti durante il primo anno di liceo.

Questo linguaggio si caratterizza per la semplicità di apprendimento, l'ampia diffusione in rete di materiale di supporto e la disponibilità di librerie pensate per il calcolo scientifico. Per queste caratteristiche, si ritiene che questo linguaggio si presti in modo particolare per essere introdotto a livello di scuola superiore. Per una descrizione più approfondita del linguaggio dal punto di vista didattico si vedano [1]) e [2].

L'approccio didattico utilizzato è stato laboratoriale suddividendo in gruppi gli studenti all'interno dell'aula informatica della scuola.

La prima esperienza didattica è consistita nell'ideare un esperimento scientifico da realizzare sulla stazione spaziale internazionale (ISS) avvalendosi del computer Raspberry Pi, scheda Sense Hat dotata di sensori, matrice led e di una telecamera sensibile anche al vicino infrarosso posizionata davanti a un oblò della ISS in direzione della Terra.

La proposta è stata quella di realizzare un semplice classificatore di immagini in grado di individuare in tempo reale le classi mare, suolo, nuvole/ghiaccio e contorno dell'oblò dietro il quale era fissata la telecamera. L'algoritmo di classificazione, sviluppato interamente dagli studenti a partire da immagini di test acquisite da precedenti esperimenti di AstroPi, è stato un semplice algoritmo a soglie di valori applicato alle bande delle immagini trasformate però nello spazio dei colori denominato HSV (Hue Saturation Value). Questo spazio è stato utilizzato perché, basandosi sulla percezione che si ha di un colore in termini di tonalità, saturazione e valore, rendeva più semplice individuare le soglie per le diverse classi. Successivamente, l'esperimento proponeva di calcolare "a terra" la misura frattale delle eventuali nuvole acquisite durante le tre ore di durata dell'esperimento e

cercare di verificare se questa misura fosse collegabile ad eventuali differenti tipologie di nuvole.

L'esperimento, superata l'iniziale selezione da parte dell'Agenzia Spaziale Europea, è stato effettivamente realizzato con successo sulla ISS e gli studenti hanno potuto analizzare le immagini acquisite inviate dall'ESA e presentare un report finale (si veda: `http://esamultimedia.esa.int/docs/edu/AstroRussel_final_report.pdf`. Una descrizione dettagliata di questo percorso didattico è disponibile qui [3].

Sempre nella stessa classe è stato sperimentato un percorso interdiscplinare con il docente di lettere relativo alla analisi dei testi letterari. In questo caso il linguaggio Python è stato utilizzato per:

- importare file testuali contenenti opere letterarie (Manzoni, Verga, ecc..),
- preprocessare i testi (per esempio eliminando articoli e congiunzioni)
- applicare delle misure di similarità come la distanza di Jaccard, la distanza euclidea e la similarità del coseno.

In questo modo gli studenti hanno potuto calcolare la similarità fra diversi testi letterari di diverse epoche osservando che opere di autori dello stesso periodo e stile letterario risultavano fra loro più simili. Come ulteriore applicazione di questo percorso, un gruppo di studenti ha partecipato al Concorso Internazionale ISLP per Poster Statistici dell'ISTAT analizzando la similarità fra i discorsi dei Presidenti della Repubblica Italiana realizzando, come da indicazioni del concorso, un poster (si veda qui: `http://crf.uniroma2.it/wp-content/uploads/2020/12/Russell-Poster-ISLP-italiano.pdf`). Maggiori dettagli su questo percorso sono disponibili in questo articolo [4].

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Cos'è il Liceo Matematico

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Il Liceo Matematico è un progetto didattico fondato sulla collaborazione tra Università e Scuola, ispirato all'insegnamento interdisciplinare e laboratoriale nelle scuole di secondarie di secondo grado e adottato già da più di 130 istituti in tutta Italia. La Matematica è usata come ponte tra le discipline e, viceversa, le discipline umanistiche permettono di esplorare campi matematici esterni al tradizionale perimetro scolastico. In questa breve presentazione verrà illustrato il progetto e verranno mostrate alcune delle attività svolte in questi anni, nella cornice del Liceo Matematico del Liceo Scientifico Majorana di Roma.

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