GIMC SIMAI YOUNG 2022

Book of abstract

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UNIVERSITÀ DI PAVIA

GIMC Gruppo Italiano di Meccanica Computazionale

SIMAI SOCIETÀ ITALIANA DI MATEMATICA APPLICATA E INDUSTRIALE

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Plenary Speakers

The GIMC-SIMAI worskhop will be kicked-off on Thursday morning by six plenary talks, two given by established researchers and four by young speakers. The topics of the talks cater to the broad interests of the the GIMC and SIMAI communities, and highlight both the common background of the two societies as well as the respective peculiarities. The four young speakers have been selected as a recognition of their scientific merits:

- Francesco Regazzoni was the winner of the ECCOMAS Award for the best PhD thesis in 2020 (as SIMAI candidate);
- Lorenzo Tentarelli is the winner of the SIMAI Young Investigator Prize 2022;
- Giulia Bertaglia was the winner of the GIMC award for best PhD thesis in 2020, and the winner of the ECCOMAS PhD olympiads in the same year.
- Alessia Patton was the winner of the GIMC award for best PhD thesis in 2021.

Title

The Material Point Method and beyond

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Abstract

While the Finite Element Method (FEM) represents a recognized, well established and widely used technique in many engineeing fields, both in academia and industry, unfortunately it shows some limitation when dealing with problems where large deformation occurs. In the last decades many possible solutions and alternatives have been proposed and developed to overcome this drawback, among them one possiblility is the use of the so called *particle-based methods*. Among them, we can find Lagrangian finite element techniques with remeshing, such as the Particle Finite Element Method (PFEM), or mesh-less techniques, such as the Smoothed Particle Hydrodynamics (SPH). Another alternative, presented in this talk, is the development of hybrid techniques, such as the Material Point Method (MPM), to blend the advantages of both mesh-based and mesh-less methods. MPM uses two different discretizations: a background mesh for calculation purposes (as in classical FEM) and a set of moving material points, acting as integration points, to store the hystorical information. MPM avoids the problems of mesh tangling while preserving the accuracy of Lagrangian FEM and it is especially suited for non linear problems in solid mechanics and fluid dymanics. The talk will show some recent advances in MPM formulations [1], presenting both an irreducible and mixed formulation stabilized using variational multiscale techniques, as well as the partitioned coupling strategies with other techinques such as FEM or DEM [2, 3].

References

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[3] Singer, V., Sautter, K.B., Larese, A., Wüchner, R. and Bletzinger, K.U.,, *A Partitioned Material Point Method and Discrete Element Method Coupling Scheme* , Under revision in Advanced Modeling and Simulation in Engineering Sciences (2022).

Title

Space-time IGA

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Monica Montardini, Università di Pavia
Mattia Tani, CNR-IMATI Pavia
Paolo Tesini, Università di Pavia

Abstract

The idea of using high-degree and continuity splines (or NURBS, etc.) as a basis for a new high-order method appeared promising from the beginning [1], and received confirmations from the following developments. The k-method leads to higher accuracy per degree-of-freedom, but, at the same time, the k-method brings significant challenges at the computational level: using standard finite element routines, its computational cost grows with respect to the degree, making degree raising computationally expensive. However, recent ideas allow a computationally efficient k-method. In this talk we present our experience (based on [2] and more recent work) on the k-method in Galerkin space-time isogeometric discretization of the heat equation. That is, we use smooth splines in space and time. Exploiting the tensor product structure of the basis functions in the parametric domain, we propose a preconditioner that is the sum of Kronecker products of matrices and that can be efficiently applied thanks to an extension of the classical Fast Diagonalization method. The preconditioner is robust w.r.t. the polynomial degree of the spline space and the time required for the application is proportional to the number of degrees-of-freedom, in our numerical tests with serial execution.

References

[1] T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs, *Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement*, Comput. Methods Appl. Mech. Engrg., Vol. 194, pp. 4135-4195 (2005).

[2] G. Loli, M. Montardini, G. Sangalli, and M. Tani, *An efficient solver for space-time isogeometric Galerkin methods for parabolic problems*, Computers & Mathematics with Applications 80(11), 2586–2603, (2020).

Title

Automatic discovery of low-dimensional dynamics underpinning time-dependent PDEs by means of Neural Networks

Author(s)

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Abstract

In this talk, we present a novel Machine Learning technique able to learn differential equations that surrogate the solution of time-dependent PDEs. Our method exploits a finite number of latent variables, which provide a compact representation of the state of the system. These variables allow for the reconstruction of the spatial outputs at each temporal instant through a mesh-less decoder based on Artificial Neural Networks (ANN). We propose an algorithm able to learn in a simultaneous way the latent variables, their dynamics and the mesh-less decoder. Remarkably, our method allows building, in a fully non-intrusive manner, surrogate models for evolutionary equations, accounting for the dependence on parameters and time-dependent inputs. Numerical tests for both parabolic and hyperbolic PDEs show that very accurate numerical results are obtained, even for a reduced size of the ANNs, in a computationally efficient manner.

Title

Advanced isogeometric methods with a focus on composite laminated structures

Author(s)

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Abstract

The design and optimization of engineering products demand faster development and better results at lower costs. These challenging objectives can be achieved by readily evaluating multiple design options at the very early stages of the engineering design process. To this end, accurate and cost-efficient computational modeling techniques for solids and fluids offer a reliable support and enable a better understanding of the underlying complex physical phenomena. The present study focuses on the development of advanced computational tools in the context of Isogeometric Analysis (IgA) [1], trying to exploit its higher-order continuity properties and typically excellent accuracy-to-computational-effort ratio.

Here, we first focus on an accurate and cost-efficient computational strategy to model laminated structures comprising solid plates, bivariate Kirchhoff's plates, and solid shells. In brief, we first calculate an efficient and accurate approximation of the displacement field (and its derivatives) using a single-element through the thickness of the laminate in combination with either a layer-by-layer integration rule or a homogenized approach. This relatively inexpensive calculation renders an excellent approximation of the laminate in-plane stresses only. Instead, to recover the out-of-plane stress components, we propose a pointwise post-processing technique that is based on the direct integration of the equilibrium equations in strong form, involving the straightforward computation of high-order derivatives of the displacement field, which can be computed relying on the properties of IgA shape functions.

Then, we further develop a novel solution technique for phase-field modeling of crack propagation using IgA. One of the key features of a crack evolution process is that a fracture cannot heal and, therefore, it is a non-reversible process. Thus, we propose a novel approach for a rigorous enforcement of the irreversibility constraint, which grants non-negative damage increments under prescribed displacements and may be efficiently resolved further providing a reduction of the computational time with respect to state-of-the-art methods to solve phase-field brittle fracture.

Finally, we explore new IgA collocation (IgC) formulations in the context of fluid-structure interaction (FSI). Computational fluid dynamics problems are a paradigmatic example in which IgC can provide the superior geometric capabilities of IgA with a lower computational cost and comparable accuracy with respect to standard IgA Galerkin discretizations. Thus, to obtain a geometrically compatible coupling fluid-structure interface for FSI problems, we propose to adopt a common spline description of the interface, combining IgC on the structural side and boundary-conforming finite elements (like the so-called NURBS-enhanced finite elements) on the fluid side.

References

[1] T.J.R. Hughes, J.A. Cottrell, Y. Bazilevs, *Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement*, Computer Methods in Applied Mechanics and Engineering, Elsevier, 2005, 194 (39-41), pp.4135-4195.

Title

Uncertainty quantification methods for PDEs with applications to biomathematics.

Author(s)

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Abstract

Various deterministic numerical techniques have been and are currently being developed to solve, as efficiently and accurately as possible, problems related to physical, biological, social and economic systems. The use of such numerical schemes, though, requires that initial conditions, boundary conditions and all the parameters involved in the mathematical model describing the phenomenon of interest are known. However, in practical applications this assumption is rarely true. Indeed, our knowledge is limited by the ability to measure, bias in observations and, in general, an incomplete understanding of processes, especially when dealing with biological and social sciences. In this context, our numerical simulations present uncertain inputs that give rise to uncertainty in the outputs of interest, which must be clearly identified and quantified in order to correctly interpret numerical results and draw meaningful conclusions.
In this talk, different Uncertainty Quantification (UQ) techniques, widely used in response to these issues, will be presented, highlighting the advantages and drawbacks of each. Examples of applications of these methods in the biomathematical field will also be discussed. In particular, problems such as the quantification of uncertainties related to geometric and mechanical parameters involved in the study of human cardiovascular fluid dynamics and uncertainties in initial conditions in the analysis of the spatial spread of infectious diseases will be addressed.

Title

Metric graphs: a mathematical model for quantum technologies

Author(s)

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Abstract

As problems related to the physical limits of silicon–based devices increase, the scientific community has begun to search for alternative technologies, possibly not founded on electron transport. One of the approaches suggested by the physics literature in the last years concerns the development of quantum–based technological frameworks, which exploit either fine quantum properties of new materials (such as, for instance, graphene) or completely new ways to transfer information. This also drove the rise of the new research field of Atomtronics, which aims at the construction of devices in which currents are generated by matter waves, instead of electrons, supplied by Bose–Einstein Condensates (BEC). One of the mathematical models proposed to study the features of circuits designed in this perspective is the NonLinear Schrödinger (NLS) equation on networks, or more precisely on *metric graphs*. The talk will provide an overview on some of the most relevant achievements on this model, obtained in the last decade, and a hint on future developments, possibly toward multidimensional structures known as *hybrids*.

MS01 - Efficient linear solvers for coupled geophysical simulations

Proposers

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Abstract

The construction of complex coupled models is of paramount importance to reach a high level of fidelity and reliability in numerical geophysical simulations. Examples of such models include compositional flow with wells and thermal effects in oil reservoirs, flow and mechanics in fractured porous media, multiphase flow and reactive transport, etc. As these numerical models become larger and larger to address the increasing complexities, specialized solvers are needed. Indeed, the linear solver is the main computational bottleneck for many large-scale simulations. Moreover, the rise of next-generation supercomputers sheds light on the efficiency of the solvers. This minisymposium seeks to gather the latest idea on efficient and scalable linear solvers for coupled geophysical simulations. The focus is on both general algebraic approaches and application of ad-hoc preconditioners.

Title

A solution technique for Darcy flow in fractured porous media that ensures local mass conservation

Author(s)

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Abstract

Constructing fast solution schemes often involves deciding which errors are acceptable and which approximations can be made for the sake of computational efficiency. Herein, we consider a mixed formulation of Darcy flow and take the perspective that the physical law of mass conservation is significantly more important than the constitutive relationship, i.e. Darcy's law. Within this point of view, we propose a three-step solution technique that guarantees local mass conservation [1].
In the first step, an initial flux field is obtained by using a locally conservative method such as the TPFA Finite Volume Method. Although this scheme is computationally efficient, it lacks consistency and therefore requires a suitable correction. This correction will be divergence-free and so the Helmholtz decomposition ensures us that it can be described as the curl of a potential field. The second step therefore employs an H(curl)-conforming discretization to compute the correction potential and update the flux field. The pressure field is computed in the final step by using the same TPFA system from the first step.
We present our technique in the context of structure-preserving discretization methods and use finite element and virtual element methods of lowest order as our leading examples. In terms of computational cost, each of the three steps involves solving an elliptic problem posed on either the cell centers or the edges of the mesh.
The procedure guarantees local mass conservation regardless of the quality of the computed correction. Thus, we relax this computation using tools from reduced order modeling. In particular, we introduce a reduced basis method that is capable of rapidly producing a potential field for given permeability fields. By applying the curl to this field, we ensure that the correction is divergence-free and mass conservation is not impacted.
Finally, we extend the method to solving Darcy flow in fractured porous media. We rewrite the equations in terms of the mixed-dimensional divergence and identify the problem as a mixed-dimensional Darcy flow system. In turn, the solution procedure directly applies. The mixed-dimensional curl ensures that the correction step is divergence-free and we show the performance of our technique in the context of flow in three-dimensional, fractured media.

References

[1] W. M. Boon and A. Fumagalli, *A Reduced Basis Method for Darcy flow systems that ensures local mass conservation by using exact discrete complexes*, arXiv preprint arXiv:2205.15626, 2022.

Title

Scalability Results for the Solution of the Richards Equation

Author(s)

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Abstract

Groundwater flow in the unsaturated zone is a highly nonlinear phenomenon that can be modeled by the Richards equation, and there is a significant amount of research concerning different formulations and algorithms for calculating the flow of water through unsaturated porous media. We consider here a cell-centered finite difference approximation of the Richards equation in three dimensions,

$$\rho\,\phi\frac{\partial s(p)}{\partial t} - \nabla\cdot K(p)\nabla p - \frac{\partial K(p)}{\partial z} = f,$$

for $p(t)$ the pressure head at time t, $s(p)$ the water saturation at pressure head p, ρ the water density, ϕ the porosity of the medium, $K(p)$ the hydraulic conductivity, and f any water source terms containing the elevation z.
To discretize it we average for interface values the hydraulic conductivity K, a highly nonlinear function, by arithmetic, upstream and harmonic means. The nonlinearities in the equation can lead to changes in soil conductivity over several orders of magnitude and discretizations for space variables often produce stiff systems of differential equations. A fully implicit time discretization is provided by *backward Euler* one-step formula; the resulting nonlinear algebraic system is solved by an inexact Newton Armijo–Goldstein algorithm, requiring the solution of a sequence of linear systems involving Jacobian matrices. We prove results concerning the distribution of the Jacobians eigenvalues and the explicit expression of their entries [1] while exploring connections between the saturation of the soil and the ill-conditioning of the Jacobians. We propose a new software framework called PSCToolkit [2] to experiment with scalable and robust preconditioners suitable for efficient parallel simulations at very large scales.
This work has been partially supported by the EU under the Horizon 2020 Project "Energy oriented Centre of Excellence: toward exascale for energy (EoCoE-II)", Project ID: 824158.

References

[1] D. Bertaccini, D'Ambra, P., Durastante, F. and S. Filippone, *Preconditioning Richards Equations: spectral analysis and parallel solution at very large scale*, arXiv: `https://arxiv.org/abs/2112.05051`, 2021.

[2] D'Ambra, P., Durastante, F. and S. Filippone, *AMG preconditioners for linear solvers towards extreme scale*, SIAM Journal on Scientific Computing 43.5 (2021): S679-S703.

Title

An iterative solving strategy for 3D-1D coupled problems under an optimization based approach

Author(s)

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Abstract

Coupled 3D-1D problems arise in many practical applications, in an attempt to reduce the computational burden in simulations where cylindrical inclusions with a small section are embedded in a much larger domain. For example, in geological reservoir simulations, small natural inclusions, as well as artificial wells, can be modeled as one dimensional manifolds interacting with the surrounding porous matrix. Nevertheless, the mathematical treatment of the coupling between a 3D and a 1D problem is non trivial, as no bounded trace operator is defined when the dimensionality gap between the interested manifolds is higher than one. For this reason, in [1] and [2], we proposed a novel framework for 3D-1D coupling, based on a well posed mathematical formulation and ending up in a method which is highly robust and flexible in handling geometrical complexities. In [1], the problems in the porous matrix and in the inclusions are coupled by imposing the continuity of the solution and the conservation of the flux at the interface, which is supposed to be perfectly permeable to the quantity of interest. This is achieved by a three-field domain decomposition strategy. In [2] the interface is instead supposed to be a semipermeable membrane and the exchanged flux is proportional to the jump of the solution across the interface. Hence only flux conservation is imposed. In both cases the resulting formulation is then recast into a PDE-constrained optimization problem: a cost functional accounting for the error committed in the fulfillment of the matching conditions is introduced and minimized subject to the 3D and the 1D equations.
This talk will be mostly focused on the solving strategies for the resulting optimization problem, in particular at the increase of the number of the inclusions and hence of the complexity of the problem. An iterative solver based on a conjugate gradient scheme will be proposed and ad-hoc built preconditioners for the continuous [3] and the discontinuous [2] case will be presented.

References

[1] Berrone, S. and Grappein, D. and Scialò, S., *3D-1D coupling on non conforming meshes via a three–field optimization based domain decomposition*, Journal of Computational Physics, 448, 2022.

[2] Berrone, S. and Grappein, D. and Scialò, S., *A PDE-constrained optimization method for 3D-1D coupled problems with discontinuous solutions*, https://arxiv.org/abs/2203.01732v1, 2022.

[3] Berrone, S. and Grappein, D. and Scialò, S. and F. Vicini, *A gradient based resolution strategy for a PDE-constrained optimization approach for 3D-1D coupled problems*, Int J Geomath, 13(1), 2022.

Title

A high order parallel semi-implicit DG scheme for linear elasticity on staggered unstructured meshes.

Author(s)

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Abstract

In this talk we present a new high order accurate space-time discontinuous Galerkin (DG) finite element scheme for the solution of the linear elastic wave equations in first order velocity-stress formulation. The algorithm is presented in two and three-space dimensions on *staggered* unstructured triangular and tetrahedral meshes. The method reaches arbitrary high order of accuracy in both space and time via the use of space-time basis and test functions. Within the staggered mesh formulation, we define the discrete velocity field in the control volumes of a primary mesh, while the discrete stress tensor is defined on a face-based staggered dual mesh. The space-time DG formulation leads to an *implicit* scheme that requires the solution of a linear system for the unknown degrees of freedom at the new time level. The number of unknowns is reduced at the aid of the Schur complement, so that in the end only a linear system for the degrees of freedom of the velocity field needs to be solved, rather than a system that involves both stress and velocity. Thanks to the use of a spatially staggered mesh, the stencil of the final velocity system involves only the element and its direct neighbors and the linear system can be efficiently solved via matrix-free iterative methods. Despite the necessity to solve a linear system, the numerical scheme is still computationally efficient. The chosen discretization and the linear nature of the governing PDE system lead to an unconditionally stable scheme, which allows large time steps even for low quality meshes that contain so-called sliver elements. The fully discrete staggered space-time DG method is proven to be *energy stable* for any order of accuracy, for any mesh and for any time step size. For the particular case of a simple Crank-Nicolson time discretization and homogeneous material, the final velocity system can be proven to be symmetric and positive definite and in this case the scheme is also exactly *energy preserving*. Althrough the derived method is unconditionally stable, for real geometries the mesh may contain sliver elements, leading to an ill-conditioned linear system. We then present a simple and efficient physics-based preconditioner that is useful in the presence of sliver elements. Since we use a matrix-free iterative Krylov subspace method for the solution of the main linear system, the parallelization of the algorithm is straightforward using the MPI standard. The involved matrix-vector multiplication is then based on a simple domain decomposition that takes advantage from the small stencil size of the linear system. The new scheme is applied to several test problems in two and three space dimensions, providing also a comparison with high order explicit ADER-DG schemes. We present also several numerical comparison with other reference solutions.

References

[1] M. Tavelli, M. Dumbser, *Arbitrary high order accurate space-time discontinuous Galerkin finite element schemes on staggered unstructured meshes for linear elasticity*, Journal of Computational Physics, 366, 346–414, 2018.

MS02 - Polygonal and polyhedral methods: theory and applications

Proposers

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Abstract

Galerkin methods based on polytopal meshes are becoming an established technology in the framework of PDEs discretisation, thanks to the advantages that they entail compared to standard simplicial/quadrilateral finite element methods (FEMs). Amongst others, we recall the following upsides: natural design of structure preserving schemes; more efficient mesh refinement/coarsening (due to the automatic use of hanging nodes); robustness to mesh distortion and in material design simulations; easy handling of geometries featuring highly heterogeneous micro-structures and inner interfaces. In this mini-symposium, we aim at gathering young researchers working with different polytopal methods (discontinuous Galerkin, hybrid high-order, virtual elements, hybridizable discontinuous Galerkin, ...). Both theoretical advancements and more practical, engineering-oriented applications, as well as challenges in code development (including solvers and advanced solution techniques), are welcome.

Title

The virtual element method for bulk-surface PDEs and its application to battery modeling

Authors

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Abstract

We present the Bulk-Surface Virtual Element Method (BSVEM) for the spatial approximation of stationary and time-dependent coupled bulk-surface PDEs in three space dimensions, thereby extending previous work on the two dimensional case [3]. The method combines the polyhedral VEM for the bulk equations [1] and the surface Virtual Element Method (SVEM) for the surface equations [2]. We provide a geometric error analysis of polyhedral meshes independent of the method. Then, we provide a full error analysis in the lowest order case that holds even in the presence of curved boundaries, provided the exact solution is $H^{2+3/4}$ in the bulk and H^2 on the surface. The method brings all the advantages of general polyhedral meshes into the context of bulk-surface PDEs. We show the application of the method to a novel bulk-surface PDE system for battery modeling.

References

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Title

Hybrid mimetic finite-difference and virtual element formulation for coupled poromechanics

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Abstract

Simulations of physical phenomena in porous media often require handling domains with geometrical complexities. The flexibility of polytopal meshes can help the generation of meshes conforming to the changes in physical properties.
We introduce a coupling between multiphase flow and mechanics based on Mimetic Finite Differences and Virtual Element Methods, capable of handling general polygonal and polyhedral meshes. The coupling is performed via a fully implicit approach and suitable preconditioning strategies are proposed, together with stabilization strategies designed to avoid the presence of spurious pressure modes in undrained conditions. The method is validated on standard test cases.

References

[1] Andrea Borio, François P. Hamon, Nicola Castelletto, Joshua A. White, and Randolph R. Settgast. Hybrid mimetic finite-difference and virtual element formulation for coupled poromechanics. *Computer Methods in Applied Mechanics and Engineering*, 383, 2021.

Title

A stabilization free virtual element method.

Author(s)

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Stefano Berrone, Politecnico di Torino

Abstract

In this talk, we present a new family of Virtual Element Methods (VEM), that we call Enlarged Enhancement Virtual Element Methods (E^2VEM), designed to allow the definition of a coercive bilinear form that involves only polynomial projections. In [1], we introduce and analyse the first order of this method, which is based on the exploitation of higher order polynomial projections in the discrete bilinear form, maintaining the same set of degrees of freedom of the discrete space, with respect to the standard one [3]. We provide a proof of well-posedness and optimal order a priori error estimates. Numerical tests on convex and non-convex polygonal meshes confirm the criterium for well-posedness and the theoretical convergence rates. Finally, we present a comparison of the behaviour of standard VEM and E^2VEM, with the focus on some elliptic test problems whose solution and diffusivity tensor are characterized by anisotropies. These results are detailed in [2].

References

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[3] L. Beirão da Veiga and F. Brezzi and L. D. Marini and A. Russo , *Virtual Element Methods for General Second Order Elliptic Problems on Polygonal Meshes*, Mathematical Models and Methods in Applied Sciences, 26(04):729-750, 2015.

Title

Virtual Element Method for image-based domain approximation

Author(s)

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Abstract

We consider the problem of solving the Poisson problem in 2D on domains with curved boundaries, approximated by polygonal domains that are the union of squared elements. We consider a VEM discretization combined with a projection approach similar to [2, 3] and we show, both theoretically and numerically, that resorting to the use of polygonal elements allows to satisfy the assumptions required for the stability of the projection approach. Thus the potential of higher order methods can be fully exploited. The resulting approach represents an effective alternative to the use of finite element method, thanks also to an efficient strategy that allows to reduce the number of degrees of freedom that do not actively contribute to the consistency of the method. The proposed approach can be extended to the three dimensional case. We present numerical experiments to assess the well behaviour of our strategy.
The results presented are taken from [1].

References

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[3] J. H. Bramble, T. Dupont and V. Thomée, *Projection method for Dirichlet's problem in approximating polygonal domains with boundary-value corrections*, Math. Comp. 26 (120), (1972) 869-879.

Title

Artificial Neural Network evaluation of Poincaré constant for Voronoi polygons

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Abstract

We propose a method, based on Artificial Neural Networks, that learns the dependence of the constant in the Poincaré inequality on polygonal elements of Voronoi meshes, on some geometrical metrics of the element. The cost of this kind of algorithms mainly resides in the data preprocessing and learning phases, that can be performed offline once and for all, constructing an efficient method for computing the constant, which is needed in the design of the a posteriori error estimates in numerical mesh-based schemes for the solution of Partial Differential Equations.

Title

A family of Virtual elements for 3D elasticity problems

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Abstract

The Virtual Element Method (VEM) is a recent technology for the approximation of partial differential equation problems, which shares the same variational background of the Finite Element Method (FEM). The main features of this technique are its robustness to deal with general polygonal and polyhedral meshes, including hanging nodes and non-convex elements, and its flexibility to handle some interesting properties of the problem.
In this talk, we focus on the resolution of linear elasticity problems. More precisely, we consider the variational formulation based on the Hellinger-Reissner principle. In this framework it is well known that, for classical Galerkin schemes, designing a suitable method that preserves both the symmetry of the stress tensor and the continuity of the tractions at the inter-element is typically not a simple task. The principal reason behind this difficulty lies in the rigid structure of the polynomial approximation space. Therefore, our idea is to exploit the great flexibility of the VEM to avoid these troubles and design stable methods. Recently, some Virtual Element schemes have been proposed and analyzed both for two and three-dimensional problems [1, 2, 3].
The aim is to present an extension to the three-dimensional case for a family of Virtual Element Methods. Some numerical tests are provided in order to show the validity and the potential of our analysis [4].

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Title

Machine Learning based refinement strategies for polytopal grids with applications to Virtual Element and Discontinuous Galerkin methods

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Abstract

We propose new strategies based on Machine Learning techniques to handle polygonal and polyhedral grid refinement, to be possibly employed within an adaptive framework. Specifically, Convolutional Neural Networks (CNNs) are employed to classify the "shape" of an element so as to apply "ad-hoc" refinement criteria. CNNs can be used to enhance existing refinement strategies at a low online computational cost. The k-means clustering algorithm is used to refine polytopes with unknown shapes in a robust manner. This strategy is a variation of the well known Centroidal Voronoi Tessellation. We test the proposed algorithms considering two families of finite element methods that support arbitrarily shaped polytopal elements, namely the Virtual Element Method (VEM) and the Polytopal Discontinuous Galerkin (PolyDG) method. We demonstrate that these strategies do preserve the structure and the quality of the underlying grids, reducing the overall computational cost and mesh complexity.

Title

A space–time virtual element method for the heat equation.

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Abstract

We present the first space–time virtual element method for the heat equation [1], which generalizes the finite element method proposed by Steinbach in [2] to polytopal meshes.
Local test and trial discrete functions are solutions to a heat equation with polynomial data. Global virtual element spaces are constructed in a nonconforming fashion, as this allows for a unified analysis that is independent of the spatial dimension and possible Trefftz variants.
As the method can easily deal with nonmatching space-like and time-like faces, it is very suitable for space-time adaptivity.

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Title

Discontinuous Galerkin approximation of the fully-coupled thermo-poroelastic problem

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Abstract

Poroelasticity inspects the interaction among fluid flow and elastic deformations within a porous medium. In several applications in the context of environmental sustainability, such as geothermal energy production and CO_2 sequestration, temperature plays a key role in the description of the physical phenomena. Thus, in order to correctly describe these geological processes, the differential problem should also take into account the influence of the temperature, leading to a fully-coupled thermo-poroelastic (TPE) system of equations [1]. We present and analyze a polytopal discontinuous Galerkin (PolyDG) method for the numerical modelling of the quasi-static fully-coupled thermo-poroelastic problem. The geometric flexibility and the arbitrary-order accuracy featured by PolyDG methods ensure a high-level of flexibility and precision that are needed to properly represent the solutions. As a starting point for the design of the numerical scheme, we adopt a four-field weak formulation inspired by [2], where an additional total pressure variable is added in order to ensure robustness in the quasi-incompressible limit and inf-sup stability. We perform a robust stability analysis for the linearized semi-discrete problem under mild requirements on the problem data. A priori *hp*-version error estimates in suitable energy norms are also derived. Finally, a complete set of numerical simulations is presented in order to validate the theoretical analysis, to inspect numerically the robustness properties, and to test the capability of the proposed method in a practical scenario inspired by a geothermal problem.

This research work has been funded by the European Commission through the H2020-MSCA-IF-EF project PDGeoFF (Grant no. 896616).

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Title

BDDC preconditioners for 3D divergence free virtual element discretizations of the Stokes equations.

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Abstract

The balancing domain decomposition by constraints (BDDC) preconditioners are domain decomposition methods based on the subdivision of the computational domain of a partial differential equation (PDE) into non-overlapping subdomains. BDDC methods represent an evolution of balancing Neumann-Neumann methods, that have been used extensively in the past to solve large scale finite element problems.
In our work, we apply BDDC to solve PDEs where the space discretization is performed by Virtual Element Methods (VEM), a new family of methods introduced in 2013, which could be considered as a generalization of finite element methods to arbitrary element-geometry. The advantage of these methods is that we can apply them on a wide choice of general polygonal/polyhedral meshes without integrating complex non-polynomial functions on the elements, keeping a high degree of accuracy.
Following our previous work on the two-dimensional case [4], we present here a BDDC algorithm [1, 2] to solve the Schur complement system obtained from a recent divergence free VEM discretization of the three-dimensional Stokes equations [3]. Firstly, we briefly present the VEM mathematical framework, then we analyze theoretically the convergence of the proposed BDDC preconditioners and finally we report some computational results that validate the theoretical estimates.

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MS03 - Additive manufacturing: challenges and perspectives

Proposers

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Abstract

Additive Manufacturing (AM) technologies are undergoing exponential growth in many engineering fields, from aerospace to biomedical applications, from fashion to the food industry. The main benefit of this technology is the possibility to design the product such that it is optimized for a specific function. The manufacturing constraints are dramatically reduced and the designer can finally focus more on the intended application of the part rather than on its manufacturability. As a direct consequence of AM diffusion, there is an increasing necessity of a deeper understanding of the complex process-structure-property relationships occurring in AM to optimize the manufacturing process parameters as well as to generate an optimal design of 3D printed structures. This Symposium aims at presenting and discussing the most recent results in the field of AM both from an experimental and a numerical point of view. The Symposium addresses, but is not limited to, the following topics:

1. Ontologies for AM
2. AM material modelling
3. Topology optimization and AM design
4. Advanced numerical techniques for AM process and product simulations
5. AM metrology and sensing
6. Uncertainty Quantification for AM

Title

Defect prediction in laser powder bed fusion based on thermographic features utilizing convolutional neural networks

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Abstract

The appearance of irregularities such as keyhole porosity is a major challenge for the production of metal parts by laser powder bed fusion (PBF-LB/M). The utilization of thermographic in-situ monitoring is a promising approach to extract the thermal history which is closely related to the formation of irregularities [1]. In this study, we investigate the utilization of convolutional neural networks to predict keyhole porosity based on thermographic features. Here, the porosity information calculated from an x-ray micro computed tomography scan is used as reference. Feature engineering is performed to enable the model to learn the complex physical characteristics of the porosity formation. The model is examined with regard to the choice of hyperparameters, the significance of thermal features and characteristics of the data acquisition. Based on the results, future demands on irregularity prediction in PBF-LB/M are derived.

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Title

Multi-scale approach for the estimation of the stress-strain response of laser powder bed fusion lattice structure

Authors

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Abstract

In the last few years additive manufacturing (AM), in particular laser powder bed fusion (LPBF), gave the possibility to easily obtain structural components with complex geometrical features. In this regard, lattice structures represent a good opportunity since these latter allow to realize lightweight components with enhanced mechanical properties. In a large number of papers available in the literature, the mechanical properties of AM material are studied but, regarding lattice structures obtained by LPBF, its mechanical behavior is still difficult to predict, due to microstructure modifications as a consequence of the scanning strategy and building direction. This study proposes a novel multi-scale approach to predict the effective σ–ε curve within the lattice structure, consisting in local measurements carried out by nano-indentation, in different regions of the lattice structure, and along different orientations to estimate the effective behavior of the component. In this way, possible modifications of the microstructure induced by the process have been captured. Based on the experimental investigations at both macro and nano-scale, a numerical model for stainless steel 316L octet-truss lattice specimen has been calibrated, and, in order to improve the accuracy of the simulations, the geometrical model was built starting from the real component, analyzed through μ-CT.

Title

Uncertainty Quantification for Additive Manufacturing

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Abstract

The present paper aims at the application of Uncertainty Quantification (UQ) techniques for a thermo-mechanical model of an Inconel 625 beam using PBF-LB/M (Laser-based Powder Bed Fusion of Metals) technology. In particular, we propose an UQ approach to reduce the uncertainties of the activation temperature, gas convection coefficient and powder convection coefficient involved in the simulation of the PBF-LB/M process. First, we perform a variance-based Global Sensitivity Analysis (GSA) to study the sensitivity of the uncertain parameters by observing their influence on the displacement prediction. The GSA results allow us to conclude that the gas convection coefficient does not influence the displacements and can therefore be kept constant for subsequent analyses. Secondly, we conduct an inverse UQ analysis, based on the Bayesian approach on synthetic displacement data, to calibrate the PBF-LB/M parameters; afterwards, we perform a forward UQ analysis, based on the posterior uncertainty, to accurately estimate residual strains. Moreover, to reduce the computational costs of PBF-LB/M process simulations, we adopt a surrogate modeling approach based on the Sparse Grid method. The results show the ability of the proposed approach to reduce the uncertainties of the activation temperature and powder convection coefficient, which in turn implies that the uncertainty in residual strain prediction using the PBF-LB/M model can be significantly reduced.

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Title

An Ontology-based Approach to Defect Detection in Additive Manufacturing

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Abstract

Developing control systems for automated Additive Manufacturing (AM) services that are capable of addressing both data integration and semantic interoperability issues, as well as monitoring and decision making tasks, is a key challenge for Industry 4.0 applications [1]. To this goal, principled knowledge representation approaches based on formal ontologies have been proposed as a foundation to information management and maintenance in presence of heterogeneous data sources for AM processes [4]. In addition, ontologies provide reasoning and querying capabilities to aid domain experts and end users in the context of constraint validation and decision making [3]. Finally, ontology-based approaches to AM services can support the explainability and interpretability of the behaviour of monitoring, control and simulation systems that are based on black-box machine learning algorithms [5]. In this work, we focus on metal AM processes, providing a novel ontology for the classification of process-induced defects known from the literature [2]. Together with a formal representation of the characterising features and sources of defects, we integrate our taxonomy with state-of-the-art ontologies in the field [6]. Our knowledge base aims at enhancing the modelling capabilities of metal AM ontologies by adding further defect analysis terminology and diagnostic inference features. Towards future research directions, we also illustrate our ontology in the context of a broader control architecture envisioned for automated AM production services, to be developed together with a neural network component for run-time defect detection.

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Title

Space-time *hp*-finite elements for heat evolution in laser powder bed fusion additive manufacturing

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Abstract

Laser powder bed fusion is an additive manufacturing technique where three-dimensional parts are printed by successively stacking layers of metal powder and melting the areas inside the geometric model using a high-powered laser. Various defects can arise during the process, such as residual stresses after cooling, geometric inaccuracies due to lack of fusion and overheating, or an inconsistent microstructure with varying mechanical properties. Numerical simulations can help identify potential flaws and improve the printing process, but they are challenging due to the vast differences in spatial and temporal scales.
We address this challenge using four-dimensional space-time hp-finite elements [1] that we refine locally in space-time towards the laser spot. This way, we simultaneously reduce the element size and duration, whereas classical time-stepping approaches only reduce the element size in space. We discuss a Petrov-Galerkin [2] and least-squares formulation [3] of the nonlinear heat equation with an apparent heat capacity model. By dividing the entire duration of the simulation into consecutive time slabs, we reduce the individual problem sizes until we can compute them on personal computers.
We validate our model for single laser strokes on bare metal substrates, where we compare the predicted melt pool dimensions to the data obtained from experiments [2] and discuss the limitations of thermal models. We then compare the performance of our Petrov-Galerkin and least-squares formulations to a time-stepping approach with an equivalent spatial resolution.

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MS04 - Largescale linear algebra problems: solvers for scientific challenges

Proposers

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Abstract

Many solution strategies for challenges in applied mathematics produce large scale linear algebra problems. They range from the most common solution of (sequences of) extremely large and sparse linear systems, to the efficient computation of more general matrix functions, and the solution of ill-posed problems. Consequently an interaction between specialists in the application domains and the linear algebra community is pivotal for reaching satisfactory results. The main goal of this minisymposium is showcasing success stories that come from this interaction. The discussed applications will focus on – but are not limited to – the approximation of the numerical solution of Partial Differential Equations, analysis of Complex Networks, and data-retrieval challenges. The contributions will, on one hand, address how to translate real-world applications into the numerical linear algebra setting. On the other, they will focus on the newest development in solvers techniques both from the implementation and theoretical sides.

Title

Improved parallel-in-time integration via low-rank updates and interpolation.

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Abstract

This work [2] is concerned with linear matrix equations that arise from the space-time discretization of time-dependent linear partial differential equations (PDEs). Such matrix equations have been considered, for example, in the context of parallel-in-time integration leading to a class of algorithms called ParaDiag [1]. We develop and analyze two novel approaches for the numerical solution of such equations. Our first approach is based on the observation that the modification of these equations performed by ParaDiag in order to solve them in parallel has low rank. Building upon previous work on low-rank updates of matrix equations, this allows us to make use of tensorized Krylov subspace methods to account for the modification. Our second approach is based on interpolating the solution of the matrix equation from the solutions of several modifications. Both approaches avoid the use of iterative refinement needed by ParaDiag and related space-time approaches in order to attain good accuracy. In turn, our new approaches have the potential to outperform, sometimes significantly, existing approaches. This potential is demonstrated for several different types of PDEs.

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Title

Symbol–based multigrid methods for linear systems in saddle–point form

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Abstract

A variety of applications requires the solution of linear systems in saddle–point form. In these cases, it is possible to formulate the problem in such a way that the system matrix is symmetric, but indefinite. Therefore, Ruge–Stüben theory – usually used to prove multigrid convergence – cannot be directly applied [4]. Powerful smoothers are often used to take into account the special coupling, represented by the off-diagonal blocks [1, 2]. Instead of altering the smoother, a different algebraic approach has been recently presented [3].
In this talk, we analyse the case where the blocks of the saddle–point coefficient matrix have a particular Toeplitz structure. In this way the associated generating functions play a central role in the formulation of the Two–Grid method convergence analysis. The resulting symbol–based approach provides sufficient conditions for convergence that are feasible to check in applications. In addition, a strategy to choose the optimal smoothing relaxation parameter is included.
Finally, we show that the presented approach preserves the same matrix structure at coarser levels and that it possesses a "level independence" property. The numerical tests on V–cycle and W–cycle methods confirm that also the recursive application of the proposed strategy is effective.

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Title

Minimal-norm Gauss–Newton method for large scale problems.

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Abstract

In this work, we will describe a regularized Gauss–Newton method for the computation of the minimal-norm solution to underdetermined nonlinear least-squares problems [1, 2]. The approximate solution of the iterative method is obtained from that of Gauss–Newton by adding a correction vector, and depends on two relaxation parameters which are automatically estimated. We will focus on medium and large scale problems. In this case, the iterative method projects each linearized step in a suitable Krylov space. Numerical experiments concerning imaging science will be presented to illustrate the performance of the method.

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Title

A comparison of different graph-theoretic measures for identifying low- and high-density forms of liquid water

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Abstract

Water is a complex liquid with anomalous properties. Various models have been hypothesized to explain many of these peculiarities, the most popular is centered on the existence of two liquid forms of water with different densities: the low-density liquid (LDL) and the high-density liquid (HDL). In the simplest models, a box containing water molecules can be represented as a graph, where the nodes correspond to the molecules, and the edges of the graph denote the chemical bonds. In our previous work [3], we presented a new order parameter based on graph theory, in particular on the Total Communicability (TC) [1] to identify these two density forms. Given a node v_i, the TC is defined as $TC(v_i) = [e^{\beta A}\mathbf{1}]_\mathbf{i}$, where $\mathbf{1}$ is the vector of ones, A is the adjacency matrix of the network, and $\beta > 0$ is a parameter. This quantity has an interpretation in terms of walks on the graph, it takes into account the global properties of the network, and it can be computed efficiently using algorithms for computing the action of a matrix function on a vector. In this talk, we propose to investigate additional centrality measures [2] for the structural characterization of liquids: the closeness centrality and the betweenness centrality, which are based on the shortest paths in the network, the Katz centrality and the subgraph centrality, which can be rewritten in terms of matrix functions and take into account the spectral properties of the network. Since these centrality measures are descriptors of the structural properties at the molecular level, we also explore their ability to identify clusters of water molecules at very high local density.

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Title

Monolithic solution strategies for large-scale computational problems from physiology and astrophysics

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Abstract

Currently, many problems in applied mathematics result in large-scale computational challenges which require the use of massively parallel machines and scalable solution strategies to minimize the time to solution. In this talk we present monolithic strategies to numerically solve partial differential equations, for various applications. These strategies consists in framing, whenever possible, a computational problem in a large and possibly sparse (non) linear system which can be solved, in parallel, combining efficient preconditioning techniques and Krylov methods. By contrast, many traditional staggered approaches are based on the solution of a sequence of smaller computational problems. An example of such a paradigm can be found when solving evolutionary problems, where a monolithic strategy (also known as all-at-once approach) can be used, resulting in the assembly of large a space-time system with a block Toeplitz structure, in contrast to standard sequential time-stepping techniques. In this context, we consider the space-time discretization of the anisotropic diffusion equation, using isogeometric analysis in space and a discontinuous Galerkin approximation in time. Drawing inspiration from a former spectral analysis of space-time operators [1], we propose a parallel multigrid preconditioned GMRES method [2]. The application of this multilevel space-time strategy to a non-linear reaction-diffusion problems from electrophysiology (i.e. the monodomain equation and the EMI model) will be also discussed, considering comparison with other recently developed methods. Moreover, we present a monolithic approach to simulate radiative transfer in stellar atmosphere; in this scenario we present a matrix-free implementation of a multi-fidelity preconditioner [3]. Through simulations on massively parallel systems, we show how monolithic strategies can improve software scalability and discuss the trade-offs of this approach.

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MS05 - Advances in spline constructions for geometric modeling & processing and numerical simulations

Proposers

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Abstract

Thanks to their great theoretical and applied developments over the last years, splines can be considered an excellent tool for approximation, [1, 2]. Yet, their potential is not exhausted, they are still thriving and several problems need to be tackled, both for theory and applications. The minisymposium aims to gather early career researchers in different spline fields to discuss the open problems and challenges in numerical simulation, approximation theory, and geometric modeling. In particular, the construction of curves and surfaces with high smoothness still poses significant difficulties, therefore, suitable multi-patch representations should be addressed, both theoretically and practically. Additionally, more flexible schemes, deriving from the combination of approximation and spline interpolation could be explored. Specific topics for the contributions include (but are not limited to): mathematical properties and analysis of diverse spline models, evaluation and comparison of existing strategies, software development and applications of spline based methods to real industrial problems.

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Title

An interpolatory view of spline weighted least squares approximation

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Abstract

Least squares approximations are ubiquitous in applications when trying to reconstruct an unknown function from its observations. In this talk, we consider the more general framework of weighted least square methods. We derive a formula for weighted spline least squares approximation where we express the approximate as a convex combination of its interpolates. We also discuss recent results on two related problems: the truncated weighted least-square spline approximation and the optimal choice of weight functions for the weighted least squares problem. The analytical results are complemented by numerical experiments.

Title

3D data stream interpolation with PH quintic splines for path planning applications

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Abstract

The design strategy of path planning for autonomous vehicles should consider several aspects, from the accuracy and smoothness of the trajectory to the efficency of the control algorithm. In the specific case of 3D data stream points, the versaltility and locality of the interpolating trajectory design is fundamental. For this aim, an interesting choice is to rely on Pythagorean Hodograph (PH) splines, thanks to their low computational cost features [1].
In this talk we first present an efficient local data stream interpolation algorithm to successively construct each spline segment as a quintic PH biarc interpolating second and first order Hermite data at the initial and final end-point, respectively. The locally required second-order derivative information is taken from the previous segment. Consequently, the data stream spline interpolant is globally C^2 continuous and can be constructed for arbitrary C^1 Hermite data configurations. We than propose a simple and effective selection of the free parameters that arise in the local interpolation problem.
A path planning and guidance module design is than presented, responsable for the motion of vehicles along a certain trajectory [2]. We introduce a path following guidance law, capable to give a robust response to unknown constant disturbances even in the case of under-actuated vehicles. A selection of numerical experiments, based on different data sets, validates the effectiveness of both the trajectory design and the guidance strategy, when the target position of the vehicle is computed with the PH spline interpolation algorithm mentioned above and when, considering only input point streams, local rules for derivative approximations has been coupled with the inteprolation scheme [3].

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Title

A spline-based regularized method for the reconstruction of geological models from sparse data

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Abstract

The construction of a geological numerical model is a key step in the study and exploration of the subsurface. These models are constructed from seismic or well data. Often the available data are sparse and noisy, which makes this task difficult, mainly for reservoirs where the geological structures are complex with distinct discontinuities and unconformities.
In this presentation, we propose a new method to compute an implicit function of the stratigraphic layers. In this method, the data are interpolated by piecewise quadratic C1 Powell-Sabin splines and the function is regularized via a diffusion partial differential equation PDE. The method is discretized in finite elements on a triangular mesh conforming to the geological faults.
Compared to classical interpolation, the use of piecewise quadratic splines on a mesh has three major advantages. First, a better handling of stratigraphic layers with strong curvatures. Second, a reduction in the resolution of the mesh, allowing a considerable gain in computation time. Third, a local adaptivity to the geometry of the data, taking faults into account.
The regularization of the function is the most difficult component of any implicit modeling approach. Often, classical methods produce inconsistent geological models, in particular for data with high thickness variation, and bubble effects are generally observed. To address these problems, we propose a new scheme in which a diffusion term is introduced and iteratively adapted to the shapes and variations of the data, while minimizing the fitting error.

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Title

A Quantitative Comparison of Smooth Multi-patch Constructions for Isogeometric Analysis

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Abstract

One of the main advantages of isogeometric analysis (IGA) is the use of splines as the basis for numerical simulations, which allows for increased smoothness across element boundaries. Among several advantages of this increased smoothness is the ability to work with higher-order derivatives in variational formulations, which enable simplified discretizations for problems like the rotation-free Kirchhoff-Love shell model. However, for multi-patch spline representations - which are used for representations of more complex geometries - higher-order continuity is only achieved by modifying either the patch-wise defined basis functions or the variational formulation. In the former case, penalty or Nitsche-like strategies can be used, among others. Such methods gained a lot of popularity and provide a relatively easy formulation in existing assemblers. In the latter case, unstructured spline constructions as the D-patch [1], Argyris-like coupling methods [2, 4] or the recently developed almost-C^1 [3] construction can be employed. In the present work, we aim to provide a quantitative comparison of the aforementioned smooth multi-patch constructions for isogeometric analysis. The comparison presented here consists of a more theoretical part based on the bi-harmonic equation, as well as a more practical part applied to Kirchhoff–Love shells. In the theoretical part, convergence rates and computational times are compared. In the practical part, the applicability of the methods is assessed on a car geometry and their accuracy is evaluated.

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Title

Isogeometric Analysis with C^1-smooth functions for multi-patch Kirchoff-Love shells

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Abstract

We present an isogeometric method for the analysis of Kirchhoff-Love shell structures which are composed of multiple patches and which possibly possess extraordinary vertices, i.e. vertices with a valency different to four. The proposed isogeometric shell discretization is based on the one hand on the approximation of the mid-surface by a particular class of multi-patch surfaces, called analysis-suitable G^1 [1], and on the other hand on the use of the globally C^1-smooth isogeometric multi-patch spline space introduced in [2]. We use our developed technique within an isogeometric Kirchhoff-Love shell formulation [3] to study linear and nonlinear shell problems on multi-patch structures. Thereby, the numerical results show the great potential of our method for the Kirchhoff-Love shell analysis of geometrically complex multi-patch structures which cannot be modeled without the use of extraordinary vertices.

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Title

Construction and Analysis of a G^1-smooth polynomial family of Approximate Catmull-Clark Surfaces

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Abstract

Subdivision surfaces are a widely used numerical method to reconstruct smooth surfaces starting from a polyhedral mesh of any topology. However, in presence of the so-called extraordinary vertices, i.e. vertices with valence $N \neq 4$, the limit surface presents a loss of regularity like, for instance, the Catmull-Clark surface. To recover smoothness around these particular points the multipatch approach can be used, for instance, imposing tangent plane continuity (G^1 smoothness) around the extraordinary patches. Starting from the work of Loop and Shaefer [3] which presents an approximate bicubic Bézier patching of the Catmull-Clark limit surface defined by local smoothing masks, employing quadratic glueing data functions I modify the previous scheme to obtain G^1 continuity around the EVs. This construction leads to a family of surfaces that are given by means of explicit formulas for all involved control points. Moreover, I conduct a curvature analysis in order to assert the quality of the resulting surfaces, both visually and numerically.

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MS06 - Enabling technologies for uncertainty quantification and optimization in real-world applications

Proposers

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Abstract

Sevel problems of practical interest arising in the field of physics, engineering, and natural sciences in general, require complex physics-based models to accurately assess the behavior of the phenomenon under investigation. Such models usually depend on several variables/parameters accounting for the physical and geometrical properties of the system. In many applications, e.g., uncertainty quantification (UQ) analysis and optimization, the design/uncertain parameter space needs to be accurately explored and exploited. This easily results in a large number of simulations, especially in the case of high-dimensional spaces (curse of dimensionality). Even if, on the one hand, the increase of the available computational resources makes the simulations of such complex systems feasible in theory, in practice costs and time constraints makes high-fidelity UQ and optimization unfeasible for most users and projects. Therefore, methods and approaches to reduce the computational cost of UQ and optimization are required and have been proven to be crucial, especially when the mapping between the parameter space and the output quantity of the simulations is highly nonlinear. Hence, the aim of this mini-symposium is to discuss some of the recent developments regarding methods for enabling uncertainty quantification analysis and optimization in real-world applications (such as supervised and unsupervised machine learning, dimensionality reduction, multi-fidelity approaches, etc.).

Title

Operator network approximations for some elliptic parametric PDEs.

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Abstract

The application of neural networks (NNs) to the numerical solution of PDEs has seen growing popularity in the last five years: NNs have been used as an ansatz space for the solutions, with different training approaches (PINNs, deep Ritz methods, etc.); they have also been used to infer discretization parameters and strategies.
In this talk, I will focus on the convergence of operator networks that approximate the solution operator of linear elliptic PDEs. I will, in particular, consider operator networks that, given a fixed right-hand side, map sets of diffusion-reaction coefficients into the space of solutions (coefficient-to-solution map). When the coefficients are smooth and with periodic boundary conditions, the size of the networks can be bounded with respect to the H^1-norm of the error, uniformly over the parameter set. Specifically, the number of non zero weights grows at most poly-logarithmically with respect to the error. By concatenating neural netowrks, we can extend the analysis to parametric coefficients, depending on a potentially infinite number of parameters.

Title

Uncertainty Quantification for parametrized PDEs using Deep Orthogonal Decomposition

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Abstract

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, UQ becomes extremely challenging and computationally expensive whenever dealing with high-dimensional and complex systems, such as those driven by PDE models. In these cases, one way to go is to resort to Reduced Order Models (ROMs), a class of model surrogates that can efficiently replace expensive routines, such as numerical solvers, at a negligible compromise in accuracy [1]. Here, we consider models described by parameter dependent PDEs and we address both forward and inverse UQ problems. To counter the computational cost, we propose a novel approach based on Deep Neural Networks (DNNs) that we call Deep Orthogonal Decomposition (DOD). The latter is an adaptation of the so-called Principal Orthogonal Decomposition [4], where a DNN model is used to describe the solution manifold in terms of an adaptive local basis. The approach results in a nonlinear strategy that can also benefit from some of the properties that are typical of linear methods. In particular, as we demonstrate over a broad range of numerical experiments, DOD allows for new and nonintrusive ways of performing UQ. The experiments considered include applications to oxygen perfusion in biological tissues [2, 3], advection-diffusion-reaction systems and fluid flow in complicated domains.

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Title

Deep-learning based ROMs for fast transient dynamics.

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Abstract

In recent years, large-scale numerical simulations played an essential role in estimating the effects of explosion events in urban environments, for the purpose of ensuring the security and safety of cities. Such simulations are computationally expensive and, often, the time taken for one single computation is large and does not permit parametric studies.
The aim of this project is to facilitate real-time and multi-query calculations by developing a non-intrusive Reduced Order scheme. Reduced Order Models (ROM) allow us to reduce the computational time employed by a single simulation by reducing the dimension of the system. The scheme hereby proposed is based on a combination of traditional methods, such as the Proper Orthogonal Decomposition (POD), and deep learning techniques. In the case of blast waves, the parametrised PDEs are time-dependent and non-linear and represent a transient and fast event. For such problems, the Proper Orthogonal Decomposition (POD), which relies on a linear superposition of modes, cannot approximate the solutions efficiently. Therefore, we add a nonlinear reduction step based on Autoencoders (AE), which are a type of artificial neural network. The efficacy of this method is shown in an example consisting of an explosion happening in the vicinity of a building. We show that the deep-learning based ROM introduced can reconstruct the solutions efficiently and performs better than the traditional POD method.

Title

Non-intrusive surrogate modeling of frequency response surfaces via locally adaptive sparse grids

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Abstract

Numerical methods for time-harmonic wave propagation phenomena are often computationally intensive. In this framework, model reduction methods can be used to obtain a cheap and reliable approximation of the frequency response of the system. In this talk, we consider parametric frequency response problems, where the high-fidelity problem depends not only on the (complex) frequency $\omega \in \mathbb{C}$, but also on additional design/uncertain parameters $\theta \in \mathbb{R}^{n_\theta}$, $n_\theta \geq 1$. More precisely, we will seek an approximation of a Hilbert-space-valued map of the form

$$u : \mathbb{C} \times \mathbb{R}^{n_\theta} \ni (\omega, \theta) \mapsto u(\omega, \theta) \in \mathcal{V},$$

where $\mathcal{V}$ is the Hilbert space containing the solution of the frequency-domain problem of interest, e.g., $\mathcal{V} = H^1(\Omega)$ (or a suitable finite element discretization) for the solution of the Helmholtz equation over the physical domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. In practice, $u(\omega, \theta)$ is defined as the solution of a PDE which depends parametrically on ω and θ. For instance, the parameters θ may be employed to model material or geometric properties of the system under consideration.
Our method [1] first builds a database of frequency-response surrogate models via minimal rational interpolation [2], by freezing the extra parameters. Then, the different frequency-dependent surrogate models are combined over parameter space. This requires special care due to the rational nature of the surrogates. The exploration of the (potentially, high-dimensional) parameter space is carried out via locally adaptive sparse grids, through which one can weaken the curse of dimension while sampling parameter configurations in an adaptive way.
All of this is carried out in a non-intrusive way: our algorithm may be applied even without knowledge of (or access to) the structure of the problem that yields u as solution. This is in contrast with some other popular model reduction techniques like the "reduced basis" method, and is of practical interest for several reasons, e.g., when the (finite element) solver that computes u is a black box (which is the case when closed-source proprietary code is used), or when the data comes from lab experiments rather than from numerical simulations.

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Title

State augmentation method for buffeting analysis of structures subjected to non-stationary wind

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Abstract

Extreme wind events such as hurricanes and thunderstorms always exhibit considerable non-stationary characteristics, having time-varying mean wind speeds and non-stationary wind fluctuations. The rapid changes in these flows can potentially amplify aerodynamic loads on structures and result in higher non-stationary buffeting responses. When considering aeroelastic effects, the aerodynamic damping will be time-dependent due to the time-varying mean wind speed, and the wind-structure coupled system can be thus represented as a linear time-varying (LTV) system [1].

In view of these non-stationary effects, many attempts have been made to develop random vibration theory for non-stationary buffeting, including the Monte Carlo method, generalized frequency-domain method, and pseudo excitation method. However, some methods may need intensive calculations due to time-integration process, and some may be difficult to consider time-dependent system properties.

Based on the theory of Itô's stochastic differential equation, Grigoriu [2] proposed the state augmentation method to calculate the stochastic response of linear systems subjected to stationary excitations. With this method, the moments of any order of the response can be directly obtained by solving a system of linear differential equations with high efficiency. Although this method has been applied in several wind engineering problems, it has not been reported for non-stationary buffeting analysis.

The aim of this paper is to extend the state augmentation method to investigate the non-stationary buffeting of a bridge tower under non-stationary winds. The non-stationary wind speed is characterized as a time-varying mean and uniformly modulated wind fluctuations. By using the Ornstein–Uhlenbeck process to approximate wind fluctuations, the augmented states of the system and the excitation are written as an Itô-type stochastic differential equation. Based on Itô's lemma, the moments equation of the non-stationary response is derived as a system of first-order ordinary differential equations. The proposed method is validated by comparisons with the Monte Carlo method and the pseudo excitation method. The result shows that the state augmentation method has higher accuracy and efficiency than the well-accepted time-frequency techniques.

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Title

Retrieval of surface emissivity from FORUM-EE9 simulated measurements: optimization of constraints

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Abstract

FORUM (Far-infrared Outgoing Radiation Understanding and Monitoring, [1]) is a satellite mission selected in 2019 as the ninth ESA (European Space Agency) Earth Explorer mission. FORUM will provide interferometric measurements in the spectral interval encompassing the Far-InfraRed (FIR) part of the spectrum which is responsible for about 50% of the outgoing longwave flux [2] lost by our planet into space. None of the existing sounders is able to measure the Top of the Atmosphere (TOA) resolved spectrum in the FIR and this unique contribution will reduce the uncertainties in the Earth energy budget (i.e. the Earth global warming). The observations will also improve the knowledge of some atmospheric variables such as tropospheric water vapour, ice cloud properties and land emissivity in the FIR. In the early stages of the mission development, an End-to-End Simulator (E2ES) has been devised as a support tool for demonstrating proof-of-concept of the instrument and to evaluate the impact of instrument characteristics and scene conditions on the quality (precision, accuracy) of the reconstructed atmospheric products [3].
The retrieval is the inversion of the radiative transfer equation. In the retrieval step, performed in the E2ES by the CLAIM (CLouds and Atmosphere Inversion Module) code, the atmospheric state that best reconstructs the simulated measured spectrum is determined. The inversion is a severely ill-conditioned problem, and is solved using a Gauss-Newton (GN) method combined with the Optimal Estimation (OE) approach, a Tikhonov regularization scheme based on a Bayesian approach that is standard in the remote sensing community. The retrieved profiles may anyway present unphysical oscillations, so that an a-posteriori regularization has been applied after the GN method convergence: the Iterative Variable Strength regularization (IVS). In this seminar I will focus on the retrieval of the surface emissivity, in particular on the choice of the retrieval grid step and the IVS parameters, using the FORUM simulated measurements in different latitude bands [4].

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Title

Multifidelity Optimization for Engineering Design: Space Application

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Abstract

The design and optimization of space engineering systems requires the implementation of costly high-fidelity models capable to accurately represent complex physical phenomena. Examples are computational fluid dynamic models for the numerical solution of partial differential equations that permit to capture the aerothermodynamic interaction during the re-entry of a space vehicle from an interplanetary transfer. However, simulation-based optimization usually requires a large number of model evaluations during the search for the optimal design, which makes the use of high-fidelity models unfeasible due to their high computational cost. To address this challenge, we discuss a multifidelity strategy for the design and optimization of complex systems capable to combine multiple models at different levels of fidelity in order to contain the computational cost and achieve a better design solution. We propose a strategy for multifidelity active learning that leverages low-fidelity models to explore design configurations and refines the quality of the design solution through the principled query of the high-fidelity model. The active learning scheme is formulated to merge data-driven and domain-aware sources of information and is implemented for the multidisciplinary design optimization of an Orion re-entry capsule. The optimization goals are the minimization of the propellant mass burned during the re-entry, the minimization of the structural mass of the thermal protection system and the minimization of the temperature reached by the heat shield, all referred to the baseline design configuration. The results illustrate that our multifidelity framework leads to a design improvement of the 15% with respect to the baseline solution with a fraction (7%) of the overall computational cost that would be required by a single-fidelity optimization based on high-fidelity models only.

Title

Aft form optimization of ships using surrogate models

Author(s)

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Abstract

Surrogate based optimization is an efficient tool for accelerating the design stage in hydrodynamic optimization which requires high fidelity analysis to explore the relation between system of inputs and outputs. Especially for the aft form optimization which makes the design optimization problem quite challenging since time consuming viscous effects become dominant in this flow region. Accordingly, the demand for high computational facilities increase and results in the use of surrogate strategies are inevitable in order to reduce computational burden. Therefore, it is aimed here to establish a methodology for minimum viscous resistance for the aft form optimization where the viscous effects become dominant within reasonable time. Kriging surrogate model is chosen for aft form optimization problem which constitutes many advantages; such as being a proper approach to multi-dimensional problems and being able to produce error estimates. Design of experiments (DoE) required for the training of the metamodel is achieved here by a high-fidelity flow solver. In this context, 15% of the ship's length is selected in the aft part as the optimization zone and the wetted surface geometry of the prescribed zone is defined by a limited number of control points. In this study, when generating DoE, ±10% and subsequently ±15% variations are allowed in the half-breadths of the control points. Hull form transformations are obtained by using Akima interpolation technique. Akima methodology is a continuously differentiable interpolation, built from piece-wise third order polynomials and applicable to successive intervals of the given points. Then, the metamodeling stage started to find the relation between the control point variation of the hull form and corresponding physical output of the hull form.
Accordingly, double-body, fully turbulent viscous flow computations were performed for all of the variant hull forms. Since the study focused on the minimization of viscous resistance, wave resistance is excluded from the computations to see the net viscous pressure effect of the variant hull forms on viscous resistance. The present optimization study started with a set of data, x1 to x6 (represents for half-breadths of the selected control points), which correspond to multidimensional design input of each variant hull form, with observed responses, R (presently the viscous resistance). The optimization study is then carried out for minimum viscous resistance by genetic algorithm (GA).
The approach implemented here points out that, applied metamodel is able to reduce computational time and achieve at sound results from viscous resistance point of view. Besides the differences in the predictions of the flow solver and the surrogate model on the resistance values, there is a good agreement between the surrogate model and the flow solver on the flow characteristics. In addition, from the viscous resistance results, we can say that the optimal aft is able to make the flow relatively better streamlined as compared to initial form. It can be seen from the results that the separation problem is reduced in considerable amount and 5% decrease in viscous pressure resistance is achieved in the end.

Title

Space-time shape uncertainties in the forward and inverse problem of electrocardiography

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Abstract

In electrocardiography, the "classic" inverse problem is the reconstruction of electric potentials at a surface enclosing the heart from remote recordings at 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.

The purpose of this work is to 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 several numerical experiments on a simplified but physiologically grounded two-dimensional geometry to illustrate the validity of the approach. The tested parametric dimension ranged from 100 up to 600. For the forward problem, the sparse quadrature is very effective. In the inverse problem, the sparse quadrature and the quasi-Monte Carlo method perform as expected, except for the total variation regularisation, where 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.

Title

A sequential data-integration approach to reduce uncertainty on land subsidence modeling.

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Abstract

One of the main anthropogenic causes of subsidence, i.e. the loss of land elevation, is the fluid withdrawal from the underground. In order to forecast and contrast excessive subsidence, numerical models are used. The accuracy and reliability of these tools have become fundamental in last years. In this context, correctly dealing with the uncertainties that affect the numerical models is a crucial aspect. The traditional approach to study land subsidence consists on defining a number of deterministic scenarios as input for a numerical model, whose outcomes are combined to identify confidence intervals. The clear limit of this procedure is that it cannot account for uncertainties and exploit the increasing availability of monitoring data. To overcome these deficiencies, we propose a sequential comprehensive workflow, which combines the numerical model with data assimilation techniques.
The workflow starts with the identification of the most influential sources of uncertainty. Then, the forward numerical model is used to propagate the uncertainties from the input to the output, creating a set of ensembles of Monte Carlo realizations. At this stage, three data assimilation steps are carried out, namely the χ^2-test, the Red Flag and the Ensemble Smoother. The aim is first to evaluate the representativeness of the ensembles and then constrain them with the available measurements, thus reducing the uncertainties. The application of the workflow is repeated in time according to the availability of the monitoring data in order to dynamically update the model.
The entire workflow requires a significant computational effort, especially when dealing with real cases. For this reason, we consider the use of surrogate models based on either the generalized polynomial chaos expansion or physics-informed neural networks to replace a full finite element geomechanical model.
We apply this procedure for an off-shore hydrocarbon reservoir, buried in the Northern Adriatic basin, Italy. In addition to the complexities that usually affect the modeling of a real-world case, this application is of particular interest because of the simultaneous availability of different kinds of measurements during the reservoir development. The outcome of the experimentation proves the robustness of the proposed integrated approach, the effectiveness of using the available measurements to reduce uncertainties and the efficiency of the surrogate models for geomechanics applications.

Title

Stochastic Korteweg-de Vries equation: structure-preserving numerical issues

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Abstract

In this talk, numerical issues for the stochastic Korteweg-de Vries equation [5] are analyzed under a *structure-preserving* perspective. It is well-known, indeed, that the exact solution of this stochastic partial differential equation satisfies some invariant laws [6]. In particular, the expected spatial integral of the first moment of the solution is constant in time, while the expected spatial integral of the second moment of the exact flow grows linearly in time. Here, we aim to understand whether such characterizing properties exhibited by the exact dynamics are well reproduced also along numerical approximations provided by a central finite difference scheme for the spatial discretization [7] and by stochastic ϑ-methods for time integration [4]. The long-term analysis, also confirmed by numerical experiments, reveals a linear or quadratic error growth in time [1]. Also, an ε-expansion of the exact solution [2, 3] allows us to gain insights on the behaviour of general first-order approximations to such problem, in terms of numerical invariants preservation.

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MS07 - Mathematical model in biomedicine: from optimization to machine learning

Proposers

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Abstract

In many fields of biomedicine, it is often the case that a phenomenon needs to be described starting from non-invasive indirect measurement by solving an inverse problem. To this end two paradigms may be used: on the one hand, optimization techniques exploit the knowledge of the physical model behind the phenomen to find the best solution that fits the measured data, on the other hand machine learning and deep learning techniques aim at learning the model from a huge amount of experimental data. However, the last decades have seen an increased interaction among these two paradigms. First of all, most machine learning approaches are based on the minimization of an objective function thus requiring robust and efficient optimization algorithms to be implemented. Additionally, the physical model may be used to inform machine learning approaches, by e.g. learning from a set of solutions of the inverse problem obtained via optimization. The aim of this minisymposium is to collect some new trends describing the increasing interplay between machine learning and optimization techniques with a focus on those methods that have been successfully applied in biomedical applications. Specifically the biomedical applications covered by the talks include the estimation of neural activity and connectivity from non-invasive measurement of the brain electro-magnetic field, modeling of ultrasound beam patterns, and image reconstruction from computed tomography, diffuse optical tomography, electrical impedance tomography, and limited angle tomography. Both parts of the minisymposium end with a presentation on more methodological aspects related to the topic.

Title

Data-optimized models for reconstruction in Magnetic Particle Imaging with realistic magnetic fields.

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Abstract

We present a data-optimized 3D model for Magnetic Particle Imaging (MPI) that is able to incorporate realistic magnetic fields to reconstruct the spatial distribution of para-magnetic tracers. In real MPI scanners, the generated magnetic fields have distortions that lead to deformed magnetic low-field volumes with the shapes of ellipsoids or bananas instead of ideal field-free points (FFP) or lines (FFL), respectively. Most of the common model-based reconstruction schemes in MPI use however idealized assumptions of an ideal FFP or FFL topology and, thus, generate artifacts in the reconstruction. Our approach allows to incorporate calibration measurements of the magnetic fields into the imaging model. The new data-optimized model is able to deal with distortions and can generally be applied to dynamic magnetic fields that are approximately parallel to their velocity field. We show how this 3D model can be discretized and inverted algebraically in order to recover the magnetic particle concentration. To model and describe the magnetic fields, we use decompositions of the fields in spherical harmonics. We complement the description of the new model with several simulations and experiments exploring the effects of magnetic fields distortions and of model parameters on the reconstruction.

Title

Sparse optimization of neural cross-power spectrum from indirect electromagnetic data

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Abstract

Magnetoencephalography (MEG) is a non-invasive neuroimaging technique that provides recordings close to the head surface of the brain magnetic field generated by intracranial neural currents. From a mathematical perspective, the neural activity can be described by a multivariate stochastic process, $\mathbf{X}(t) = (X_1(t), \ldots, X_n(t))^T$, whose components $X_i(t)$, $i = 1, ..., n$, model the dynamic activity of n brain areas. $\mathbf{X}(t)$ can be indirectly observed through MEG data, represented by another stochastic process, $\mathbf{Y}(t) = (Y_1(t), \ldots, Y_m(t))^T$, being m the number of employed MEG sensors. Specifically, the relationship between $\mathbf{X}(t)$ and $\mathbf{Y}(t)$ is assumed to be a linear inverse problem with additive Gaussian noise, i.e.

$$\mathbf{Y}(t) = \mathbf{G}\mathbf{X}(t) + \mathbf{N}(t),$$

where $\mathbf{G}$ is the gain matrix of size $m \times n$, and $\mathbf{N}(t) = (N_1(t), ..., N_m(t))^T$ represents measurement noise. Furthermore, this model is the starting point for the estimation of the cross-power spectrum of the unknown neural sources, $\mathbf{S}^{\mathbf{X}}(f)$, a powerful tool in the study of brain connectivity which consists in quantifying the statistical relationship between the time-series associated to different brain areas.
In the first part of this talk, I will explain how to derive a linear inverse problem that directly relates the cross-power spectrum of brain sources, $\mathbf{S}^{\mathbf{X}}(f)$, to that of the data, $\mathbf{S}^{\mathbf{Y}}(f)$ [1]. I will then show how to use Lasso regularization and the FISTA (Fast Iterative Shrinkage-Thresholding Algorithm) algorithm to get a sparse estimate of $\mathbf{S}^{\mathbf{X}}(f)$ [2]. Eventually, I will illustrate the results obtained by applying the proposed method on a set of simulated MEG data, highlighting the improvement obtained in the estimation of connectivity with respect to more standard approaches.

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Title

Biomedical Ultrasound Beam Patterns Optimization: from a stochastic approach to neural networks.

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Abstract

Medical Ultrasound Imaging is the most widespread real-time non-invasive imaging system: it exploits the ability of human tissue to reflect ultrasound signals. Thanks to advances in technology the machine performance, image quality and computational power have increased the development of new strategies, techniques and methods. In particular, in the recent decades several quantitative modalities have been developed, allowing measuring physical parameters of tissues with diagnostic significance [1]. The performance of each modality (either image quality or measurement precision) is deeply dependent on how the transmission and reception phases are tuned. The two phases are characterized by some parameters such as pulse shape, central frequency, transmission focus, transmission and receiving apodization and so on. In this work we present a novel formulation for the transmit Beam Pattern optimization problem in the narrow band case. Standard transmit beam pattern is based on a focused transmission at a fixed focal depth: this results in well-known drawbacks like non-uniform beam width over depth, presence of significant side lobes and quick energy drop out after the focal depth. To overcome these limitations we propose to optimize the transmit delays considering them as free variables, i.e. no longer linked to a specific focal depth. We formulate the problem as a Least Squares problem between the beam pattern corresponding to a set of transmit delays and a prescribed one. The problem is non linear and non convex: we present some results obtained by using Particle Swarm Optimization [2] and a possible strategy that involves neural networks.

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Title

A new converging approach for learnt optimization in CT image reconstruction

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Abstract

Medical image reconstruction from low-dose tomographic data is an active research field, recently revolutionized by the advent of deep learning. In fact, it typically yields superior results than classical optimization approaches, but its ability to properly compute the inverse problem solution is still questionable. In addition, the clinical applicability of tomographic precedures imposes constraints that must be taken into account and further undermine the stability of learning-based approaches.
In this talk, we present a new scheme, called RISING, embedding deep learning tools in an optimization approach. It is a two-step framework: the first phase executes few iterations of a model-based optimization algorithm whereas, in the second step, a pre-trained convolutional neural network improves the reconstructed images playing the role of the iterations required to achieve the convergence solution. The network training is ground-truth free. The framework exploits the computational speed and flexibility of a data-driven approach and inherits stability from the model-based problem statement, while fitting clinical requirements.

Title

Optimizing while training: Score Oriented Losses (SOLs)

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Abstract

In the framework of deep learning, the training of a model is performed by minimizing a certain *loss function*. On the other hand, the assessment of the classification performances is achieved by considering different *skill scores*, which are built upon the entries of the so-called *confusion matrix* and are usually chosen according to the specific application. Since they are discontinuous functions with respect to the predictions given by the model, they can not be directly maximized in the training process, and they are usually optimized after the training of the network by varying the value of a threshold.
In this talk, we discuss a new class of score-oriented loss functions [1]. 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 our findings.

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Title

Quantitative imaging and radiomics: assessment of radiomics feature reliability in medical imaging

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Abstract

The rationale beneath radiomics relies on the assumption that quantitative information about morphological and functional descriptors can be computationally extracted from medical images. Such quantitative features are the so called radiomics features. We focused our radiomics analysis on MR images of meningioma, the most common primary intracranial tumor in adults. The availability of these radiomics features allows the search of correlation with tumor-related genomic information. For example, investigations suggest a role for PD-L1 expression in meningioma microenvironment immune suppression, which could favour tumor recurrence: in principle, it is possible to exploit the informative content of radiomics features to classify tumors with PD-L1 mutation, and also for prognostic purposes. For these reasons, radiomics features have to be reliable, robust and accurate. From a mathematical view-point, there are very few studies about the robustness of feature extraction procedure. In this talk we present some of the computational challenges that arise in the assessment of radiomics feature reliability in medical imaging.

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Title

Learned SVD approach for Diffuse Optical Tomography

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Abstract

Diffuse Optical Tomography (DOT) is an emergent medical imaging technique which employs near–infra–red (NIR) light to estimate the spatial distribution of optical coefficients inside biological tissues for diagnostic purposes, in a non-invasive and non-ionizing manner. At present, the widespread of DOT imaging is hindered by the inherent difficulty of reconstructing the absorption coefficient due to prevalent scattering in the NIR band. This, in turn, implies that the related inverse problem for coefficient reconstruction is severely ill-conditioned and regularization procedures are mandatory. Regularization methods based on ℓ_2 norm, on sparsity–promoting functionals (*e.g.*, ℓ_1 norm), on Total Variation functional or even on Bregman techniques [1] have been used in the past, but they are not flawless: the main issues regard the regularization parameter tuning.

The paradigm shift which is taking place in imaging due to machine learning [2] opens new paths also for DOT reconstruction. With its severe ill-posedness, this is indeed a challenging candidate to explore new automatized regularization procedures. In this presentation, we refer about our research in deep learning techniques to perform regularization in an automatized manner. We explore fully data–driven and hybrid physics–driven/data-driven approaches [3] and we analyze pros and cons of each technique.

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Title

Deep Neural Networks for Inverse Problems with Pseudodifferential Operators: An Application to Limited Angle Tomography

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Abstract

Sparsity promotion is a popular regularization technique for inverse problems, reflecting the prior knowledge that the exact solution is expected to have few non-vanishing components, for example, in a suitable wavelet decomposition. In this talk, I will present a novel convolutional neural network, called ΨDONet, designed for sparsity-promoting regularization for linear inverse problems. Such a network is able to replicate the application of the Iterative Soft Thresholding Algorithm (ISTA), a classical reconstruction algorithm for sparsity promoting regularization, and to actually outperform it, by learning a suitable pseudodifferential correction. By a combination of techniques and tools from regularization theory of inverse problems, multi-resolution wavelet analysis, and microlocal analysis, we are able to theoretically deduce the architecture of the network and to prove some convergence results. Our case study is limited-angle computed tomography: we test two different implementations of our network on simulated data from limited-angle geometry, achieving promising results.

Title

Classification of strokes in electrical impedance tomography: from the inverse problem to a neural networks approach

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Abstract

Reconstruction of conductivity images in electrical impedance tomography (EIT) requires the solution of a nonlinear inverse problem on noisy data. This problem is typically ill-conditioned and solution algorithms need either simplifying assumptions or regularization based on a priori knowledge. This work considers a different strategy, it aims at training two types of Neural Networks (NN) with absolute EIT measurements on a computational head model [1], in order to binary classify the type of stroke occurred: haemorrhagic, if there is a blood leak in the brain tissue, or ischaemic, when a blood clot stops the blood supply to a certain area of the brain. Although this approach solves the easier problem of classification, it could however be extremely beneficial for emergency use.
The networks (Fully Connected NN and Convolutional NN) are trained on a dataset with 40000 samples of simulated measurements that take into account different kinds of possible errors in the measurement setup: slight variations in the background conductivity and in the contact impedances, misplaced electrodes and mismodeled head shape [2]. On most test datasets we achieve $\geq 90\%$ average accuracy with fully connected neural networks, while the convolutional ones display an average accuracy $\geq 80\%$. Despite the use of simple neural network architectures, the results obtained are very promising and motivate the applications of EIT-based classification methods on real phantoms and ultimately on human patients.

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Title

Neural architecture search via standard machine learning methodologies

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Abstract

In the context of deep learning, the more expensive computational phase is the full training of the learning methodology. Indeed, its effectiveness depends on the choice of proper values for the so-called hyperparameters, namely the parameters that are not trained during the learning process, and such a selection typically requires an extensive numerical investigation with the execution of a significant number of experimental trials. The aim of the paper is to investigate how to choose the hyperparameters related to both the architecture of a Convolutional Neural Network (CNN), such as the number of filters and the kernel size at each convolutional layer, and the optimisation algorithm employed to train the CNN itself, such as the steplength, the mini-batch size and the potential adoption of variance reduction techniques. The main contribution of the paper consists in introducing an automatic Machine Learning technique to set these hyperparameters in such a way that a measure of the CNN performance can be optimised. In particular, given a set of values for the hyperparameters, we propose a low-cost strategy to predict the performance of the corresponding CNN, based on its behavior after only few steps of the training process. To achieve this goal, we generate a dataset whose input samples are provided by a limited number of hyperparameter configurations together with the corresponding CNN measures of performance obtained with only few steps of the CNN training process, while the label of each input sample is the performance corresponding to a complete training of the CNN. Such dataset is used as training set for a Support Vector Machines for Regression and/or Random Forest techniques to predict the performance of the considered learning methodology, given its performance at the initial iterations of its learning process. Furthermore, by a probabilistic exploration of the hyperparameter space, we are able to find, at a quite low cost, the setting of a CNN hyperparameters which provides the optimal performance. The results of an extensive numerical experimentation, carried out on CNNs, together with the use of our performance predictor with NAS-Bench-101 [1], highlight how the proposed methodology for the hyperparameter setting appears very promising.

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MS08 - Physics-based machine learning for engineering simulation and digital twin

Proposers

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Abstract

Machine Learning (ML) models, which have already found tremendous success in several applications, are beginning to play an important role in advancing scientific discovery in several engineering domains, traditionally dominated by the numerical solution of PDEs [1]. The use of ML models is particularly promising in scientific problems involving processes that are not completely understood, or where it is computationally infeasible to run simulations at desired resolutions in space and time. Moreover, tasks such as inverse modeling, calibration, optimization, parameters identification and uncertainty quantification - necessary towards a Digital Twin approach - require advanced surrogate and reduced order models techniques. Neither an ML-only nor a Physics-based-only approach can be considered sufficient for complex scientific and engineering applications, in particular in computational mechanics. Therefore, the research community is beginning to explore the continuum between ML and Physics-based models (PINN, Deep Learning ROM, Autoencoders just to name a few examples [2]), where both scientific knowledge and ML are integrated in a synergistic manner. However, several challenges are still present and need to be addressed both from a theoretical and practical point of view. The aim of this Minisymposium is to present and share the latest improvements in this field, exploring future possible developments and applications. Moreover, the Minisymposium aims also to connect academic research, spin-off and corporate vision to boost the research on this topic, in particular in the Italian ecosystem.

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Title

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

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Abstract

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 speedup training times, and decrease the network complexity, substantially. Accuracy and efficiency of the DL-ROM technique are assessed on different parametrized PDE problems in cardiac electrophysiology, 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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Title

Deep learning-enhanced model order reduction in nonlinear structural mechanics.

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Abstract

High-fidelity approximations of solutions to nonlinear, time-dependent, parameterized PDEs can be computed by means of so-called full order models (FOMs), e.g. the finite element method, at a great computational cost. To speed-up the numerical simulations, especially when interested in the repeated evaluation of the parameters-to-solution map, it is of paramount importance to develop emulators or reduced order models (ROMs) featuring smaller complexity or lower dimension.
The reduced basis (RB) method [1] represents a well known projection-based ROM which yields approximations that fulfill the physical problem at hand. It consists of a Galerkin projection of the FOM onto a linear low-dimensional subspace - built by performing, e.g., proper orthogonal decomposition (POD) on a set of sampled FOM solutions - thus obtaining, at each time step, a reduced nonlinear system that can be efficiently solved by means of Newton method. Nonetheless, for problems characterized by (high-order polynomial or nonpolynomial) nonlinearities, intrusive and expensive hyper-reduction stages are required to make the assembling of the ROM independent of the high-fidelity dimension.
To overcome this computational bottleneck, we rely on deep neural networks (DNNs) [2] for learning the low-dimensional residual vectors and Jacobian matrices arising at each Newton iteration, therefore recovering the efficiency of the RB method. The resulting hyper-reduced model, to which we refer to as *Deep-HyROMnet* [3], is a physics-based ROM, that still relies on the POD-Galerkin approach, however employing DNNs for predicting the low-dimensional nonlinear operators. Numerical results of nonlinear structural mechanics problems, including the contraction and relaxation of a patient-specific left ventricle, show that our novel approach is able to speed-up the FOM solution several orders of magnitude than POD-Galerkin ROMs equipped with standard hyper-reduction techniques, such ad the discrete empirical interpolation method, still keeping good level of accuracy.

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Title

PINN-based models for coupled hydro-poromechanics simulations

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Abstract

Physics-Informed Neural Networks (PINNs) are particular neural networks that in addition to data consider information from the physics by involving the residual of the governing PDEs as a constraint in the training. Therefore, PINNs make it possible to integrate data and simultaneously solve PDEs. This hybrid nature of PINNs reconciles data-driven machine learning models with traditional ones: they inherit the NN ability to learn complex structures from data, while gaining prediction reliability and physical consistency from PDEs. For this reason, PINNs are particularly interesting for parameter estimation and design support in large-scale problems, hence they have been selected for modeling the main coupled hydro-poromechanical processes of interest in reservoir simulations.
A PINN-based approach is implemented for coupled hydro-poromechanics and investigated on classical benchmarks. An analysis of the influence of the hyper-parameter selection in PINN setup has been performed to identify the most appropriate and accurate architecture, then the results have been applied to more practical cases for PDE solution and parameter identification. The goal is to assess and validate the approach, thus laying the foundation of the method in the field. The PINN-based model developed in the present work is the starting point for future applications to challenging test cases typically encountered in reservoir modeling and real-world cases with data recorded by sensors.

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Title

Physics-informed Neural Networks for parametric partial differential equations and optimal control

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Abstract

The talk focuses on an extension of physics informed supervised learning approach to parametric partial differential equations. These models, even if exploited in many application fields, might be computationally expensive. This aspect can be an issue in real-time and many-query settings. Thus, we propose a physics informed learning strategy to provide simulations in a small amount of time. We exploit the physics information in different ways: in the loss function (standard physics informed neural networks), as informative input (extra features), and as a guideline to propose an effective structure for the neural network itself (physics informed architecture). These three aspects will lead to a faster training (offline) phase and a more accurate parametric (online) prediction. Among the test cases, we will show an application in an optimal control context, too [1].

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Title

Nonlinear manifold Reduced Order Models with Convolutional Autoencoders and Reduced Over-Collocation method

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Abstract

Non-affine parametric dependencies, nonlinearities and advection-dominated regimes of the model of interest can result in a slow Kolmogorov n-width decay, which precludes the realization of efficient reduced-order models based on linear subspace approximations. Among the possible solutions, there are purely data-driven methods that leverage autoencoders and their variants to learn a latent representation of the dynamical system, and then evolve it in time with another architecture. Despite their success in many applications where standard linear techniques fail, more has to be done to increase the interpretability of the results, especially outside the training range and not in regimes characterized by an abundance of data. Not to mention that none of the knowledge on the physics of the model is exploited during the predictive phase. In order to overcome these weaknesses, we implement the nonlinear manifold method introduced by Carlberg et al [1, 3] with hyper-reduction achieved through reduced over-collocation and teacher-student training of a reduced decoder [2]. We test the methodology on a 2d nonlinear conservation law and a 2d shallow water models, and compare the results obtained with a purely data-driven method for which the dynamics is evolved in time with a long-short term memory network.

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Title

Neural network-based, structure-preserving entropy closures for the Boltzmann moment system

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Abstract

Direct simulation of physical processes on a kinetic level is prohibitively expensive in many large scale applications due to the extremely high dimension of the solution spaces. Thus, the moment system of the Boltzmann equation, which projects the kinetic physics onto the hydrodynamic scale, is often considered. The unclosed moment system can be solved in conjunction with the entropy closure strategy, which provides structural benefits to the physical system of partial differential equations. Usually computing such closure of the system spends the majority of the total computational cost, since one needs to solve an ill-conditioned constrained optimization problem for each grid cell and each time step.
This work [1] presents neural network based minimal entropy closures for the moment system of the Boltzmann equation to accelerate the solution process. The described method embeds convexity of the moment to entropy map in the neural network approximation to preserve the structure of the minimal entropy closure. Two techniques are used to implement the methods. The first approach approximates the map between moments and the minimal entropy of the moment system and is convex by design. The second approach approximates the map between moments and Lagrange multipliers of the dual of the minimal entropy optimization problem, which present the gradients of the entropy with respect to the moments, and is enforced to be monotonic by introduction of a penalty function. We derive an error bound for the generalization gap of convex neural networks which are trained in Sobolev norm and use the results to construct data sampling methods for neural network training. Numerical experiments are conducted, which show that neural network-based entropy closures provide a significant speedup for kinetic solvers while maintaining a sufficient level of accuracy. The methods are efficiently implemented in a hybrid kinetic solver, which is described in [2].

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Title

Physics-informed neural networks on parameterized shapes: a new tool for surrogate modeling for shape optimization

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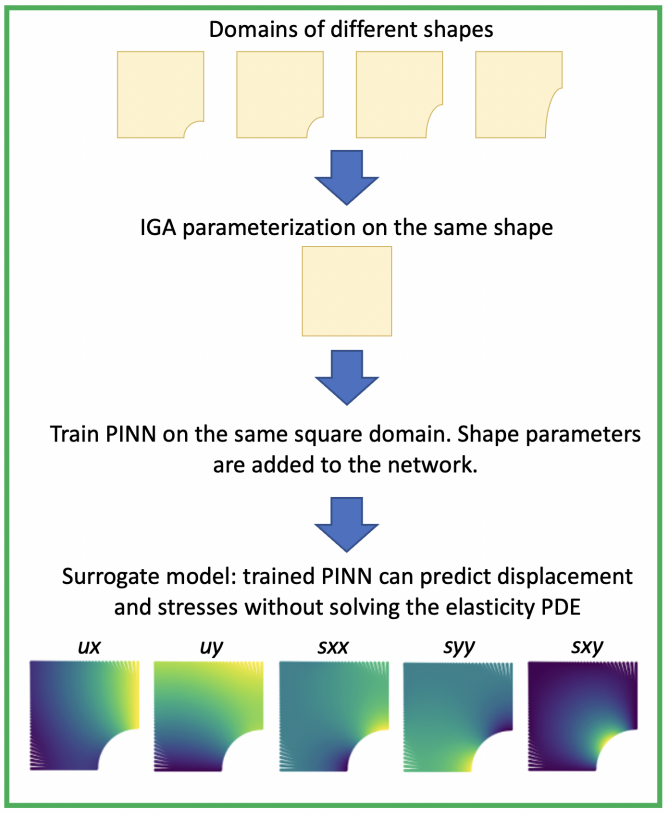
Abstract

In this talk, we discuss the formulation of a physics-informed neural network (PINN) that incorporates shape information among its variables. The shape is included in the network by means of the coordinates of the control points of an IGA parameterization.
We formulate the network and discuss its applicability to build surrogate models for shape optimization. In particular, we focus on the linear elasticity equation and show that our network can be successfully trained using IGA data generated for different shapes, which differ from the coordinates of the control points of the used parameterization. Furthermore, we discuss the ability of the trained network to predict displacements and stresses in shapes that were not included in the training dataset. This finally affords to use the predicted solution fields to solve shape optimization problems.
The talk is based on joint work with Prof. Xiaoping Qian at the University of Wisconsin-Madison (U.S.A.).



Title

Variational Physics-Informed Neural Networks: an a posteriori error analysis

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Abstract

Physics Informed Neural Networks (PINNs) are neural networks trained to solve forward or inverse partial differential equations (PDEs), eventually exploiting some data or external knowledge. After the development of the first PINN in [1], several adaptations have been proposed in order to improve its stability and efficiency and to solve specific engineering problems.
In this talk, we focus on a specific type of PINN denoted as Variational Physics Informed Neural Network (VPINN) and in which a neural network is trained using only the variational formulation of the PDE. Such a method has been firstly proposed in [2].
In particular, we propose an a posteriori error estimator for second order elliptic problems (see [3]). Such estimator is both efficient and reliable and is computed by combining residual-type terms and data oscillation terms with the loss function used during the training. This is an important feature since it allows the user to distinguish between the different sources of error and act on the neural network or on its training accordingly, in order to improve the model accuracy or efficiency.
Numerical experiments are in agreement with the theoretical analysis and show that the estimator behaviour is very similar to the one of the H^1 error both during the training of a single VPINN and when multiple VPINNs are trained on different meshes.

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MS09 - Mechanics of biological systems: models and experiments

Proposers

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Abstract

Unveiling and predicting the behaviour of biological systems is a very difficult task, that poses challenging research questions. Specifically, the field of biology is characterized by the very complex nature of living organisms: they display strong multiscale and hierarchical structures, ranging from the sub-cellular to the organ level, which need to be properly addressed both from the experimental and the theoretical point of view. In this respect, the interest in biological systems has grown exponentially in the last few decades and the possibility of studying and deducing models describing such complex structures was made possible by the advent of innovative techniques for single molecule experiments. Thus, according to the experimental evidence, theoretical and applied mechanics come into play in gaining a better understanding of complex biological systems with a twofold aim: as a matter of fact, the role of mechanical and thermal fields has to be taken into account to develop meaningful models describing such systems as well as they provide a framework to accelerate the research process in the field of biology.

The aim of our mini-symposium is to bring together young researchers working in the field of biomechanics in all its shades, to share ideas and insights on their works possibly developing new fruitful collaborations. The symposium is divided in two sessions. The first session is mainly devoted to the theoretical modelling of biological structures, where many open questions are still to be unveiled. The mechanobiology of the cells, the thermo-mechanical response of bio and bioinspired materials and their link with human physiology and pathology, are only a few examples of open issues that will be tackled within this session. The second session is focused on the experimental response of biological systems, in which the comparison with computational and analytical descriptions is crucial to correctly validate the introduced models. Indeed, only the shared contribution of both the experimental tests and the theoretical approaches may open new frontiers in the comprehension and design of novel bioinspired materials and structures.

Title

A continuum multiphase model to predict growth and invasion of brain tumours

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Abstract

The purpose of the present work is to investigate the progression of a brain tumour, in order to acquire more details about its anisotropic nature, which follows the orientation of surrounding white matter tracts. Indeed, mathematical models of cerebral tumour growth can help in understanding the physiology and the progression of this disease, for the purpose of predicting the evolution of cancer shape and volume and quantifying its aggressiveness. In this perspective, we try to reproduce the evolution of this highly malignant brain tumour evaluating its mechanical impact on the surrounding healthy tissue. A mathematical multiphase model, based on Continuum Mechanics, is developed, where both the healthy and the diseased regions are treated as a saturated biphasic mixture, comprising a solid and a fluid phase. Moreover, the region occupied by the tumour is considered to be completely separated from the host tissue by a sharp moving interface. The cell phase is supposed to behave as a Mooney-Rivlin hyperelastic solid, with different material parameters between healthy and diseased zone. Instead, the liquid phase is considered constitutively as an ideal fluid. With the aim to describe the mechanical effect of tumour growth onto tissue deformation, theory for materials with evolving natural configurations and the multiplicative decomposition of the deformation gradient tensor are employed. For what concerns the growth tensor, which appears in this decomposition, we focus on its anisotropic evolution, in order to enforce the different cases of monodirectional, planar and spherical growth. Furthermore, it is necessary to introduce in the model an equation describing the evolution of nutrients in the domain, since their amount affects the cells capability to duplicate. After having set the mechanical model, we solve it through numerical simulations. For this purpose, the Lagrangian formulation is derived from the Eulerian model. Later, a weak formulation of the Lagrangian model is obtained in order to numerically solve the model using FEniCS, a Python-based PDE finite element solver. Afterwards, numerical simulations on the real three-dimensional brain geometry are performed, using available data from MRI and DTI to build the computational domain and account for patient-specific anisotropy. From a numerical point of view, the obtained algorithm is stable and it allows to represent discontinuous deformation gradients, through the use of a mesh conforming to the material host-tumour interface. On the other hand, from a modelling point of view, with respect to available models in the literature, the anisotropy has also been included in tumour growth and the model is able to describe how the brain tracts are modified due to the tumour mass expansion.

Title

On mathematical models and methods for 1D fluid-structure interaction problems in computational hemodynamics

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Abstract

For several decades, computational models have contributed to increasing our knowledge of human haemodynamics, providing efficient approaches for the quantification of fluid-dynamic phenomena in the cardiovascular network and meaningful data that would otherwise require invasive techniques or would simply not be available from general clinical measurements.
In recent years, mathematical models of biofluid-dynamics have been consistently developed, focusing on several fundamental aspects and issues that need to be addressed in order to successfully model the circulatory system. Among these, it has to be considered that blood flow mechanically interacts with vessel walls and tissues, resulting in complex fluid-structure interactions whose mathematical analysis is difficult to describe correctly and simulate numerically efficiently.
In this talk, a 1D blood flow model capable of correctly capturing the fluid-structure mechanism acting within the arterial and venous system is discussed [1, 3, 4]. The proposed model allows both elastic and viscoelastic configurations of the vessel walls to be considered, the elastic regime being easily recovered from the viscoelastic one in the zero relaxation limit [2]. The system is solved numerically with an efficient and robust second-order Implicit-Explicit (IMEX) Runge-Kutta Finite Volume method that benefits from the asymptotic-preservation property, meaning that the consistency of the scheme with the asymptotic regime is guaranteed and the order of accuracy is preserved in the stiff limit.

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Title

Multi-scale modelling of cell-matrix interactions

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Abstract

We develop a mathematical model to study the quasi-static decohesion occurring in cell-matrix complexes, with a specialization to integrin-mediated systems, as is the case of focal adhesions [1]. The latter are the first sites that support the attachment of cells to the extra-cellular matrix (ECM) or promote their detachment, thereby strongly condition several cell functions, such as cell motility or cell re-orientation [1]. In the present work, we consider a one-dimensional model and, based on a shear lag approach, we design a three-layer scheme, consisting of mechanical components representing the focal adhesion, the ECM and the integrin receptors [1,2,3,4]. The latter are supposed to transmit a linear fragile force to the other two elements, i.e., when the shear reaches a threshold value, the force drops to zero [2,3]. With reference to a Griffith-like criterion of rupture, we analytically determine how the system evolves from a fully attached state to the nucleation of a decohesion front, up to full decohesion. More specifically, we are able of detecting two different types of decohesion: one, ductile, is characterized by a progressive rupture of the integrin receptors, while the other one, fragile, represents a discontinuous transition from the fully attached to the fully detached state [2]. In doing this, we introduce an internal length, defined through the elastic parameters characterizing the focal adhesion, the ECM and the integrin receptors, which allows us to determine the size of the zones at which the loads between the system's components are transmitted [2,3,4]. Moreover, we display how such characteristic length regulates the transition from the ductile to the fragile rupture [2,3]. Finally, we compare our results with experimental data, and we show a good agreement between them, both qualitatively and quantitatively [2].

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Title

Harnessing tonotopy: bio-inspired spiral structures

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Abstract

The cochlea organ possesses unique characteristics which allow mammalians to perceive sounds in wide frequency and amplitudes ranges, comprising nearly ten octaves and 120 decibels, possessing also a tonotopic organization which yields a shift in excitation peaks according to the frequency components of signals. Although the use of locally resonant structures is widespread in the context of wave manipulation, the bandwidth of local resonance effects is typically narrow. To overcome this drawback, a possible approach is to combine several elements with distinct resonant frequencies to create a rainbow effect, thus encompassing a wider frequency range, which however leads to difficult in experimental realization, since it requires the combination of multiple structures. Thus, the design concepts present in the cochlea structure are of interest in the field of bio-inspired metamaterials, since its tonotopic structure may present multiple resonant frequencies and be used to discriminate frequencies along its spatial profile.
A cochlea-inspired structure can be modeled by sweeping a rectangular area along a curve described in the cylindrical coordinate system, which can be considered planar, for the sake of simplicity (Figure 1a). For a given set of boundary conditions, the total out-of-plane (z-direction) elastic energy associated with each vibration mode can be computed and maximized, through the adjustment of the parameters which control the curvature and cross-section of the cochlea-inspired structure, to yield an optimal distribution of peaks in the vibration modes. The tonotopy of the obtained structure can be assessed by applied transient pulses centered at different frequencies. It is possible to compare the location of the response peak for each input frequency and verify that these have a frequency-dependent location (Figure 1b). These features encourage applications such as energy harvesting, non-destructive testing, and vibration attenuation.

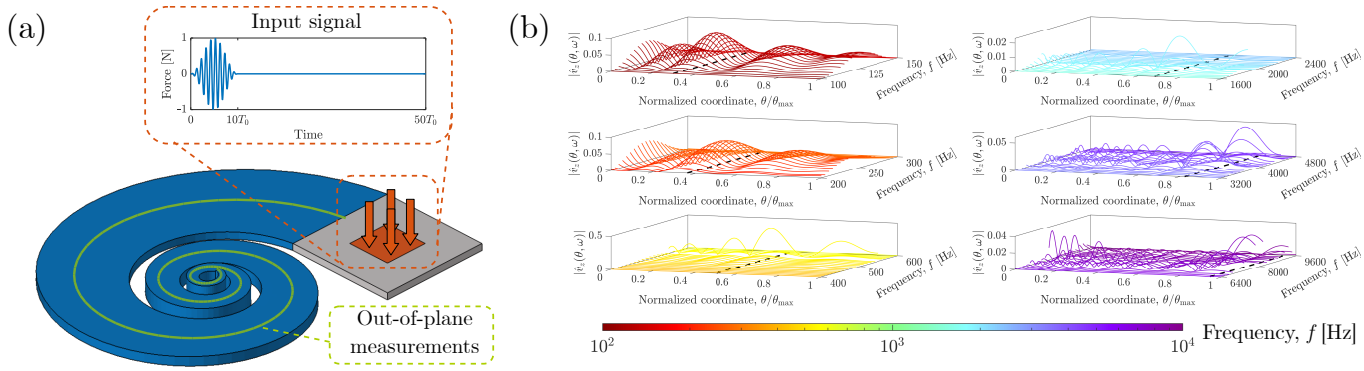

Figure 1

Title

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

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Abstract

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

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Title

A biphasic elasto-plastic model for the compression-release test of multicellular aggregates.

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Abstract

Cells that are clustered together and adhere to each other, by the means of protein filaments, form the so called multicellular aggregates (MCSs). Depending on the radius of such aggregates, they can comprise from a few hundreds to hundreds of thousands of cells. Despite their apparent simplicity, multicellular aggregates can be of help to reach a deeper comprehension on processes in which bio-mechanical factors play an important role, such as tumour progression [1], since MCSs are able to capture essential features of dedicated *in vivo* experiments [2].

With respect to [3], we reformulate the model to include the mechanical contributions of the interstitial fluid allocated between cells. We propose a three-dimensional, elasto-plastic biphasic model of multicellular aggregate and we specialize it to a compression-release experiment [4]. Hence, the MCS is described as a saturated biphasic medium comprising a soft porous matrix, which includes the ECM, cells and the various constituents, and an interstitial fluid, for which we assume Darcian regime. Moreover, the solid phase of the MCS undergoes remodelling, a stress-driven process that reorganizes the micro-structure of the material and that is described through the onset of plastic-like distortions.

Finally, we study the evolution of the coupled system that comprises the MCS and the experimental apparatus, in which mechanical interactions are exchanged through the contact surface. The results of our numerical simulations permit to evaluate, both qualitatively and quantitatively, some of the consequences of the coupling between the remodelling and the flow of the interstitial fluid. Finally, our numerical results are qualitative coherent with experimental data [2].

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Title

Experimental nanomechanics of natural or artificial spider silks

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Abstract

Spider silks are materials that have attracted the attention of the intellectuals in every epoque[1]. This was mainly due to their exceptional mechanical properties, which outperform many artificial fibers. In order to bring these materials at the industrial level, however, spiders cannot be used because of their cannibalistic nature. This has elicited the creation of artificial counterparts, which are commonly based on bio-inspired concepts obtained from native spider silks[2]. In particular, the use of specific aminoacidic sequences in the spider silk proteins (spidroin) directly taken from the natural repeats is one of the key aspects that is frequently investigated[3].

In this context, a broad and deep knowledge of the mechanical properties of different spider silk types, which have different aminoacidic sequences and thus mechanical properties, is crucial to improve the properties of the artificial counterparts.

In this talk, we present some of our recent works regarding the use of nanomechanical experimental techniques to find suitable candidates for artificial production. Nanotensile and nanoindentation tests have been deeply used in these years to investigate the mechanical properties of different spider silk types (both natural and artificial). In particular, the challenges in testing pirifirom silk will be highlighted[4], as well as the importance in creating specific dataset of mechanical properties[5,6].

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Title

On the interplay between activity, elasticity and diffusion in self-contractile biopolymer gels

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Abstract

Biopolymer active gels are fabricated by distributing a myosin motors concentration on a network of actin filaments. The composite forms an homogeneous thin sheet of acto-myosin bonds, which is suspended in a liquid bath. This system undergoes spontaneous contraction in condition of free-swelling (i.e. without need of external stimuli), developing a variety of steady states, which depend on sheet geometry and on evolution of the stress-diffusion dynamics, as it experimentally observed [1]. These self-contracting materials have many potential clinical applications, ranging from artificial muscle manufacturing, wound healing speed up, to control of drug delivery in pharmaceutics. The main issue about the developing of bio-devices exploiting that behaviour concerns the controllability of the contraction process toward a desired achievement, in terms of end-shape and its reversibility. Facing to this, a detailed understanding of stress-diffusion phenomena in presence of active remodeling is a crucial starting point. We propose a continuum mechanical model, based on an augmented stress-diffusion theory, which describes liquid release under bulk contraction and includes bulk sources to mimic molecular motors which cause self contraction [2]. The model is thermodynamically consistent, and the evolution is governed by a dissipative dynamics, as dictated by the dissipation inequality over the augmented kinematic of the activity. We have performed some numerical simulations, carried out on a minimal model, in terms of constitutive choices of gel elastic response and myosin motors activation, to analyze the interplay between liquid outflow and stress-strain evolution inside the gel. The results show that a proper tuning of geometrical properties of gel sheets, together with the resistance to remodeling, are already enough to catch the main experimental findings: the liquid outflow velocity related to gel boundary contraction, the transversal-planar time scales separation during boundary contraction, and the stress-strain relaxation induced by the active remodeling; as well as to reproduce the shape transition toward a dome-like, or a wrinkle-like, end-shapes which are likewise found in experiments [1].

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Title

Mechanobiological insights into receptor dynamics

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Abstract

Ligand-receptor chemical interplays underlie several specific cellular behaviors. Consistently, these protein interactions also play a pivotal role during the phenomenon of angiogenesis, i.e. the new blood vessels formation from pre-existing ones. Particularly, the sprouting of new blood vessels is promoted by the proliferation and migration of Endothelial Cells (ECs) covering the inner wall of the vessels that already exist; such a complex biological machinery is triggered through the interaction between appropriate receptors on the cell membrane (e.g. VEGFR2) of ECs and suitable growth factors (e.g. VEGF-A, gremlin, etc.) located in their extracellular environment. Nevertheless, despite the biochemical pathways resulting from several receptor activation is well documented, the role of cell mechanics during angiogenesis deserves additional quantitative studies. In this work, we are focused on angiogenesis at cellular level studying how the mechanical behavior of a single Endothelial Cell (EC) can affect the chemo-diffusive activities, on its lipid membrane, of those transmembrane proteins (e.g VEGFR2, integrin) that are mainly involved for the triggering of the angiogenic stimulus. Hence, we present a chemo-transport-mechanical model, embedded in the field of continuum thermodynamics, which takes into accounts for ligand-receptor chemical reactions, mechanical deformation of the EC and diffusion of the receptors along the advecting cell membrane. Constitutive relationships have been deduced from suitable Helmholtz free energies by means of the Coleman-Noll procedure both for membrane and bulk physical processes [1]. Subsequently, the governing equations have been written in weak form as a prelude to the approximation schemes implemented in the finite element library *deal.ii*. Finally, co-designed in-vitro and in-silico experiments trying to identify which are the physical laws that mainly affect the relocation and activation of specific receptors along the membrane of an EC that spreads on a ligand-enriched substrate.

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Title

Predictive multi-scale models for hysteresis, induced anisotropy and residual stretches in soft biomaterials

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Abstract

The mechanical characterization of soft biomaterials is fundamental in current materials science and engineering. In order to fine-tune and develop new materials one must bridge the molecular scale with the macroscopic behavior.
Our multiscale approach deduces, starting from the description of the constituent macromolecules, macroscale constitutive laws for the whole macroscopic network. In the framework of statistical mechanics, it is possible to express the macromolecule Helmholtz free energy as a function of the chain entropy, which is in turn related to the possible configurations of the monomers. Additional tube-like terms must be introduced aiming at limiting the possible path of single monomers once they are immersed in a complex network.
Traditional chain models consider only reversible deformations, whereas we state new evolution laws which are derived from the thermodynamics of macromolecule folding/unfolding of chain regions which can undergo a morphological transition from hard folded domains to amorphous ones due to strain [1].
With the filament models in hand, we show how to characterize the soft material three-dimensional mechanical behavior, depending on the oriented distribution of macromolecules, and in particular the anisotropic accumulation of damage and the internal hysteresis dissipation. This is done by considering both a finite number of possible chain orientations and continuous distributions which require quadrature rules on the microsphere.
The resulting macroscale predictions are assessed by performing parameter identification for different biomaterials tested in uniaxial traction [2, 3]. Novel experimental data are also presented for biaxial and pure shear modes.

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Title

Modeling metastatic tumor evolution, numerical resolution and growth prediction

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Abstract

In this work we have introduced a generalized metastatic tumor growth model that describes the primary tumor growth by means of an Ordinary Differential Equation (ODE) and the evolution of the metastatic density using a transport Partial Differential Equation (PDE), [3]. The numerical method is based on the resolution of a linear Volterra integral equation (VIE) of the second kind, which arises from the reformulation of the ODE-PDE model, [2]. The convergence of the method is proved and error estimates are given. The computation of the approximate solution leads to solve well conditioned linear systems. Here we focus our attention on two different case studies: lung and breast cancer. We assume five different tumor growth laws, [1], for each of them, different metastatic emission rates between primary and secondary tumors, and last that the new born metastases can be formed by clusters of several cells.

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MS10 - Advanced methods and computational approaches for the mechanics of heterogeneous materials

Proposers

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Abstract

This minisymposium embraces all topics related to the mechanical behaviour of heterogeneous materials and their structures. The mechanical response of complex materials is significantly influenced by the heterogeneous microstructure and by the nonlinear multiphysics phenomena occurring in their constituents. An active and constantly increasing research effort toward innovative and highly efficient computational techniques allows to model microstructured materials with a higher level of reliability. Moving from such considerations, the present symposium welcomes contributions highlighting advanced methods and computational approaches for analysing the mechanics of heterogeneous material in a wide range of applications (e.g., civil, mechanical, biomedical engineering). Key topics of discussion will include but are not limited to: new methods for the analysis of the mechanical material response up to failure; data-driven approaches; multiscale and multiphysics simulations; phase field approaches; structural optimization for computational design.

Title

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

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Abstract

The phase field approach to fracture has received a major attention by the scientific community as a new method for modelling crack nucleation, diffuse damage and complex patterns of crack growth in materials [1,2]. The basic mathematical framework requires the solution of a Poisson-type partial differential equation describing the evolution of damage in tension, coupled with the equations of the elastic or the elasto-dynamic equilibrium. Moreover, the majority of the formulations introduce a split of the strain history function to allow damage evolution only in tension.

As a further progress, multi phase-field approaches have been recently proposed to simulate the evolution of damage associated to different mechanisms. For instance, in tension, a multi phase-field approach to fracture has been exploited in [3] for fibre-reinforced composites to simulate different damage evolution scenarios in the fibres and in the matrix.

Here, we propose a multi phase-field approach where two phase-field variables are introduced to: (i) model damage due to tensile stress states leading to crack growth, and (ii) simulate damage in compression due to material crushing.

The mathematical differential problem, which leads to a system of two Poisson partial differential equations coupled with the elastic equilibrium equation of the damaged material, is herein solved from the computational point of view by proposing a numerically efficient staggered solution scheme within the finite element method.

The methodology is herein applied for the first time to the simulation of damage phenomena occurring in concrete specimens in compression, by considering their meso-structure composed of mortar matrix and aggregates. Experimental trends in [4] are also correctly captured.

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Title

Multiscale And Multiphysics Computational Mechanics of Nuclear Fusion Magnet Systems

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Abstract

A tokamak is a reactor which extracts energy from nuclear fusion processes. In order to induce them, the fuel must be brought to and kept at the plasma state ($\approx 10^6$ K), and one of the two possibilities to accomplish this is through magnetic confinement. The magnet system of a tokamak is based on three groups of magnets, the Toroidal Field Coils (TFCs), the Poloidal Field Coils (PFCs) and a Central Solenoid (CS), each devoted to specific roles [1], and comprising a heterogeneous internal organisation of current-carrying conductors which for advanced fusion experiments are bound to be superconducting and operated at 4K. The strategy to design and/or assess the magnet system of a tokamak must take into account on the one hand the spectrum of geometrical scales, from the macroscopic dimensions of an assembled coil (≈ m) to the internal structure of a conductor (≈ mm), and on the other the different physics involved, ranging from a partial magneto-mechanical coupling to coolant flow and neutron heating. This talk will address the principal aspects of the methodology to tackle the study of a magnet system, drawing on real case studies where several computational techniques have conveniently been applied (homogenisation of material properties, contact nonlinearities, fatigue effects) to capture as closely as possible the behaviour of the magnets in normal and off-normal conditions.

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Title

Unsupervised discovery of constitutive laws: experimental validation for hyperelastic materials

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Abstract

As a result of the enormous data collection capacity of modern instruments, data-driven methods are being increasingly explored in computational solid mechanics. In the area of automatic constitutive law discovery, a new approach, called EUCLID (Efficient Unsupervised Constitutive Law Identification and Discovery), was presented in [1]. The approach is able to discover the material model from a large library of possible candidates using only data acquired from experimental tests, such as the applied force and displacement field of the sample measured throughout the test.

This approach combined with digital image correlation (DIC) techniques allows the model to be discovered and calibrated using a single specimen. This must locally guarantee the presence of multi-axial stress states, which can be achieved through a complex geometry. This is a great advantage in comparison to classical calibration procedures (e.g. [2]) which need to subject specimens to a significant amount of testing in order to obtain an accurate description of the stress-strain space.

Thus far, the EUCLID approach [1] has only been validated with data from finite element simulations; the aim of this work is to validate it with experimental data as well. Mechanical tests are performed on natural rubber specimens with geometries of increasing complexity. During the test the overall force is measured through a load cell and the displacement field is acquired through a DIC sensor. The experimentally derived model is used to predict material behavior in experimental tests not used in the model discovery phase in order to demonstrate the accuracy of the approach.

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Title

Mesh adaptation-driven inverse homogenization for multi-physics architected lattices

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Abstract

Lattice materials represent an effective solution for many structural applications, especially when conventional monolithic materials cannot satisfy the required constraints. The advancements in additive manufacturing technologies experienced in the last years have further amplified the interest towards meta- and lattice materials. As a consequence, the design of new lattices, featuring innovative combinations of physical effective properties occupies a central role in the optimal design of structures.

We present a mesh adaptation-assisted algorithm that enables the design of lightweight periodic cellular materials with prescribed properties in a multi-physics context. The formulation relies on an inverse homogenization problem, modeled through a standard density-based topology optimization at the microscale, and on an ad hoc grid generation step, driven by an anisotropic a posteriori error estimator [1]. The resulting layouts exhibit non-standard topologies compliant to the prescriptions and are characterized by clear-cut contours, thanks to the employment of anisotropic adapted meshes.

In this presentation, we focus on a thermo-elastic setting, by proposing innovative unit cells exhibiting both isotropic and/or anisotropic behaviours with respect to mechanical and thermal requirements [2]. The new cellular materials are compared with the state-of-art in engineering practice in terms of thermo-elastic properties, thus highlighting the good performance of the new layouts which, in some cases, can outperform off-the-shelf lattices.

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Title

Osteon failure mechanics: a multi-scale computational model

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Abstract

Cortical bone is a complex heterogeneous material showing a hierarchical structure over different length scales [1]. At the sub-macroscale, cortical bone is constituted by hollow quasi-cylindrical systems, called osteons, which are in turn made up of several coaxial pseudo-cylindrical layers, termed lamellae. Each lamella exhibits a defined pattern of sub-microstructural units (the sublamellae), characterized by an ordered arrangement of mineralized collagen fibrils (MCF). In turn, at the nanoscale, MCFs are constituted by Type-I collagen fibrils, hydroxyapatite mineral crystals and minor quantities of water and non-collagenous organic proteins.

The cortical bone material composition and structural organization on each length scale highly affect its mechanical behaviour and failure mechanisms at the macroscale level. As such, a detailed model for analysing the elasto-damage response of single osteons has been developed, thus paving the way towards a refined constitutive modelling of cortical bone macro-tissue. A combined analytical-numerical bottom-up multiscale strategy has been implemented to obtain equivalent elastic properties of lamellar bulk tissue. The model accounts for some peculiar features of mature cortical bone, like the interfaces present between the lamellae, and some randomly-distributed ellipsoidal micro-cavities (lacunae). A thermodynamically consistent damage-based approach has been employed to model possible occurrence of interlaminar/intralaminar failure modes. Present model has been validated by comparing available results of some benchmark mechanical tests conducted on isolated osteons with the numerical ones obtained by reproducing in-silico such experiments. A strength of the model is that it is based on physically and histologically meaningful parameters, thus making it suitable to straight describe biophysical and/or biochemical alterations (induced by ageing or diseases) by varying their corresponding values.

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Title

Algorithmic processes to generate building components with complex or heterogeneous fillings

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Abstract

The advent of industry 4.0 in the construction sector is profoundly changing procedures and products in the building construction sector. Indeed, during the last decade, the experimentation of 3D printing exploiting viscous materials opened up unprecedented possibilities of including complex geometries in building components [1]. Consequently, modern computer-aided design approaches such as parametric modelling and generative design are increasingly used in the scientific and technical world. Such techniques exploit algorithmic processes to generate complex or heterogeneous fillings starting from mathematical equations operated with visual scripting. This process provides the ability to change the shape of the model's geometry immediately when specific dimension values are modified. The proposed research exploits the use of parametric modelling to realise new bricks with complex internal geometries. The external shape is generated according to the geometry of the classical brick, while the internal geometries are developed starting from periodic minimal surfaces (a surface that locally minimizes its area). Such geometries are chosen for their well-known ability to provide effective mechanical properties and energy absorption capability [2]. In particular, the parametric modelling of the brick is achieved in 3 steps through a visual script by using Grasshopper software: i) Generation of the external shell; ii) generation of the periodic minimal surfaces from their implicit mathematical equations (Figure 1); iii) internal shape adjustment and finalization of the brick. At the end of the process, the obtained parametric model can be used to change the brick geometry as needed in terms of typology of minimal surface, internal and external walls thickness, and fill texture density.

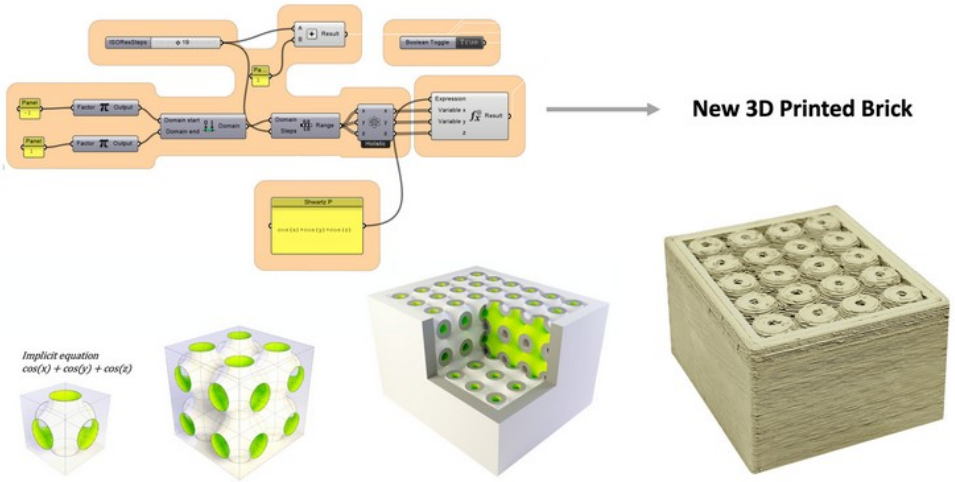

Figure 1 Generation of fill texture of the brick starting from the implicit equation of a periodic minimal surface and by using the Grasshopper visual scripting

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Title

A simple procedure for the definition of masonry strength domain

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Abstract

Numerical modeling of masonry structures has undergone a considerable development in recent years. Particularly, block-based models appear very promising to investigate the main aspects of masonry mechanics, as they can account for the actual masonry texture.

In this contribution, in the spirit of analyzing representative volume elements (RVEs) for masonry homogenization, the role of masonry texture is analyzed and discussed with a focus on its influence on material strength domains. The study is performed and validated using a block-based model, characterized by zero-thickness frictional-cohesive interfaces for mortar together with a continuum damage plasticity model for blocks, is adopted.

As a result, a simple procedure for the definition of the strength domain is presented and discussed. An arbitrary number of fracture mechanisms can be easily accounted in the strength domain, making it suitable both for masonry and for textured continua in general. The obtained formulation can also be employed within a computationally cheap textured continuum model.

Applications of the approach to regular masonry mechanical behavior are herein considered. The main features of the procedure are highlighted and the possible extension to other masonry textures is also discussed.

Title

Indentation of coated deformable layers analyzed via a new FE contact scheme.

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Abstract

When a rigid body indents a coated or layered bulk, contact stiffness is highly dependent on the elastic mismatch between the different layers as well as the thickness ratios of the materials. The FE contact scheme presented in [1] allows to accurately evaluate the combined effect of these two different agents, together with the possibility of taking into account any desired contacting geometry, from simple smooth indenters down to fully rough profiles.

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Title

An efficient computational approach for indentation-induced fracture based on the phase-field approach and interface finite elements with embedded roughness

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Abstract

Indentation experiments permit non-destructive testing of materials to evaluate their mechanical and fracture properties. The crack patterns caused by the indentation can be directly related to hardness and fracture properties of the material.
This work proposes an efficient numerical framework for simulating cracking phenomena due to indentation tests. The formation and subsequent cracks growth in the sample caused by indentation loading are modeled using the phase-field approach for fracture. The phase-field approach has been proved to be an efficient tool for failure simulations of brittle and ductile materials under different loading conditions, and it has been already applied in [1, 2] to simulate flat punch indentation tests.
The consistent computational cost related to the indenter discretization limits the simulation of more complex indenting geometries. In order to overcome this issue, the substrate phase-field model has been combined with the MPJR (eMbedded Profile for Joint Roughness) interface finite element proposed in [3] and extended in [4], which allows considering a nominally flat indenter without the need of an explicit discretization of its profile. The interface finite element considers the actual indenter profile as a correction to the normal gap at the interface between the indenter and the substrate, and solves the contact problem between the two solids. The present framework permits the evaluation of the micro-scale effect of the presence of roughness on the indenter and on the sampled surfaces, often neglected in the standard models since it can be directly introduced in the simulation through the interface finite elements.

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MS11 - Computational methods for nonlinear solid mechanics

Proposers

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Abstract

The mini-symposium invites contributions from the field of nonlinear computational mechanics of solids and structures. Discussions on the computational issues arising from the nonlinearities governing the considered problems and their solutions are encouraged. These include physical nonlinearities, such as nonlinear constitutive models, as well as geometrical nonlinearities due to buckling, large deformations and contact. The formulation of novel computational tools and the improvement of consolidated techniques are topics of great interest. Additionally, advanced design and optimisation strategies accounting for the nonlinear structural behaviour are welcome. Reduced order models for nonlinear problems are also considered with the aim of reducing the computational cost of the simulations and understanding the main parameters governing the mechanical problem. Finally, challenging full-scale case studies involving nonlinear simulations are appreciated. Main topics

- Modelling and discretisation techniques for nonlinear problems
- Integration of nonlinear constitutive equations
- Solution methods for nonlinear problems in statics and dynamics
- Buckling and instabilities in materials and structures
- Electro-elastic and thermo-elastic coupling and fluid-structure interaction
- Design and optimisation of nonlinear behaving structures
- Reduced order models
- Challenging nonlinear problems and case studies

Title

A new Lagrangian-Eulerian Particle Finite Element Method (PFEM) with automatic interface detection

Authors

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Abstract

The dynamics of fluid flows interacting with highly deformable structures and with evolving free surfaces is a complex problem, attracting considerable attention. Among the different numerical methods recently proposed in the literature, the Particle Finite Element Method (PFEM) is a mesh-based Lagrangian approach for fluid modelling, particularly suited for problems with fast changes in the domain topology. Starting from a set of fluid particles, the PFEM exploits the Delaunay triangulation and the alpha-shape method to create a new computational mesh, whenever the current one becomes overly distorted due to fluid motion [1].

In Fluid-Structure Interaction (FSI) problems involving large structure deformations and fluid free-surface flows, the PFEM represents a powerful numerical tool since fluid boundaries and FSI interfaces are tracked naturally by the position of the mesh nodes [2]. However, when non-homogeneous boundary conditions on velocities are imposed or in regions where the topology varies moderately, e.g. in confined portions of the fluid domain characterized by a fixed geometry, an Eulerian formulation turns out to be more convenient. To exploit the advantages of both formulations, a mixed Lagrangian-Eulerian description of boundary nodes has been proposed in [3]. According to this technique, nodes on the fluid free-surface and on the FSI interface, as well as all internal nodes are treated as Lagrangian, while the remaining boundary nodes are treated as Eulerian.

In many engineering applications, however, there is no need to treat all internal nodes as Lagrangian. In the present version of the mixed Lagrangian-Eulerian approach, nodes on the fluid free-surface and on the FSI interface are treated as Lagrangian, while the remaining nodes can be either Eulerian or Lagrangian. In particular, nodes in the Eulerian region are kept fixed during the whole analysis and there is no need for remeshing. Consequently, mesh generations are limited to a reduced domain only, thus significantly decreasing the computational burden. Furthermore, an algorithm to automatically detect runtime the transition zone between the two kinematic descriptions for FSI problems has been devised to increase the efficiency of the method. To validate the proposed approach, 2D numerical examples are developed and compared to those available in the literature.

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Title

A PFEM numerical model for the simulation of 3D concrete printing

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Abstract

3D Concrete Printing (3DCP) is rapidly gaining momentum in the building industry, as it could be the way to achieve a fully automatized and more sustainable construction process. However, before a large-scale adoption of this technology takes place, it is necessary to address some issues both at the practical and at the numerical simulation level. In the specific, the development of reliable computational tools would provide a better understanding of the printing process, while also enabling to predict, in a design framework, its outcomes, in terms of material, structural and process performances. In this work it is presented a 2D numerical model to simulate the extrusion and layer deposition phases of 3DCP. The model assimilates fresh concrete to a homogeneous weakly-compressible fluid and solves the Navier-Stokes equations in a Lagrangian framework with the Particle Finite Element Method (PFEM) [1],[2]. The model is applied to the printing of three rectilinear overlapped layers of cementitious mortar. The results in terms of layer's shape outline and pressure field are in good agreement with the data provided in [3]. The velocity field shows the sought behaviour in 3DCP, with the material reaching a state of rest soon after flowing out of the nozzle. Moreover, the pressure field offers some additional insights, which could be effectively exploited to prevent layer's collapse during printing and to ensure the final "quality" of the printed object.

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Title

Thermoelastic analysis of geometrically nonlinear shells using an isogeometric model

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Abstract

Temperature change in shell structures can produce relevant phenomena such as buckling and loss of stability. These effects are caused by the thermal induced stresses and by the temperature dependence of the material properties. The resulting nonlinear behaviour, which is quite complex for structures made of isotropic materials, is even more complicated when composites are brought into play. In fact, in a similar context, standard simulation tools exhibit lack of robustness or, in the most tricky cases, fail.
In this work, the problem of robustness and efficiency of geometrically nonlinear thermoelastic analyses is addressed. It starts from a solid-shell isogeometric discretisation that allows an accurate approximation of geometry and kinematics avoiding the parameterisation of finite rotations. A generalised arc-length method is proposed in which the temperature amplifier is taken as an additional unknown. Robustness is ensured by a mixed integration point (MIP) approach which expolits the advantages of mixed formulations in large displacements taking the stresses at the integration points as independent variables. Besides, to reduce the computational cost of the nonlinear analysis, a reduced order model is developed. It is based on Koiter's theory and gives the initial postbuckling behaviour efficiently for varying temperature amplifier. The main obstacle in the definition of an accurate reduced model is the the strain energy nonlinearity with respect to the temperature amplifier. This task is achieved by coherent asymptotic expansions and by an accurate evaluation of the buckling modes using a two-point mixed eigenvalue problem.
The robustness of the proposed continuation method and the accuracy of the reduced order model are demonstrated in several numerical examples. Traditional straight fibre composites are analysed as well as innovative variable stiffness materials and good results are obtained in all cases. Additionally, the proposed Koiter reduction technique opens up new possibilities for optimisation methods of thermally loaded structures and for studies on the stability under temperature changes.

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Title

A generalized path-following method for tracing the sensitivity curve in shell buckling

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Abstract

The failure of thin-walled structures is often dominated by buckling while the material is still in the elastic range. A geometrically nonlinear analysis is generally needed to estimate the load-carrying capacity taking into account the detrimental effect of imperfections, especially the geometric ones. The worst-case imperfection is usually sought among all possible combinations of assigned shapes, e.g. the first linearized buckling modes, by carrying out a large number of path-following analyses to detect the nonlinear critical point for each imperfection. With the aim of reducing the computational cost of such a procedure, an efficient continuation method is presented here for a direct evaluation of the critical point vs imperfection curve (generalized path), i.e. considering directly the subset of critical points without repeating a whole nonlinear analysis per imperfection. After a finite element (FE) discretization, the critical point is defined by a system of nonlinear algebraic equations imposing equilibrium and critical condition [1]. An arc-length equation is added to follow the path of critical points in the imperfection space. The solution of the extended system by a Newton scheme requires a Jacobian involving also the derivatives of the critical condition with respect to the FE parameters and the derivatives of all the problem equations with respect to the imperfection parameters. A closed form and efficient computation of the Jacobian is achieved by a solid-shell model and a strain-based equivalent imperfection. In addition, a mixed stress-displacement iterative scheme is devised for a highly efficient and robust solution. Exploiting the block structure of the equations, the robustness of the mixed iteration and the accurate predictor of the continuation strategy, the method requires just one factorization of the condensed stiffness matrix for each imperfection to evaluate the corresponding nonlinear critical point. Finally, the derivatives of the critical point with respect to the imperfection parameters are also obtained in closed form and can be used to generate a gradient-based generalized path for a quick search of the worst-case imperfection. All the details are available in [2].

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Title

Phase-field modeling of brittle fracture in plane stress conditions

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Abstract

The phase-field modeling of brittle fracture has gained more and more popularity in the last two decades as it can elegantly simulate complicated fracture processes, including crack initiation, propagation, merging, and branching, without the need for additional ad-hoc criteria and remeshing operations. Nevertheless, while the phase-field model provides excellent predictions in three-dimensional and plane strain conditions, a non-trivial application of the approach concerns plane stress problems. These are essential to model the mechanical behavior of structural elements such as plates and shells in a computationally efficient fashion. In the current work, a novel formulation for plane stress problems is proposed. The model presents a new free energy split where the in-plane and out-of-plane kinematic variables are conveniently separeted to correctly reproduce the fracture driving force. The resulting out-of-plane deformation provides a simple yet effective measure to assess the physical response of the model with respect to state-of-the art approaches such as [2]. Furthermore, the proposed split does not affect the structure of the phase-field problem which arise from the alternate minimisation of the total energy function and allows for a rigorous and efficient solution as proposed in [1]. Finally, the model reliability is proved through extensive numerical tests which compare three-dimensional and two-dimensional specimens in plane stress conditions.

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Title

Large displacement elastoplastic analysis of beams and shells: Finite elements and mixed iterative solution

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Abstract

This work addresses the analysis of slender structures with contemporary presence of geometric and material nonlinearities, focusing on the finite element discretization and the incremental-iterative solution. At each step of a path-following analysis the iterative solution is usually carried out at two different levels. The constitutive law is imposed locally at the integration point or element level in order to compute the internal forces. Then, the equilibrium equations are solved at the global level after assembling the finite element contributions. This strategy is well established but it is affected by an increase of the iterative burden in case of large rotations and high membrane/flexural stiffness ratios. This issue was solved for linearly elastic materials using mixed finite elements or mixed integration points [1] where the stress is considered an independent variable of the iterative process as well as the displacement. Different approaches are investigated in this work for the path-following finite element analysis of beams and shells in case of geometric and material nonlinearities, in order to identify the most efficient strategy in terms of discretization and iterative scheme. It is shown that for beam/frame structures, the most efficient solution is achieved by mixed (stress-displacement) finite elements, assuming the discrete stress DOFs of the element and the strain at the integration points as independent variables. The element state is not determined at each global iteration but the element equations are solved together with the global equilibrium equations. This approach allows to avoid the iterative issue for large rotations and high stiffness ratios and to reduce the local computational burden. Moreover, when the nonlinearity is mainly determined by the material, the mixed elements allow coarser meshes than those necessary in the displacement-based approach. On the other hand, the advantage of the mixed formulation in terms of required number of elements is lost in general shell structures, where the best choice is the use of displacement-based finite elements improved by the enhanced assumed strain technique [2]. These elements permit a faster evaluation of the element internal forces compared to mixed elements with a very similar accuracy-DOFs trend, while an efficient and robust iterative solution is achieved by solving the displacement-strain compatibility together with the global equations with the strain at the integration points as independent variables.

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Title

A novel Linear Complementarity Problem implementation for elastic–plastic structural optimisation of cable–rib satellite antennas

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Abstract

In the growing field of deployable aerospace structures, cable–rib satellite antennas are nowadays a target of increasing interest [1], fostering the need of consistent mechanical modelling and structural optimisation. The present work adopts Limit Analysis (LA) computational methods, as specific tools for structural modelling (see, e.g., [2, 3, 4]), accounting for material non–linearity, up to structural collapse, and possibly getting coupled to optimisation loops, toward maximisation of structural performance. In the contribution, a consistent mechanical formulation is proposed, accounting for rib elements with non–linear joints (exhibiting concentrated plastic deformations) and for linear tensioning cables, modelled by a common, wholly original, Linear Complementarity Problem (LCP) formulation. Such a computational approach is implemented within a self–made feasible procedure and validated on first specific antenna application examples. Moreover, optimisation scenarios of various, mechanical and geometrical, structural properties are investigated, within a coupled LA–optimisation framework, toward optimal automated design. The proposed computational modelling platform, both from a general standpoint in (Computational) Mechanics and from a specific viewpoint on such structures, allows for an innovative systematic structural description of satellite antennas, toward computationally efficient modelling and design.

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Title

Static limit analysis of masonry vaults: A generalized thrust network analysis

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Abstract

A reliable structural assessment of historical masonry constructions can be pursued by applying the static limit analysis theorem under Heyman's assumptions [1].
Here, the thrust network analysis (TNA) method is considered [2, 3]. It addresses the statics of a masonry vault under its self-weight by searching for a discrete network of internal compressive thrusts, acting along the network branches, in equilibrium with nodal weights. As the horizontal position of the network nodes is prescribed, the nodal equilibrium conditions are formulated in terms of the unknown nodal heights and force densities (i.e., the thrust-to-length ratio of the branches). After a priori solving the homogeneous horizontal equilibrium conditions, the nodal heights are expressed as nonlinear functions of the independent force densities through the vertical equilibrium ones. Accordingly, the safety assessment of the masonry vault is formulated as an optimization problem in the unknown independent force densities, under the constraint of compressive force densities and nodal heights contained within the vault thickness.
When considering the TNA, two observations arise. From a mechanical perspective, the method postulates that the stress state in a masonry vault is not more general than a membrane stress state acting on a thrust surface to be determined. From a computational perspective, the method is made demanding by its inherent nonlinear and nonconvex optimization format.
In response to such observations, a generalized thrust network analysis is proposed here for the safety assessment of vaulted masonry structures under their self-weight [4]. The crucial merits of the proposed method are the capability to account for general shell stress states in masonry vaults and the possibility to overcome the computational issues related to nonlinear/nonconvex optimization by the solution of a simple linear programming problem. Besides proving that the proposed method is a proper generalization of the classical TNA, an extensive campaign of numerical results is presented.

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MS12 - Poromechanics and fluid flows

Proposers

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Abstract

The computational simulation of a fluid flow and, possibly, its passage within a solid medium represents a mechanism common to a wide range of physical contexts, such as subsurface flows, soft tissues and hydrogels, among many others. In this minisymposium, we explore recent research in the mathematical analysis and the robust numerical approximation of these models, in order to efficiently handle their complex multi-physics and multi-scale nature.

Title

A fully dynamic poromechanics model for incompressible and nearly-incompressible materials: existence of solutions and projection scheme

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Abstract

Biological tissues can be seen as porous media in which solid constituents (such as the heart muscle, lung parenchyma, gray matter) are filled by viscous incompressible fluids (blood, lymph, cerebrospinal fluid). In this work, we consider the linearized version of a poromechanics model adapted to soft tissues perfusion [1]. This is a fully unsteady model in which the fluid and solid equations are strongly coupled through the interstitial pressure. As such, it generalizes Darcy, Brinkman and Biot equations of poroelasticity by including inertial and viscous effects both for the fluid and the solid. In [2, 3], the mathematical analysis of this model was performed for a compressible material and monolithic schemes were studied. More recently, an alternating minimization splitting scheme was proposed, leading to a solver closely related to the undrained and fixed-stress splits for Biot equations [4].

We show the existence of strong and weak solutions in the incompressible limit, which corresponds to the physiological regime. To do so, we use a semigroup approach and T-coercivity [5]. In particular, we recover an inf-sup condition independent of the porosity. Moreover, we present a projection scheme that enables to decouple the solid, fluid and pressure equations at each time step. Our approach is close to Chorin-Temam projection method but takes into account the specific saddle-point structure of the problem. We provide a convergence analysis of this scheme both in compressible and incompressible cases. Finally, we compare its efficiency with a monolithic approach and illustrate its sensitivity to the different model parameters.

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Title

Multiphysics wave propagation in porous media with polytopal Discontinuous Galerkin methods

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Abstract

In this talk, we focus on the numerical analysis of a polyhedral discontinuous Galerkin (PolyDG) scheme for the numerical simulation of multiphysics wave propagation in heterogeneous media. In particular, we address wave phenomena in poro-elasto-acoustic materials modeled by coupling the low-frequency Biot's equations and the acoustics equations. The coupling between different models is realized by means of physically consistent transmission conditions, weakly imposed at the interface between the subdomains. 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 in [1] 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.

For all models configuration, we introduce and analyze the PolydG semi discrete formulation [2], which is then coupled with implicit time marching schemes. We point out that the geometric flexibility and the arbitrary-order accuracy featured by the proposed PolyDG method are fundamental as they ensure a high-level of precision and scalability that are needed to correctly represent the solutions. For the semi-discrete problem, we present a complete stability analysis and derive a-priori *hp*-error estimates in a suitable energy norm. A wide set of verification tests with manufactured solutions are investigated in order to validate the convergence analysis. Examples of physical interest are also shown to investigate the performance of the proposed methods.

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Title

Virtual Element based geometric multrigrid solvers for the Poisson Equation

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Abstract

The potentialities of the Virtual Element Method (VEM) in the context of poromechanics and fluid flow simulations have been widely investigated and proved in the resolution of different physical and engineering problems. Indeed, the virtual element technique allows the use of very generally shaped elements and this is of fundamental importance in this type of applications involving geometrically complex domains. Nevertheless, still a lot is to be explored in the design of efficient solvers for the systems of equations stemming from the virtual element discretization of these problems. In the present contribution, we focus on the solution of the two-dimensional Poisson problem that is ubiquitous in the field of computational poromechanics and fluid dynamics. We present and analyse the convergence properties of two-level, W-cycle and V-cycle geometric multigrid schemes for the resolution of the h-version of the lowest order VEM. The sequence of grids are constructed by an agglomeration-based strategy exploiting the geometric flexibility of the VEM. Even if the meshes are embedded one in the other, the associated virtual element spaces are generally not nested. Therefore, we resort to the abstract BPX framework for non-nested multigrid schemes and possibly non-inherited bilinear forms. We propose some numerical experiments that validate the effectiveness of the proposed multigrid schemes.

Title

A contact mechanics and fracture flow: a stabilized formulation and a scalable preconditioning framework mechanics

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Abstract

For many subsurface application, such as geothermal energy production and CO_2 sequestration, a major role is played by the coupled simulation of frictional contact mechanics and fluid flow in fractured porous medium. In addition, large domains with high resolution representations of the geological structures and their heterogeneous properties are usually required to achieve the desired accuracy. These aspects naturally reflect on the growing demand for better performance of sophisticated and computationally expensive models. In this talk, the focus is on the linear solver, that is the most time consuming component of a simulation, and in particular on the design of a scalable and efficient preconditioning framework for the coupled contact mechanics and fluid flow problem. The model relies on the explicit discretization of the fractures, with the Lagrange multipliers method used to impose the contact constraints. Low order finite elements are used for the mechanics, while a cell-centered finite volume scheme has been adopted for the fluid flow. The arising system of equations has been properly stabilized to satisfy the inf-sup condition.
We design a scalable preconditioning framework for the 3x3 block matrix [1] exploiting the natural unknown subdivision and a state-of-the-art aggregation-based multigrid solver. Two different approaches have been derived with the identification of theoretical bounds for the eigenvalue distributions of the preconditioned matrices. The two methods are tested on real world cases to prove 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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Title

Variational principles for the linear viscoelastic problem

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Abstract

As observed by Tonti [4], variational formulations for initial value problems, and in particular for the non-aging linear viscoelastic problem, are not possibile in the classical context of the Calculus of Variations; this is due to the fact that the linear operators relevant to linear initial value problems are not self-adjoint with respect to the standard bilinear form.
The first true variational formulation for initial value problems dates back to Gurtin's work [1][2][3]. It is based on the use of convolution 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 extremum principles.
To the authors' knowledge, there does not appear to be any significant work in the literature concerning the use of variational formulations for the numerical resolution of the viscoelastic problem. In particular, variational principles based on convolutive bilinear forms with respect to time do not seem to have had any place so far in computational procedures for the numerical determination of the viscoelastic response of solids or structures subject to external actions.
This paper aims to fill this gap with reference to Gurtin's formulation and those related to it.
With reference to the non-aging linear viscoelastic problem, three convolutive-type variational formulations existing in the literature are critically reviewed: the Gurtin formulation, the split Gurtin formulation and the Huet formulation. The formulations are used for the numerical resolution of the hereditary viscoelastic problem through spatial and temporal discretization, both considering a finite time range and using a step-by-step method of time marching. Several numerical examples are included and numerical results are compared with the aim of investigating the effectiveness of the variational formulations in the numerical solution of the viscoelastic problem.

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Title

Pressure robust a-posteriori bounds with error-dominated oscillation

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Abstract

Pressure robust methods and estimates for the Stokes equation preserve the separation between the velocity and pressure variables imposed by the data, hence the velocity field is unaffected by pressure perturbations. This concept stimulated much research in the last decade. Recently, Verfürht and Zanotti developed new pressure robust quasi-optimal methods (e.g. [1]).
We shall present a pressure robust a-posteriori estimator suited for these methods, which is also robust with respect to the natural data regularity: Building upon [2], the oscillation is dominated by the error, which prevents overestimation. If the data is evaluable on polynomials the estimator can be computed exactly. Therefore, the method as well as the a-posteriori bounds prevent the danger of poor approximation or estimation properties because of pressure perturbations and missing regularity.

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MS13 -In silico approaches to advance and personalize cardiovascular medicine

Proposers

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Abstract

In silico modeling and image-based analysis are moving towards having an effective and crucial role in diagnosis, prognosis and treatment of several cardiovascular pathologies. Advanced three-dimensional (3D) and time-resolved imaging techniques are increasingly employed to deepen the severity of cardiovascular disfunctions and design patient-specific treatments, with percutaneous and minimally invasive procedures being the preferred solution. To this purpose, patient-specific numerical simulations can be exploited to assess procedure feasibility in complex clinical scenarios or to predict the post-operative biomechanics, while advanced processing of medical imaging can inform pre-operative planning, facilitate patient stratification and improve procedural timing. Thanks to the recent advancements in cardiovascular imaging, in terms of scanners' technology and acquisition protocols, a large amount of data is now available to enhance the realism and completeness of computational models as well as to extract additional morphometric and functional in vivo measurements, e.g., patient-specific hemodynamic changes over the cardiac cycle or non-invasive measures of vessels' distensibility. Cutting-edge approaches based on machine learning algorithms have already been proposed to fully exploit this amount of data automatizing and fastening predictive analytics for novel interventions and improving treatment plans. The mini-symposium has been designed for young scientists ($\leq$ 35 years old) and aims to gather and share state-of-the-art approaches able to translate computer-based solutions into daily clinical practice.

Title

Self-expandable transcatheter aortic valves: Impact of Nickel-Titanium super-elastic material properties on the device mechanical performance

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Abstract

Self-expandable transcatheter aortic valves (TAVs) elastically resume their initial shape during the implantation procedure without the need for balloon expansion, owing to the super-elastic properties of their Nickel-Titanium (NiTi) frame. Experimental findings report that the NiTi mechanical properties are highly variable depending on the chemical composition and processing of the alloy. Within this context, a computational framework is here presented to study the impact of the NiTi super-elastic material properties on the TAV mechanical performance and, accordingly, on the procedural outcomes. Finite element (FE) simulations of TAV implantation were performed, accounting for two commercial devices and three different idealized aortic root anatomies, and the mechanical response in terms of two FE outputs, namely the pullout force magnitude exerted by the frame and peak maximum principal stress within the aortic root was evaluated. Multi-parametric sensitivity analysis and a multi-objective optimization study of the TAV mechanical performance were performed in relation to the parameters of the most largely adopted NiTi super-elastic constitutive model. As main findings of the study we report that: (1) only five out of eight material model parameters were characterized by a significant correlation with both the two FE outputs (a clear indication for streamlining the design process); (2) the geometry of the TAV frame and the aortic root anatomy had a marginal impact on the influence that each NiTi material constitutive model parameter has on the mechanical performance of the device; (3) NiTi alloy candidates with pareto-optimal characteristics in terms of TAV mechanical performance were successfully identified. In conclusion, the proposed framework could support the TAV design phase, providing precious information to manufacturers on the relationship between the material properties of the supplied NiTi alloys and the TAV mechanical response. Moreover, this study has the potential to be extended to other cardiovascular devices and to account for additional features, including NiTi manufacturing data and geometrical shape optimization of the TAV frame.

Acknowledgement

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Title

A comprehensive study to develop a numerical model of the left atrial appendage occlusion

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Abstract

Left Atrial Appendage Occlusion (LAAO) with Nitinol devices is a percutaneous procedure to prevent thrombus formation generating over 90% in left atriums affected by atrial fibrillation. Real-world clinical outcomes proved how LAAO is a non-inferior alternative to oral anticoagulants. Nonetheless, the LAA morphological complexity hinders the device sizing and positioning. In this regard, Finite Element (FE) modeling is a robust tool in guiding clinical decisions among the available strategies (e.g. 3D imaging modalities, 3D printed anatomical phantoms). To date, the works available in the literature on FE modeling of LAAO [1] define the optimal device positioning without providing evidence about a thorough investigation of the crucial features affecting the procedural outcomes. The current study proposes a comprehensive approach to build a FE model of LAAO, including virtual models of the device and LAAs.

A physical sample of the Watchman device (Boston Scientific) was available. CT images were used to ensure a high-fidelity reconstruction and the built CAD model was discretized. In-vitro tests were designed to characterize the Nitinol frame and validate the FE model. Based on CT images, a number of patient-specific anatomies were reconstructed throughout the cardiac cycle and discretized. Wall properties were investigated: FE simulations were performed to calibrate a normalized stiffness, assuming from the literature both the atrial pressure gradient and the wall thickness. Finally, device deployments were simulated.

The validation of the device FE model and the characterization of patient-specific anatomies led to develop a numerical tool for investigating the influence of anatomical features (i.e. wall thickness and elastic modulus) and the procedural variability (position of the crimped device) on the outcome of the procedure.

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Title

Patient-specific computational fluid dynamics simulation before and after surgery in stenotic carotid arteries

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Abstract

Hemodynamics plays a significant role at the carotid bifurcation because of the preferential development of atherosclerosis. The present study considered patients with an internal carotid stenosis. We developed a patient-specific (PS) computational fluid dynamics (CFD) model to compute luminal area exposed to atherogenic biomechanical stimuli and to assess the impact of the stenosis on the local hemodynamics of the contralateral side. Patients were divided into two groups based on the Peak Systolic Velocity (PSV) measured in the stenotic vessel. Angio computed tomography (CT) images were used to reconstruct PS 3D model (Fig. 1A). PC-MRI data were analyzed to define PS boundary conditions (BC) for the CFD simulation (Fig. 1B). Two slices below and above the carotid bifurcation were acquired to extract the flow of the common carotid artery (CCA), the internal carotid artery (ICA) and the external carotid artery (ECA). CCA flow measured was directly imposed as inlet BC. Both measured flows of ICA and ECA were corrected to enforce conservation of mass [1]. In the branch with the highest flow, we imposed the corrected flow as outlet BC, while a stress-free BC was used in the other one. Pulsatile flow simulations were run for three cardiac cycles. Area exposed to low Time averaged wall shear stress (TAWSS) was evaluated (Fig. 1C). Pre- and post-operative results of non-stenotic vessels were compared. Considering the group with a hemodynamically relevant stenosis (PSV $\geq$ 230 cm/s), the results showed that the stenosis created a hemodynamic crosstalk that reconfigured the local hemodynamics in the contralateral vessel (Fig. 1D). We hypothesize that hemodynamically relevant stenoses may have an atheroprotective effect on the opposite side. This hypothesis will be investigated in future studies.

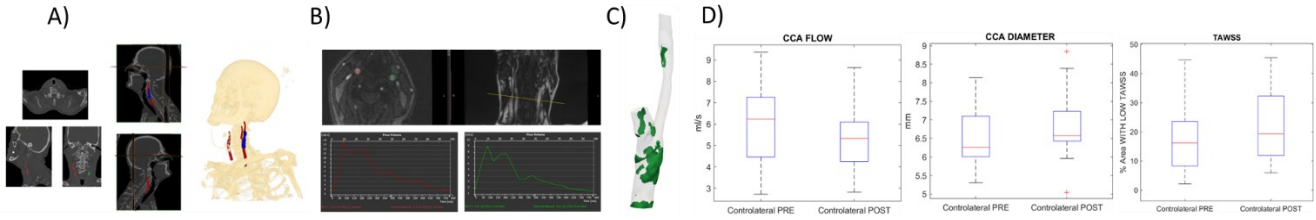

Figure 1 – A) PS 3D model reconstruction from CT; B) Flow extraction from CP-MRI; C) Area with low TAWSS; D) Boxplot of CCA flow, CCA diameter and % Area of low TAWSS pre and pos- operative in contralateral carotid arteries

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Title

Evaluation of the Double Outlet Right Ventricle (DORV) through numerical simulations.

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Abstract

The Double Outlet Right Ventricle (DORV) is a rare congenital heart malformation where both arteries that carry blood from the heart to the body and lungs come from the right ventricle only. Also, in DORV, there is a hole between the two ventricles, called Ventricular Septal Defect (VSD), which allows blood to mix through the VSD into the two ventricles with exit through the artery. The first approach of this study is to quantify the oxygenated and non-oxygenated blood that actually leave the aorta and pulmonary artery, in different conditions, to improve knowledge of this malformation and the surgical strategy [1]. The geometries of the analyzed cases are extracted from 4D-transesophageal echocardiography and the flow analysis is performed through Direct Numerical Simulations (DNS) [2]. The results made it possible to identify in detail the real diversification of blood generated by the passage in the VSD and expelled in the two vessels and the presence of a different combination of the subvolumes [3, 4, 5] which, in the long term, can lead to severe cardiac degeneration. This can help in assessing this rare malformation, the urgency and the type of surgery to be performed.

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Title

Non-invasive pressure estimation in abdominal aortic aneurysm: comparison among 4D flow MRI, CFD and 4DVar

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Abstract

Non-invasive methods for estimating 3D distributions of intravascular pressure would significantly benefit the clinical practice for a wide range of vascular diseases. Intravascular pressure fields can be derived directly from computational fluid dynamics (CFD) or from 4D flow-based velocity fields by solving the Poisson pressure equation (PPE). However, both techniques still have limitations. Variational data assimilation (VarDA) can be used to find optimal boundary conditions, effectively minimizing a misfit cost with respect to measured data and concurrently forcing consistency with physical and constitutive laws. In this work, a 4D (3D space and time) VarDA algorithm was employed to combine CFD with 4D flow MRI, improving 4D flow-derived pressure estimation.

A 4D flow MRI acquisition of a subject with an abdominal aortic aneurysm (AAA) was processed using previously developed in-house tools. A transient blood flow CFD simulation was carried out using a finite element method implemented through FEniCS, discretizing the Navier-Stokes equations in time using a θ time-stepping scheme. Zero-pressure was applied as outlet boundary condition while a plug velocity profile was prescribed at the inlet. The 4DVar algorithm was developed through the dolphin-adjoint library. The 4DVar optimization routine was carried out for 30 iterations in order to minimize a cost functional formed by the combination of mean-square-error with respect to 4D flow observations and spatiotemporal regularization terms. In order to avoid near-wall region errors of 4D flow MRI acquisition the cost functional was defined over an inner subdomain at distance s from the original boundaries according.

The velocity fields obtained with the CFD simulation using a plug velocity profile were in good qualitative agreement with the 4D flow velocity data. After 30 optimization iterations, the 4DVar algorithm allowed to obtain velocity fields that better resembled 4D flow data, successfully resulting in a lower RMSE. 3D pressure maps obtained from 4D flow were significantly lower than CFD and 4DVar results. However, lower discrepancies were observed in terms of pressure between 4DVar and 4D flow at systolic peak.

Estimating pressure from 4D flow by solving the PPE is known for underestimating true pressure values. CFD can result in low fidelity velocity fields and pressure distributions. Our results show that by assimilating 4D flow data into CFD, one can obtain velocity fields and 3D pressure maps that are in better agreement with 4D flow-derived values.

MS14 -Young developments on dynamical low-rank approximation

Proposers

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Abstract

The numerical approximation of time-dependent high-dimensional problems is a challenging task. The storage and computational effort required for an effective numerical approximation scales exponentially with the dimensions of the problem, the so-called *curse of dimensionality*. The present minisymposum discusses an important emerging approach: the dynamical low-rank approximation (DLRA).

Dynamical low-rank approximation finds its origins in the Dirac-Frenkel variational principle for the time-evolution of large dimensional problems for quantum-molecular dynamics, and it has been further extended to the general setting of ODEs: The evolution of the dynamics is projected on a search space of lower storage complexity, resulting in consequent benefits of memory efficiency and computational effort. Robust first-order in time numerical integrators for fixed-rank matrices, tensors in Tucker format and tensor train format have been recently proposed and analyzed. The notion of rank-adaptivity and high-order convergence is a central topic in the improvements of current numerical integrators for DLRA. Therefore, during the first part of the mini-symposium, innovative results from the young DLRA community will be presented.

Dynamical low-rank approximation does not constrain itself to the ODE setting. The extension to the PDE setting has been already introduced and recently, the method has been successfully applied for iterative methods in linear algebra and data-science. The second part of the MS will focus on recent uses of DLRA for kinetic problems and data-science. Important contributions to radiation therapy and the Vlasov-Poisson equations will be presented. Finally, recent fundamental applications of robust numerical integrators for dynamical low-rank approximation to the field of machine learning are going to be discussed.

Title

Dynamical low-rank integrators for second-order matrix differential equations

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Abstract

In this talk, we introduce a new dynamical low-rank integrator for second-order matrix differential equations [2]

$$A''(t) = F\big(A(t)\big), \qquad A(0) = A_0, \quad A'(0) = B_0, \quad t \in [0, T],$$

typically stemming from space discretizations of wave equations. The integrator is constructed by combining the projector-splitting integrator introduced in [1] with a Strang splitting ansatz. We also present a variant of the new integrator which is tailored to stiff second-order problems. The performance of the new schemes is illustrated by numerical experiments.

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Title

Rank-adaptive time integration of tree tensor networks.

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Gianluca Ceruti , EPF Lausanne

Abstract

In many applications it is of interest to solve numerically high-order tensor differential equations, e.g. the many-body Schrödinger equation in quantum physics or discretized high-dimensional time-dependent partial differential equations. Tree tensor networks turned out to be a promising ansatz to overcome the so-called "curse of dimensionality" as they are an efficient hierarchical data sparse format to approximate tensors. Recently, based on the dynamical low-rank approximation, a rank-adaptive integrator for tree tensor networks has been proposed in [1], which allows to numerically solve tensor differential equations, even for very high orders of the tensors.
In a recursion from the leaves up to the root of the tree, the integrator updates bases (leaves) and then evolves connection tensors by a Galerkin method in the augmented subspace spanned by the new and old bases. Therefore the hierarchical data sparse format is preserved throughout the full propagation. The rank-adaptivity allows the integrator to dynamically choose the ranks at each time step, which is important as the optimal ranks required for a given approximation accuracy may vary strongly with time.

In the present contribution we introduce the concept of dynamical low-rank approximation, tree tensor networks and the rank-adaptive integrator of [1]. Furthermore, robust error bounds and the norm and energy preservation for the many body Schrödinger equation are discussed. Numerical experiments validating the theoretical results are shown.

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Title

A robust collision source method for rank adaptive dynamical low-rank approximation in radiation therapy

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Abstract

Computational methods in radiation therapy require a discretization of the six-dimensional phase space, composed of energy, spatial position and direction of flight. The dimensionality of the problem further increases when considering uncertainties. This prohibits fine numerical discretizations which are essential for the construction of accurate and robust treatment plans.
We use a dynamical low-rank approximation (DLRA) of the particle density to evolve the solution of the continuous slowing down approximation to the transport equation on a low-rank manifold in time. Here the energy is treated as a pseudo-time and a rank adaptive integrator is chosen to dynamically adapt the rank in energy. To facilitate the use of boundary conditions and reduce the overall rank, the radiation transport equation is split into collided and uncollided particles through a collision source method. Uncollided particles are described by a directed quadrature set guaranteeing low computational costs, whereas collided particles are represented by a low-rank solution. The resulting method is more efficient concerning both run-time and memory than conventional radiation transport solvers and agrees well with conventional deterministic solvers as well as state-of-the-art Monte Carlo codes.
We further extend the method to directly include uncertain parameters and therefore quantify even complex and time-dependent uncertainties efficiently. We observe good agreement of the computed expected value and variance of the delivered dose with collocation methods already at a significantly reduced rank for simple Gaussian errors. A higher rank is required for highly irregular time-dependent uncertainties derived from patient CT data, however the complexity is still reduced compared to standard collocation based approaches.

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Title

Efficient 6D Vlasov simulation using the dynamical low-rank framework `Ensign`

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Abstract

Efficiently solving kinetic equations is important in applications ranging from plasma physics to radiative transport. In their numerical simulation, one of the main challenges is the up to six-dimensional phase space, and the associated unfavorable scaling of computational cost and memory requirements.
In the context of Vlasov–Poisson equations, it has been shown that dynamical low-rank algorithms can drastically reduce the required simulation effort, while still accurately resolving important physical features such as filamentation and Landau damping (see, for example, [1]).
In this talk, we present a new second order projector-splitting dynamical low-rank algorithm for the full six-dimensional Vlasov–Poisson equations, which has been introduced very recently in [2]. An exponential integrator based Fourier spectral method is employed to obtain a numerical scheme that is unconditionally stable but still fully explicit.
The resulting method is implemented with the aid of `Ensign`, a C++/CUDA software framework, introduced again in [2], which facilitates the efficient implementation of dynamical low-rank algorithms on modern multi-core CPU as well as GPU based systems. In dynamical low-rank context, providing a software package is arguably really important, as the resulting evolution equations are somewhat more complex than the original model. The usage and features of `Ensign` are briefly described in the talk as well.
We finally conclude the presentation by discussing numerical and performance results on linear Landau and two stream instability problems, which demonstrate that 6D simulations can be efficiently run on a single workstation and highlight the significant speedup that can be obtained using GPUs.

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Title

Dynamical low-rank training of neural networks

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Abstract

Neural networks have achieved tremendous success in a large variety of applications. However, their memory footprint and computational demand can render them impractical in application settings with limited hardware or energy resources. At the same time, overparametrization seems to be necessary in order to overcome the highly non convex nature of the training optimization problem. An optimal trade-off is then to be found in order to reduce networks' dimension while mantaining high performance. Popular approaches in the current literature are based on pruning tecniques that look for subnetworks able to mantain approximately the initial performace [4].
Nevertheless, these tecniques often are not able to reduce the memory footprint of the training phase. In this talk we will present DLRT [1], a training algorithm that looks for "low-rank subnetworks" by using DLRA theory and tecniques [2, 3]. These subnetworks and their ranks are determined and adapted already during the training phase, allowing the overall time and memory resources required by both training and evaluation phases to be reduced significantly. I.e., a memory reduction up to more than 90% is achieved during the training phase. The efficiency of the proposed method is demonstrated through a variety of numerical experiments both on fully-connected and convolutional networks.

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MS15 - Computational models as enabling technologies for (bio)printing design and tissue engineering applications

Proposers

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Abstract

Bioprinting (BioP) is a biofabrication technique that consists in the 3D printing of a bioink (i.e., that is a combination of cells, growth factors, genes, and drugs incorporated within a biocompatible hydrogel) to create three-dimensional biological construct for regenerative medicine and tissue engineering applications. The BioP process begins with the ladening of cells into the hydrogel to form the bioink. Then the bioink is printed and the fabricated construct is crosslinked to ensure structural stability and biological constraints. Finally, the construct is placed in the incubator improve and speed up the process. Several process manufacturing variables must be fixed in the pre-printing phase for defining the settings of the printing process, such as the design of the final geometrical structure, the definition of the printing pattern, as well as decisions on the composition of the bioink (e.g., rheological properties of the biomaterial, number of cells, etc.), crosslinking protocols, and cell nutrition. These variables are influenced by complex mechanisms related to mechanics, chemistry, and biology. For this reason, a balance between the constraints of technological engineering and the biological and biotechnological requirement is need. To this end, computational approaches have been developed to provide in silico answers to decisions on BioP process variables to limit experimental tests that are time-consuming, expensive, and often turn out to be impractical. In this context, the proposed symposium focuses on the discussion of the key role of computer modeling and simulations for the bioprinting process optimization.

Title

In silico Approaches Towards Biofabrication of Human Eardrum Scaffolds

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Abstract

The thin and concave tissue of tympanic membrane (TM) or more commonly known as the eardrum, captures sound pressure waves from the environment and transforms them into mechanical motion. The successful transmission of these acoustic vibrations is accredited to its intricate three-dimensional (3D) architecture comprising of radial and circumferential collagen fibers aligned within a conical shape [1]. In this work, we investigated the influence of this precise geometrical construction on its mechanical and acoustic response by applying relevant *in silico* and *in vitro* tissue models [2].

A Python script was developed for generating 3D models highlighting the key anatomical features of the human TM. Three test cases along with a plain control were chosen to decouple some of these dominant structural attributes. A dual-scale fabrication strategy combining electrospinning and additive manufacturing was carefully optimized for manufacturing the chosen designs. Preliminary computational modeling performed on COMSOL Multiphysics suggested a geometrical dependence over their mechanical and acoustic responses, where the presence of radially aligned fibers was observed to have a more prominent effect as compared to their circumferential counterparts. The experimental characterizations conducted using macro-indentation and laser Doppler vibrometry also confirmed similar vibro-acoustic results. Finally, human mesenchymal stromal cells and human dermal fibroblasts cultured on the TM scaffolds demonstrated a desirable alignment and collagen deposition along the fabricated patterns.

This work synergized theoretical and experimental approaches toward understanding the significance of geometry in tissue engineered TM scaffolds [2]. Furthermore, with the optimized biofabrication strategies, a radical improvement has been achieved in the previously reported limits for manufacturing human TM.

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Title

Computational modelling of a milli-scale perfusion bioreactor for vascular applications

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Abstract

Introduction – Vascularization is one of the most critical challenges of tissue engineering (TE) and it is fundamental to establish complex and long-term reliable three-dimensional (3D) models. Current technologies for biomanufacturing the vessel structure still lack standardization to enable a wider adoption of such systems, calling for further activities dealing with the deeper characterization of different physiological or pathophysiological conditions [1]. To fill this gap, a novel 3D-printed modular and versatile perfusion bioreactor, capable of replicating 3D tissue-like vascularized constructs, has been proposed. To this aim, we describe the computational simulation-based study conducted to support the first steps in bioreactor design and its parameters tuning, by avoiding a trial-and-error procedure.

Materials and methods – The device, designed with Fusion 360 (Autodesk) and fabricated with a FDM printer (Creality CR6 SE), was conceived to easily interchange its components, allowing for the generation of tunable vessels in length and diameter. An in-silico model of the bioreactor was created considering a channel with a diameter and length equal to 2.5 and 5mm, respectively. Numerical simulations to assess the fluid-dynamics of the medium flowing inside the bioreactor and O_2 diffusion were performed. In particular, for the numerical fluid-dynamic assessment, two domains were identified: i) a free flow domain (i.e., the channel) modeled with Navier-Stokes equation; ii) a porous flow domain, replicating the hydrogel around the channel, modeled with Stokes-Brinkman equation. Regarding the diffusion part, Fick's law was used to describe oxygen diffusion through the medium and hydrogel, and Michaelis–Menten kinetics to model O_2 consumption of HUVECs, around the channel, and of hepatocytes, within the hydrogel-based construct. Different flow rate values at the inlet were taken into consideration. Velocity and pressure fields, shear stress, and O_2 concentration distribution throughout the perfusion system were computed and analyzed. Preliminary validation in static with only HUVECs was performed.

Results and discussion – The flow pattern, represented by velocity streamlines, is always able to reach internal regions of the scaffold with the value of hydrogel's permeability and porosity considered, irrespective of flow rate. Since closely related, O_2 distribution and shear stress were studied together and the related critical values of each quantity (>0.04 mM and <5 dyn/cm^2, respectively [2]) were assessed to prove that such thresholds were not reached by the proposed device. The bioreactor was successfully validated in the short term in static demonstrating its compatibility with functional endothelial cells and the wall formation around the channel.

Conclusions – In this preliminary part of computational study, the obtained results were beneficial for optimizing the design specifications and understanding relevant issues, especially in assessing whether the internal parts of the scaffold were perfused and in finding a balance between shear stress, acting directly on the vessel wall and that can provoke the detachment of endothelial cells, and O_2 distribution within the construct, responsible of the cell survival and function. Next steps will see experimental tests in term of dynamic culture in order to validate the obtained computational results and further computational analyses to study cell diffusion throughout the system given by the perfusion flow created by the bioreactor.

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Title

Computational framework for 4D bioprinting

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Abstract

Four-dimensional (4D) bioprinting refers to the fabrication via additive manufacturing of structures, designed to interact with physiological systems at cellular level, that possess the capability to shape transform over-time, when exposed to a specific external stimulus [1]. 4D bioprinting is influenced by several variables (e.g., stimulus, materials, geometries), thus being characterized by a long trial and error process. In this context, mathematical modeling assumes high relevance since it can predict the over-time structure evolution for given material properties, geometries, and stimuli, thus reducing material and time waste. Here, we present two different case studies in which finite element (FE) modeling, via Comsol Multiphysics 5.3, was implemented to study the shape morphing behavior of 4D bioprinted structures made of regenerated silk (RS) under the effect of temperature, for the development of bimorph springs for the treatment of the short bowel syndrome via distraction enterogenesis [2], and for the development of bilayer sutureless clips for intestinal anastomosis [3]. The rationale of both studies relays on the negative expansion coefficient of RS, that converts the thermal energy into the structures shape-shifting.

Bimorph springs: Core–shell coiled structures were 4D bioprinted via coaxial extrusion based bioprinting (EBB). Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) was used as shell ink, whereas four different RS compounds were used as core ink with different RS concentration and the addition of graphene nanoparticles (GNPs). FE models, featuring the solid mechanics application mode, were exploited to evaluate structure movements as a variation of the core compound. Models showed a temperature-induced self-contraction and torsion of the structures, with a greater contraction (i.e., movement along the spring axis) when the compound with the highest concentration of RS and the addition of GNPs is simulated, due to its higher Young's modulus and thermal contraction coefficient. Models have been validated via phantom testing. Briefly, the PHBV-RS/GNPs 80:20 was able to pull the flaps of a silicone intestine phantom from 3.58 to 3.49 cm due to an increase in temperature from room temperature to 37°C.

Sutureless clips: Bilayer hollow tubes were 4D bioprinted via EBB, equipping the printer with a rotating spindle. The inner layer of the structure was made of PHBV, whereas the external layer was made of RS/$CaCl_2$ or RS/$CaCl_2$/KNO_3. FE models, featuring the solid mechanics application mode, were performed to analyze the capability of the bilayer structure to radially contract under thermal stimulus. The simulations showed that at 37°C the tubes contracts radially, compressing the intestine wall, with a more pronounced compression when the RS/$CaCl_2$/KNO_3 solution is simulated, involving a radial displacement of the intestine wall–PHBV interface of 10.38 μm. Models have been validated via *ex vivo* testing. Briefly, the RS/$CaCl_2$/KNO_3 –PHBV tubes were inserted over a portion of murine intestine and their ability to resist peristaltic pressure was analyzed via bursting pressure, which reached approximately 90 mmHg, thus validating the temperature-induced anastomosis ability of the structure.

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Title

Finite Element Models of Bio-ceramic Scaffolds for Bone Tissue Engineering: design and characterization

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Abstract

Bone is a self-healing tissue, but some pathologies, aging, non-physiologic conditions and trauma may cause a critical size bone defect that cannot heal spontaneously. The implant of bio-ceramic scaffolds is a promising approach for the treatment of these pathologic conditions. Among bio-ceramics, hydroxyapatite (HAP) is considered a good candidate for bone scaffold manufacturing thanks to its high affinity with the native bone's mineral component, thus ensuring biocompatibility and promoting osteo-integration. Recent developments in 3D printing technologies allow for a wide variety of micro-structured devices meeting patient-specific needs. In particular, DLP-stereolithography is a printing technology allowing for very fine spatial resolution and high printing fidelity. However, as the technological process includes a sintering phase at high temperature, the properties of the obtained material are strongly affected by the intrinsic defects which characterize the final product. Computed micro-Tomography (μCT) based finite element (FE) analyses are suitable for assessing mechanical properties taking to account the micro defects occurring due to de manufacturing process [1].
We first assessed through μCT-based FE simulations the macroscopic stiffness and strength of high-porous trabecular-like architectures, obtained from an open-cells polyurethane foam template. The obtained macroscopic properties are validated through comparison with macroscopic experimental data already available on the same architecture and material [2].
Even if the aforementioned scaffolds match the native trabecular bone strength, mechanical and physical properties (*i.e.* permeability) can be improved by using Triply Periodic Minimal Surfaces (TPMS) microarchitectures. They are particularly suitable for bone scaffolding, where load-bearing capability and high interconnectivity of pores are needed for rapid tissue regeneration. Thereby, starting from analytic formulation of TPMS, we have designed hundreds of designs by changing the input parameters of the function. In this sense, classical optimization approaches may be unsuitable for such a complex approach in which multiple output parameters (mechanical, physical and morphological) have to be monitored simultaneously. For this purpose, Machine Learning approaches can be a suitable approach to support the selection of a design with prescribed multi-disciplinary properties.

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Title

Modelling and simulation of macroscopic flows of dense suspensions

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Abstract

The rheology of highly concentrated suspensions of solid particles dispersed in a viscous fluid features a number of surprising phenomena [1]. By varying the rate of deformation we can observe shear thinning, continuous or discontinuous shear thickening and, at very high concentrations, even the phenomenon of shear jamming. While the understanding of the microscopic origin of these phenomena has reached a significant depth [2, 3], the definition of suitable continuum–level models able to capture the rheology of dense suspensions is still the subject of active research efforts [4].
Building on a recently proposed tensorial model for shear–jamming suspensions [5], we develop constitutive relations that allow to include further effects such as shear thickening and yielding. In particular, the inclusion of rate-dependent phenomena requires the addition of evolution equations for tensorial measures of strain, akin to the conformation tensors used in viscoelastic fluid models. The presence of such evolution equations and the nonlinearities that arise in coupling them to the flow equation require appropriate computational strategies to guarantee the reliability of the numerical results [6].
Different features of the proposed continuum model are analyzed and illustrated with numerical solutions in paradigmatic examples of complex flows, in which the geometric features of the domain and the possible presence of free surfaces make it necessary to have available a fully tensorial model. In parallel, we discuss the numerical strategies employed to treat such heterogeneous flows.

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Title

Multiscale agent-based model to investigate the mechano-biological regulation of bone fracture healing inflammatory stage

Authors

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Abstract

Bone fracture healing is a complex process. Its complexity is noticeable during the initial inflammatory phase, which starts right after the injury with the activation of the immune response. As the role of *in silico* technologies is currently growing in characterizing the next generation of bone healing models [1], we are developing a computer model to investigate bone healing from the initial inflammatory stage. Once fully developed, it will provide clinical added value due to its capacity to explore the mechanical and biological aspects of therapeutic strategies that can enhance bone fracture regeneration from its earliest moments.

We developed a multiscale in silico model that combines finite element and agent-based models to simulate bone fracture healing in mechanical and biological environments, respectively. With this novel approach, the immune cells can be simulated as single entities during the inflammatory stage. Therefore, their temporal and spatial dynamics can be explored by including the stochasticity that characterizes biological processes, which are highly variable. *In vivo* immunofluorescence images from a previous work [2] will be used to perform quantitative and qualitative calibration. These images are segmented to quantify the different cell types in the bone fracture images and compare them with the simulation results. In the first instance, a sensitivity analysis is performed with the support of Taguchi's orthogonal arrays [3] applied to Design of Experiment (DoE) techniques. This preliminary analysis allows identifying the most influential parameters of the model. In the following step, those parameters will be calibrated using a genetic algorithm (machine learning).

Sensitivity analysis showed that a realistic number of macrophages within the healing region could be obtained if the following parameters are properly calibrated: (a) inactivated macrophages proliferation ratio, (b) macrophages recruitment factor, (c) pro-inflammatory macrophages proliferation ratio. In detail, while (a) has primary importance during the whole development of the inflammatory stage, the other two are observed to lose (b) or gain (c) their role through the evolution of the inflammatory stage.

The preliminary sensitivity analysis provides useful information to evaluate which parameters to focus on during the calibration of the model. This information will be the starting point to train a machine learning algorithm to find the most realistic *in silico* values to describe the inflammatory stage of bone healing.

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Title

FEM analysis for supporting the design of a bioreactor to burst *in-vitro* skeletal muscle differentiation of 3D bioprinted construct

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Abstract

Skeletal muscle diseases affect annually a total of about 107.5 million people in US with treatment costs exceeding $980.1 billion per year [1]. Drugs development for these diseases is difficult because the absence of suitable preclinical platforms. However, 3D engineered platforms are able to replicate the structural and functional complexity of tissues. In this context, we propose a protocol to create an engineered platform to replicate skeletal muscle complexity. The proposed platform is composed by: 1) PDMS rectilinear structures with a central channel in which fibrin-based hydrogel loaded with murine myoblasts (C2C12 cells) will be bioprinted [2], and 2) a bioreactor capable of mechanically stimulate structures and improve tissue maturation. PDMS Sylgard 184 (1:10) was used to fabricate structures. In order to investigate the mechanical properties of our PDMS and our stretchable structures, molds were designed with Autodesk Inventor® and 3D printed. PDMS was cast inside the mold and left to crosslink for about 1 hour at 60°C. PDMS tensile tests were performed in accordance with the standard ASTM D412. From the curves fitting, we obtained the hyperelastic constitutive coefficients of our material used for the subsequent simulations. To optimize the mechanical stimulus apply by the bioreactor, *in-silico* and experimental tensile tests of our structures were carried out. Finally, we worked on the bioreactor geometry; its prototypes were designed on Autodesk Inventor and then printed in PA12 using the HP MultiJet Fusion 580 Color. In order to reduce trial-and-error, the bioreactor geometry optimization was carried out using *in-silico* simulations. All the mechanical tests were performed using a MTS Insight 30 Instrument (10 kN load cell) while simulations were performed using Abaqus software. About tensile tests of stretchable constructs, force-displacement curves were obtained and the average experimental curve was compared with the computational one. The computational model has been validated as experimental and computational data are very close (figure 1A). Finally, to design the bioreactor cell chamber, we started by simulating a first configuration which showed the flexion of the mobile part during the stretching application (figure 1B). As this behavior was undesirable for our application, the configuration has been optimized until all the samples are stretched equally (figure 1C).
The choice of the optimal cell chamber geometry and the validation of the computational models, performed in this study, are the first step to obtain a suitable mechanical stimulation bioreactor with well-defined characteristics for skeletal muscle regeneration. The next step will be the bioprinting and the biological tests.

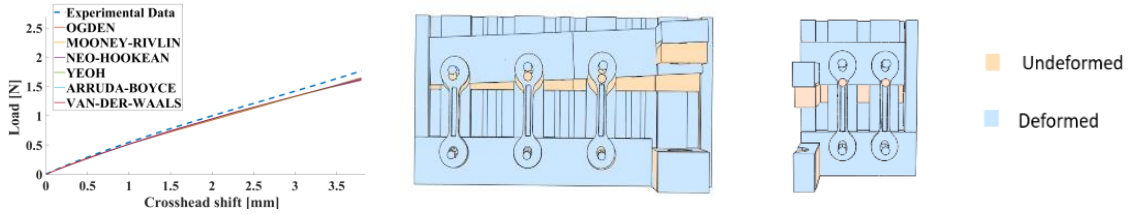

Fig. 1. A) Stress-strain curves: comparison between experimental (dot line) and computational data; Computational simulations for the bioreactor design: B) first and C) optimal configuration.

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Title

Artificial intelligence for quality control and parameter optimization in extrusion based bioprinting

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Abstract

Extrusion-based technologies represent the most wide-spread approach in Bioprinting, thanks to their simple use and hardware implementation, as well as wide variety of processable materials [1]. The implementation of quality control systems for EB bioprinting (EBB) is one of the main open challenges, as these are essential to: i) reduce the trial-and-error process and associated material consumption, ii) achieve standard results across different set-ups and laboratories to comply with relevant health standards, and iii) so accelerate the translation of Tissue Engineered products to more impactful clinical applications [2]. In this context, machine learning algorithms represent a key enabling technology that is currently being explored in literature for quality control in EBB, thanks to the ability to learn relevant features from a training dataset and generalize to new, unseen data [3-4].

In this context, we present a novel application of a deep learning model to EBB, namely a convolutional autoencoder coupled with a Support Vector Machine (SVM) classifier, to extract relevant quality measures from the printing process and classify the print result. In particular, a comprehensive dataset was built by recording videos of the process from a frontal view using a high-resolution webcam (Logitech C920). Pluronic F127 at 25% w/v was chosen as test material for all experiments. A template woodpile scaffold (10 mm sides and 5 mm height) was printed by varying multiple printing parameters (i.e., layer height, flow, infill percentage, printing speed) and using different EBB set-ups (i.e., piston-driven and pneumatic extrusion). The prints were classified after printing in three categories based on the shape of the final scaffold: “ok prints”, “under-extrusion” (i.e., not enough material is being extruded) and “over-extrusion” (i.e., an excess of material is being extruded).

Frames were extracted from each video and pre-processed to reduce the computational cost of the deep learning model. The data was then used to train the model and validate it using videos containing different types of errors (i.e., under- or over-extrusion). Results highlight that: i) the model can effectively classify the prints with high accuracy and F1 score (above 95%), and ii) the extracted quality measure is proportional to the error magnitude. Overall, these results show that the proposed method can be effectively applied as a quality control solution for the EBB process.

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Title

A computational framework for cells extrusion in bioprinting

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Abstract

In extrusion bioprinting the cell viability of the scaffold is highly influenced by several process variables, such as the dispensing pressure, the bio-ink properties, and the nozzle dimensions [1]. The introduction of the in-silico (computational) models would allow to reduce the experimental optimization costs and to increase the innovation of the bioprinting process.

So far, the theoretical and numerical models used are not specific enough to give a quantitative assessment of the main cell damage causes such as the shear stress and exposure time [2]. The aim of this work is to present a computational model for the non-Newtonian fluid extrusion which considers the presence of the cells and the interaction between the two phases.

Owing to the complex fluid-structure interaction (FSI) between the hydrogel flowing in the nozzle and the cells, as well as among the cells themselves, we have realized a multi-physics solver based on the immersed boundary technique [3].

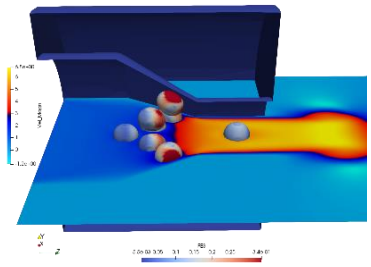

Figure 1: Velocity field along a symmetry plane and shear stress field in the nozzle at $t^* = 3$.

As a first study, a convergent-shaped nozzle with multiple immersed cells has been considered. In Fig.1 the velocity magnitude field of a nozzle symmetry plane and the shear-stress acting on the cell surface are reported. It is observed that the cells locally modify the velocity field of the fluid, and simultaneously the shear-stress and the deformation of cells are highly influenced by the presence of the other cells. This in-silico model opens then for a systematic optimization of the hydrogels material properties and of the nozzle geometries, in order to achieve a balance between the biological requests of high cell density and viability and the engineering constraint of bio-inks printability.

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MS16 - Kernel methods for computational sciences and simulation

Proposers

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Abstract

Kernel methods are powerful and flexible techniques that are used in a variety of algorithms in numerical analysis, computational physics, machine learning and stochastic processing. As other machine learning methods, they can process unstructured high dimensional data, and this makes them an attractive option to model complex simulations of physical problems. Moreover, they are grounded into a solid theory that can be often used to derive guarantees of accuracy and certification of the models. This MS aims at bringing together young researchers developing and applying kernel methods to different data-driven simulations of complex problems, tackling challenging aspects such as uncertainty quantification, surrogate modeling, reduced modeling, and inverse problems.

Title

Moving Least Square Approximation using Variably Scaled Discontinuous Weight Functions.

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Abstract

The moving least square (MLS) is an approximation (of low order) method introduced by Shepard [4] and generalized to higher approximation order by Bos and Salkauskas [**?**, **?**]. The MLS method approximates a function given at irregularly spaced points by weighted least square approximations. The smoothness of the MLS approximant is decided by the smoothness of the weight functions (cf. [5]). Moreover, the weight function are considered to be smooth functions of some order, regardless of the smoothness of the underlying function to be approximated. However, in case that the underlying functions possess some discontinuities at some points, smooth approximants become highly oscillatory near the discontinuities.
In this talk we show how to choose the weight function(s) so that the approximant reflects the discontinuities in the data. For doing so, we consider piecewise weight functions,of some order $\ell + 1$ of smoothness, that are themselves discontinuous. We take the weight functions as *Variable Scaled Discontinuous Kernels*, recently introduced in [2, 3], that enable us to reconstruct jump discontinuities. We will see that, this choice of weight functions provide tailored approximant that is useful to avoid overshoots near the edges of the underlying functions. Both theoretical and numerical analysis is provided.

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Title

Kernels and parametric fitting for first hard X-ray imaging results by Solar Orbiter STIX

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Abstract

The Spectrometer/Telescope for Imaging X-rays (STIX) is one of 6 remote sensing instruments on-board Solar Orbiter. It provides hard X-ray imaging spectroscopy of solar flares by sampling the Fourier transform of the incoming flux. With the first observations, called visibilities, we test and compare two imaging methods: the first one is an enhanced interpolation/extrapolation algorithm [3] based on the so-called Variably Scaled Kernels (VSKs) [1], while the second one is a parametric imaging approach based on forward fitting schemes [2].

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Title

Comparing Multi-Fidelity Radial Basis Function and Multi-Index Stochastic Collocation surrogates for ship resistance uncertainty quantification

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Abstract

In this talk we address the forward Uncertainty Quantification (UQ) analysis of the resistance to advancement of a ferry sailing in calm water and subject to two uncertain operational parameters, namely ship speed and payload. We present a comparison of two multi-fidelity methods to perform such analysis: Stochastic Radial Basis Functions (SRBF) and Multi-Index Stochastic Collocation (MISC). Specifically, we assess the quality of the surrogates provided by the two methods for the mapping between the parameter space and the resistance to advancement. We also discuss the estimation of expected value and probability density function of the resistance to advancement.
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. 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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Title

Probabilistic sampling for high dimensional kernel based approximation.

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Abstract

Kernel based algorithms can be formulated in Reproducing Kernel Hilbert Spaces, where functional analytical results can be used to provide guarantees on their performances.
For data-based algorithms, the problem of sampling is of utmost importance. The P-greedy algorithm [3, 4] allows one to obtain in this setting a quasi-optimal sampling of the space, that can be used in its own or as a discretization to reduce infinite dimensional problem to finite ones.
In this talk, using the result [1] from the Reduced Basis literature, we prove that the optimization step required by this algorithm may be reduced to a finite search over a sequence of randomly drawn points, thus significantly accelerating its computation especially in high dimension, while maintaining essentially the same error guarantees as the abstract algorithm, even if only in high probability.
We furthermore discuss connections to the notion of coresets for the computation of kernel maximum mean discrepancy (MMD, see e.g. [2]).

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Title

Registration-based model reduction of parameterized advection-dominated PDEs.

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Abstract

We present a nonlinear registration-based model reduction procedure for rapid and reliable solution of parameterized two-dimensional steady conservation laws. This class of problems is challenging for model reduction techniques due to the presence of nonlinear terms in the equations and also due to the presence of parameter-dependent sharp gradient regions that cannot be adequately represented through linear approximation spaces. Our approach builds on the following ingredients: (i) a general (i.e., independent of the underlying equation) registration procedure [1, 2] for the computation of a parametric mapping that tracks moving features of the solution field; (ii) an hyper-reduced least-squares Petrov-Galerkin reduced-order model for the rapid and reliable estimation of the solution field; (iii) a greedy procedure driven by a residual-based error indicator for efficient exploration of the parameter domain; and (iv) an adaptive mesh refinement technique for the definition of an accurate discretization for all parameter values. We present results for a representative nonlinear problem in steady aerodynamics to demonstrate the effectiveness and the mathematical soundness of our proposal.

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MS17 - Isogeometric methods

Proposers

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Abstract

Isogeometric Analysis (IGA) is a higher-order numerical method originally introduced by T.J.R. Hughes and coworkers in 2005 to bridge the gap between geometrical representation and numerical simulations. In addition to this, thanks to the high-regularity properties of its basis functions, IGA has shown a better accuracy per degree-of-freedom, an enhanced robustness with respect to standard finite elements, and a significant adaptability to various discretization schemes. These improvements in the analysis allow for an efficient solution of complex physical problems - ranging from solids and structures to fluids, as well as to different kinds of coupled problems - paving the way for high fidelity simulations. The purpose of this symposium is to gather experts in Computational Mechanics with interests in IGA and to discuss novel numerical approaches related to this numerical method with applications to various scientific disciplines, relevant theoretical results, and future developments in the field.

Title

Stability of space–time isogeometric methods for wave propagation problems.

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Abstract

The space–time discretization of evolution equations is a fairly recent tool that offers approximate solutions that are available at all times in the interval of interest, in contrast to semi-discretization and time-stepping techniques. Furthermore, space-time adaptivity and space-time parallelisation are available techiniques when using space-time discretizations and high-order approximation both in space and time is simple to obtain.
A variational formulation of the wave equation with integration by parts in both space and time is considered in [2]. A CFL condition $h_t \leq Ch_x$ is required for the stability of conforming tensor-product space–time discretizations with piecewise-linear polynomials. In [1] the stability of the conforming piecewise-linear FEM is addressed by first stabilizing the same discretization applied to an Helmholtz ODE initial value problem that is closely related to the wave equation. Motivated by the excellent numerical properties of the isogeometric (IgA) method, we investigate the first steps towards an unconditionally stable space–time IgA discretization for the scalar second-order wave equation by extending the techniques of [1] to high-order space–time IgA discretizations.

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Title

An improved isogeometric collocation formulation for spatial multi-patch shear-deformable beams with arbitrary initial curvature

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Abstract

This contribution presents a robust multi-patch formulation based on the Isogeometric Collocation (IGA-C) method for the solution of linear, spatial Timoshenko beam structures with arbitrary initial curvature and complex geometry. IGA-C methods have already been employed for the simulation of three-dimensional shear-deformable curved beams making use of the classical Serret-Frenet (SF) local frame for the representation of the curved geometry [1],[2]. However, this choice for the local frame prevents the generalization of the formulation since it is not suitable for geometries with zero-curvature points. To remove this limitation, the proposed approach is based on the combination of a rotation-minimizing frame (Bishop frame) with the exponential map for SO(3) (Rodrigues formula) to compute the beam curvature and its derivative. This choice not only permits bypassing the known issues related to the SF frame, but also does not require the Darboux vector and its derivative. Moreover, it is remarked that the adopted Bishop frame is immune to instabilities related to possible ill-defined torsion since it is set through an approximation technique (rotation method) as proposed in [3]. In contrast to existing isogeometric and standard finite element formulations, which are mostly based on the local SF frame, here the formulation is consistently derived by linearizing the nonlinear governing equations in the material setting. This choice permits to extend the method to the geometrically nonlinear case and to enforce the multi-patch constraints in the global reference, overcoming the known problems in formulating the multi-patch problem starting from local formulations. A primal formulation is here presented in which geometry and unknown fields (displacements and rotations) are discretized with B-spline basis functions. Numerical tests are performed on complex spatial curved beams, including a demanding biomechanical problem consisting of coronary stents, proving the accuracy and the robustness of the formulation.

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Title

Neuromechanical features of jellyfish propulsion: a mixed isogeometric/finite-difference model

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Abstract

The detailed replication of the neuro-mechanical processes contributing to locomotion can enhance the comprehension of multiple aspects of jellyfish biology and their environmental interactions. Specifically, understanding the impact of neurological events on behavioural aspects can help limiting the jellyfish outbreaks induced by seawater heating. This represents a major concern when considering the correlated increase in frequency and severity of events affecting marine fishery and aquaculture sectors [2]. In second instance, the study of the hierarchical architecture of a similar organism can inspire the development of soft actuators and biological pumps, with the aim of achieving the unrivalled scalability and versatility typical of biological tissues [1]. This work aims at clarifying the interaction between the temporal dynamics of the motor nerve net and the fluid-structure response of an oblate schypomedusa by means of a dedicated multiphysics computational model.

A sensory input triggers the electrophysiological stimulation of the endothelial tissue. This entails the solution of the monodomain problem coupled with a Hodgkin-Huxley type neuron model. The electrical activity drives the active contraction of the subumbrellar muscles, which in turn is described by the active strain approach. This is based on the multiplicative decomposition of the deformation gradient into an active and a passive part. The former provides the local coronal- and radial stretching of the muscle fibers, whereas the latter models the elastic response of the mesoglea. Both muscle activation parameters, and material properties have been tuned to match experimental observations from in-vivo experiments. In view of a conservative immersed boundary method [3], the body displacement produces the vortices at the bell margins responsible for the characteristic rowing propulsion. Such computational framework yields the possibility of a quantitative understanding of the correlation between the space-time patterns of neuronal stimulation and propulsive performance.

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Title

Topology-preservation, residual-based error estimation and adaptivity for scan-based immersed isogeometric analysis

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Abstract

Scan-based simulations contain innate topologically and geometrically complex three-dimensional domains, represented by large data sets in formats which are not directly suitable for analysis. In recent years, immersed finite element methods [1, 2] have been demonstrated to be suitable for scan-based geometries. Immersed techniques have been successfully combined with Isogeometric Analysis (IGA) [3] – a spline-based higher-order finite element framework – enabling its application to complex three-dimensional problems.

To exploit the advantageous properties of IGA in a scan-based setting, it is important to extract a smooth geometry. This can be established by convoluting the voxel data using B-splines [4]. A negative side-effect of this convolution technique is, however, that it can induce topological changes in the process of smoothing when features with a size similar to that of the voxels are encountered. An additional challenge in the context of immersed IGA is the construction of optimal approximations using locally refined splines. For scan-based volumetric domains, hierarchical splines are particularly suitable, as they optimally leverage the advantages offered by the availability of a geometrically simple background mesh. Although truncated hierarchical B-splines have been successfully applied in the context of IGA, their application in the immersed setting is largely unexplored.

In this contribution, we present a topology-preserving segmentation procedure using truncated hierarchical (TH)B-splines. Additionally, we propose a computational strategy for the application of residual-based error estimation and adaptivity for stabilized immersed IGA using THB-splines. We will study the proposed techniques using a range of test cases and scan data.

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Title

Isogeometric collocation method for cardiac muscle simulations.

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Abstract

Numerical simulations in cardiac precision medicine [1] are promising tools for therapeutic intervention planning but, as they are computationally demanding, the applicability is limited.
Isogeometric analysis has already been proven as an effective technique for cardiac thin-film modeling [2] whereas further improvements in the spatial discretization of 3D topologies can still be addressed. To this end, we propose a new isogemetric collocation approach for electrophysiological analysis that can be extended to coupled electromechanical simulations, as shown in preliminary results.
Through numerical examples, we demonstrate that the strong formulation (i) unifies the various spatial discretization strategies employed for the ionic current term [3], (ii) easily models tissue composed by different cell types, and (iii), in staggered solution schemes, enables efficient schemes for the mechanical sub-problem coarsening.

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Title

Application of optimal spline spaces for the removal of spurious outliers in isogeometric discretizations

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Abstract

The isogeometric approach for eigenvalue problems has been widely investigated in the literature and maximally smooth spline spaces on uniform grids are an excellent choice for addressing eigenvalue problems. Yet, they still present a flaw: a very small portion of the eigenvalues are poorly approximated and the corresponding computed values are much larger than the exact ones. These spurious values are usually referred to as outliers.
Outlier-free discretizations are appealing, not only for their superior description of the spectrum of the continuous operator, but also for their beneficial effects in various contexts, such as an efficient selection of time-steps in (explicit) dynamics. For a fixed degree, the challenge is to remove outliers without loss of accuracy in the approximation of all eigenfunctions.
In this talk we discuss isogeometric Galerkin discretizations of eigenvalue problems related to the Laplace operator subject to any standard type of homogeneous boundary conditions using the optimal spline subspaces of [1]. For a fixed number of degrees of freedom, all the eigenfunctions and the corresponding eigenvalues are well approximated, without loss of accuracy in the whole spectrum when compared to the full spline space [2, 3]. Moreover, there are no spurious values in the approximated spectrum. In other words, the considered subspaces provide accurate outlier-free discretizations.

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Title

Hierarchical matrices techniques for Helmholtz problem in IgABEM setting

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Abstract

Non-sparsity of system matrices obtained by Boundary Element Methods is a well-known issue, which requires approximation techniques to reduce storage and computational complexity as the dimension N of the system increases [1]. With the Isogeometric Analysis (IgA-BEM) setting, the sizes of the matrix are reduced, yet they are still dense and need to be handled with the aforementioned techniques. In this talk, hierarchical matrices theory [2] is considered to achieve simpler linear systems and the first results are presented when this approach is applied to solve numerically the Helmholtz problem on a spherical domain, which admits a smooth conformal multi-patch representation of the boundary surface. Since the symmetry of the domain allows to easily evaluate the indices partition used to build the hierarchical blocks in the matrix, the overall system solving process is improved in terms of computational efficiency, whereas the error approximation is not significantly affected. Numerical examples are given to compare the method effectiveness at different refinements levels.

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Title

Upwinding IgA.

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Abstract

Isogeometric Analysis (IgA) is introduced in the seminal paper [1] as an evolution of the classical finite element methods; in fact IgA uses spline functions, or their generalizations, both to represent the computational domain and to approximate the solution of the partial differential equation that models the problem. In this way the interoperability between computer aided design and numerical simulations are simplified and IgA benefits from the approximation properties of splines.
In space-time finite element methods an extra dimension for the time is assigned to standard finite elements and in [2] the authors focus on the heat equation and on its space-time Galerkin isogeometric discretization; in particular, they deal with smooth approximation in both space and time.
In space-time Galerkin isogeometric discretization of heat equation a problem arises: numerical spurious oscillations appear in presence of time-dependent concentrated source term.
In IgA framework we start from advection equation in the presence of layers and to improve the stability we propose a *novel upwind formulation for splines*, based on a new non-consistent term added to the plain Galerkin formulation. This term triangulates time derivative matrix, preserving the causality principle. To refine the accuracy of this non consistent formulation we add a non-linear term to obtain a *novel upwind formulation with optimal order of convergence* in order to fully activate the upwind stabilization only in the neighborhood of layers, guaranteeing the optimal order of convergence where the solution is smooth.
We apply the novel upwind formulation with optimal order of convergence also to the advection–diffusion equation and finally we consider heat equation with the novel space–time upwind formulation with optimal order of convergence, in presence of time-dependent concentrated source term.

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Title

Isogeometric multi-patch C^1-mortar coupling for the bilaplace equation

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Abstract

Mortar method, introduced by Bernardi, Maday and Patera in [1] in the context of finite element discretizations, is a domain decomposition technique in which weak regularity constraints are imposed along interfaces of the decomposition. In [2], Brivadis et al. applied mortar method to the isogeometric framework for solving second order elliptic boundary problem on multi-patch domains. In this case the mortar formulation allows to attain (weak) global C^0-continuity.
The aim of our work is to extend the isogeometric mortar method to fourth order elliptic problems. In particular we are interested in the discretization of the bilaplace equation on C^0-conforming multi-patch domains and we exploit the mortar technique to weakly enforce C^1-continuity across interfaces. In order to obtain discrete inf-sup stability, a particular choice for the Lagrange multiplier space is needed. Actually, we use as multipliers splines of degree reduced by two, w.r.t. the primal splines space, and with merged elements in the neighbourhood of the corners. In this framework, we are able to prove optimal a priori error estimate in a patch-wise H^2 broken norm.
Finally, we perform several numerical tests that perfectly reflect theoretical results.

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MS18 - Applied mathematics and computational mechanics

Proposers

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Abstract

Computational methods have by now become ubiquitous in every field of science and technology. Recent development in hardware (GPU, parallel architecture) have spurred the introduction of new algorithms, and the rise of machine learning / artificial intelligence have offered new opportunities and a shift in the computing paradigm. In this session we welcome both methodological talks, focused on the development and improvement of existing techniques, as well as talks focusing on applications of computational sciences in engineering and applied sciences.

Title

Modelling for bread preparation to avoid energy waste

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Abstract

A finite-element computational model for bread leavening and cooking will be presented. The partial differential equations that describe heat exchange and the presence of moisture, yeast and carbon dioxide are coupled with the quasi-static evolution of the growing elastic dough. The results of the detailed simulations are used to obtain a simplified model for energy consumption.

Title

An analytical framework to compute elastic waves propagation along finite-size metasurfaces

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Abstract

The propagation of elastic waves along the surface of structured media equipped with mechanical resonators, known as elastic metasurfaces, has attracted considerable attention in recent years. This interest arises from the coupling between the propagating surface waves and the localized resonators' motion, which yields peculiar wave phenomena such as surface-to-bulk wave conversion [1, 2], rainbow trapping [3], localization and focusing [4, 5]. These unique dynamic responses can find applications in multiple technologies, such as energy harvesting and vibration mitigation devices.

Currently, analytical tools for modeling elastic metasurfaces are mainly focused on the computation of dispersive properties of an unbounded metasurface, assuming periodicity along with the resonator array and using homogenization techniques. Conversely, the dynamics of a finite-size (eventually disordered) metasurface are investigated via numerical techniques (e.g. FEM) since no analytical formulation is currently available.

Therefore, in this talk, we will present an analytical framework, based on the multiple scattering technique [4, 5], to model the wave field of finite-size elastic metasurfaces. To this end, we will show how to use Green's functions of Lamb's problem to model the incident wave field and the scattered wave fields generated by the motion of a cluster of mechanical resonators atop a half-space surface. The unknown amplitudes of the scattered wave fields are computed by imposing proper boundary conditions at the interface between resonators and the half-space surface. The total wave field in the half-space is thus obtained as the summation of the incident and resonators' scattered wavefields. Using the proposed approach, we study the interplay between surface waves and resonators in both 2D and 3D contexts, showing the capability of finite-size metasurfaces for surface wave conversion, trapping, and localization.

We expect our tool and findings can serve as guidelines for future experiments on the design of devices for surface wave control with applications in vibration mitigation and energy harvesting technologies.

References

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Title

Numerical investigation of the stability of age-structured models with nonlocal diffusion of Dirichlet type.

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Abstract

Nonlocal diffusion problems can be formulated as linear integro(-partial) differential equations in which the diffusion term is represented by a convolution operator. On the one hand, compared with Laplace diffusion, nonlocal diffusion is more suitable for many biological and physical phenomena [3]. On the other hand, the analysis of models with nonlocal diffusion is more challenging since the associated semigroups are not eventually compact [2]. Neverthless, for age-structured models with nonlocal diffusion, *i.e.*, population models depending on time, age and spatial position, it can be shown that the asymptotic behaviour of the semigroup is determined by the spectral abscissa of its infinitesimal generator. The latter typically needs to be approximated numerically due to the infinite dimension of the state space. In this talk we propose a couple of relevant numerical approaches based on Legendre spectral and pseudospectrals method with several supporting numerical tests [1].

References

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