NAVE - Numerical Analysis in Veneto

Last update: May 3, 2024

List of contributions

Schedule

9:00 - 9:30	**Registration and Opening remarks**	
09:30 - 10:00	A. Franceschini	A reverse constrained preconditioner for the Lagrange multipliers method in contact mechanics
10:00 - 10:30	E. Gaburro	Structure preserving high order Lagrangian schemes for the solution of hyperbolic PDEs: from fluiddynamics to astrophysics
10:30 - 11:00	F. Marchetti	A machine learning perspective for optimized kernel-based approximation
11:00 - 11:30	**Coffee break**	
11:30 - 12:00	C. Millevoi	A reduced-split PINN approach for time-dependent parameter estimation in compartmental epidemiological models
12:00 - 12:30	F. Piazzon	Computation and constrained optimization of Wasserstein-1 distance by finite elements method
12:30 - 13:00	A. Larese	Numerical models for multiphysics simulations of the impact of natural hazards on structures
13:00 - 14:30	**Lunch break**	
14:30 - 15:00	G. Albi	Instantaneous control strategies for magnetic confinement of plasma dynamics
15:00 - 15:30	A. Alla	An online algorithm to identify and control unknown PDEs
15:30 - 16:00	G. Santin	Kernel methods for surrogate modeling of complex simulations
16:00 - 16:30	F. Cassini	Directional split exponential integrators with applications to ADR equations

Structure preserving high order Lagrangian schemes for the solution of hyperbolic PDEs: from fluiddynamics to astrophysics

Elena Gaburro
University of Verona

Abstract: In this talk I will give an overview of my research activities which concerns the development of novel high order accurate nonlinear numerical methods for the solution of hyperbolic equations, with a wide range of applicability that includes fluiddynamics, plasma flows and astrophysics. After a general introduction to explain the motivations and the difficulties of this field, I will concentrate on two topics which are central in my actual work. The first is the development of a particularly efficient and robust Arbitrary-Lagrangian-Eulerian framework on moving Voronoi meshes. The second involves the design of structure preserving techniques to guarantee the stability of the simulations of very complex models as the first order reformulation of the Euler-Einstein equations of general relativity.

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

A machine learning perspective for optimized kernel-based approximation

Francesco Marchetti
University of Padova

Abstract: Meshfree kernel methods have proved to be an effective tool in many fields of research. Their effectiveness usually depends on a shape hyperparameter, which is often tuned via cross-validation schemes. In this talk, we present a learning strategy that extends the classical single-parameter framework, and returns a kernel that is optimized not only in the Euclidean directions, but that further incorporates, e.g., kernel rotations. Then, by combining this approach with the usage of greedy strategies, we obtain an optimized basis that adapts to the data. Beyond a rigorous analysis on the convergence of the so-constructed two-layered kernel orthogonal greedy algorithm (2L)-KOGA, the benefits of the presented approach are highlighted on both synthesized and real benchmark datasets.

A reduced-split PINN approach for time-dependent parameter estimation in compartmental epidemiological models

Caterina Millevoi
University of Padova

Abstract: The study addresses the challenges of using compartmental models for analyzing disease outbreaks, particularly when model parameters, such as the transmission rate, change rapidly due to various factors. We propose employing Physics-Informed Neural Networks (PINNs), known for handling uncertain data and governing equations simultaneously, to track temporal changes in model parameters. PINNs bridge the gap between data-driven machine learning models and traditional compartmental models, enhancing accuracy by incorporating the residual of governing equations as a training constraint. A reduced-split approach is presented and applied to estimate variations in state variables and parameters in various settings of the SIR model - including the first months of the COVID-19 Italian pandemic - based on the SIR model equation and infectious data. The main idea is to split the training first on the epidemiological data, and then on the residual of the system equations. The method is systematically compared with the standard approach and outperforms it both in terms of accuracy and computational times. Results indicate that PINNs effectively capture changes in disease transmission, especially during high infection periods. The proposed approach proves robust and easy-to-implement in dealing with uncertain reported data, providing accurate estimates of the temporal changes in the state variables and parameters to monitor the initial spreading of a disease.

Computation and constrained optimization of Wasserstein-1 distance by finite elements method

Federico Piazzon
University of Padova

Abstract: The Kantorovich-Rubinstein-Wasserstein-1 distance (W_1, for short) is the metric induced on the space of probability measures by the solution of the optimal transport problem with euclidean cost. Wasserstein distances play an emerging role in many applications in fields such as, e.g., Mathematics, Statistics, Imaging, Economics, and Computer Science.

We study the problems of numerical approximation of the W_1 of two probability measures, and of the optimization of the W_1 distance of a given Borel measure among a weakly closed convex set of measures $\mathcal{C}$.

We present algorithms for the solution of such problems, and we prove their convergence. Also, some applications are proposed.

Numerical models for multiphysics simulations of the impact of natural hazards on structures

Antonia Larese
University of Padova

Abstract: In recent years, the frequency and intensity of large gravitational mass movements, including landslides, debris flows, and mudflows, have risen due to climate change and related factors. These phenomena transport vast amounts of rocks and granular materials that can damage structures and landscapes, creating significant risks that can lead to loss of life and property damage. The classical Finite Element Method (FEM) has limitations in dealing with materials undergoing large deformations as is required in this case. In recent decades, alternative solutions have been proposed to overcome this limitation, one of which involves the use of particle-based methods. Among these, the Material Point Method (MPM) blends the advantages of both mesh-based and mesh-free methods. MPM avoids the problems of mesh tangling while preserving the accuracy of Lagrangian FEM. It is well suited for nonlinear solid mechanics and fluid dynamics problems. The presentation will highlight recent MPM advancements, including granular flow and large-deformation material simulation in both compressible and incompressible regimes. Additionally, partitioned coupling strategies with other techniques like FEM or DEM will be discussed for complex multiphysics simulations.

Instantaneous control strategies for magnetic confinement of plasma dynamics

Giacomo Albi
University of Verona

Abstract: The principle behind magnetic fusion is to confine high temperature plasma inside a device in such a way that the nuclei of deuterium and tritium joining together can release energy. The high temperatures generated needs the plasma to be isolated from the wall of the device to avoid damages and the scope of external magnetic fields is to achieve this goal. In this paper, to face this challenge from a numerical perspective, we propose an instantaneous control mathematical approach to steer a plasma into a given spatial region. From the modeling point of view, we focus on the Vlasov equation in a bounded domain with self induced electric field and an external strong magnetic field. The main feature of the control strategy employed is that it provides a feedback on the equation of motion based on an instantaneous prediction of the discretized system permitting to directly embed the minimization of a given cost functional into the particle interactions of the corresponding Vlasov model. The numerical results demonstrate the validity of our control approach and the capability of an external magnetic field, even if in a simplified setting, to lead the plasma far from the boundaries.

A Reverse Constrained Preconditioner for the Lagrange Multipliers Method in Contact Mechanics

Andrea Franceschini
University of Padova

Abstract: Capturing the behavior of faults and fractures is critical to accurately simulate the geomechanical response of a complex subsurface system, such as an aquifer or a hydrocarbon reservoir. Several phenomena, such as micro-seismicity and fracture propagation, depend on the nature of these discontinuities. As a result, it is important to explicitly account for the complex behavior across these fractures and, from a modeling viewpoint, to simulate the influence of the fractures on the mechanical deformation. Dealing with frictional contact problems lies at the core of the challenge. This is one of the most challenging problems in computational mechanics, since it usually produces a stiff non-linear problem associated with a series of linear systems, that is hard to solve efficiently. We use Lagrange multipliers to enforce the constraint and we focus on two different discretization techniques, only one of which is intrinsically stable. To solve the saddle-point Jacobian matrices arising from the linearization, we propose a constraint preconditioner where the primal Schur complement is obtained by eliminating the Lagrange multipliers unknowns. Suitable augmentation is presented for the intrinsically stable case. Finally, an optimal multigrid method [2] is applied to efficiently solve the Schur complement. We provide numerical evidence of robustness and efficiency by solving large size problems from various applications.

Directional split exponential integrators with applications to ADR equations

Fabio Cassini
University of Verona

Abstract: Time marching schemes of exponential type received a lot of attention in the last years, thanks to the recent advances in efficiently computing actions of the exponential-like matrix functions needed by these integrators (known in the literature as φ-functions). In this presentation, we show how to compute those actions for matrices K that possess d-dimensional Kronecker sum structure, i.e., that are in the form $K = A_d \oplus A_{d-1} \oplus \cdots \oplus A_1$. The technique is based on a suitable directional splitting of the exponential-like matrix functions, which allows for an efficient tensor oriented evaluation through mu-mode products and Tucker operators. The implementation of such an approach is done by exploiting the high performance level 3 BLAS, which are available for basically any kind of modern computer architecture. The employment of the proposed technique allows for the effective numerical integration of many stiff problems from the applications using directional split exponential integrators. In particular, in this talk we present the results on two- and three-dimensional semidiscretized (systems of) Advection–Diffusion–Reaction equations, in comparison with state-of-the-art techniques.

An online algorithm to identify and control unknown Partial Differential Equations

Alessandro Alla
University of Venice

Abstract: We address the control of Partial Differential equations (PDEs) with unknown parameters. Our objective is to devise an efficient algorithm capable of both identifying and controlling the unknown system. We assume that the desired PDE is observable provided a control input and an initial condition. The method works as follows, given an estimated parameter configuration, we compute the corresponding control using the State-Dependent Riccati Equation (SDRE) approach. Subsequently, after computing the control, we observe the trajectory and estimate a new parameter configuration using Bayesian Linear Regression method. This process iterates until reaching the final time, incorporating a defined stopping criterion for updating the parameter configuration. We also focus on the computational cost of the algorithm, since we deal with high dimensional systems. To enhance the efficiency of the method, indeed, we employ model order reduction through the Proper Orthogonal Decomposition (POD) method. The considered problem's dimension is notably large, and POD provides impressive speedups. Further, a detailed description on the coupling between POD and SDRE is also provided. Finally, numerical examples will show the accurateness of our method across.

Kernel methods for surrogate modeling of complex simulations

Gabriele Santin
University of Venice

Abstract: Kernel methods are versatile tools for the approximation of functions from data, and they offer both flexibility and efficiency, and the possibility to derive precise error estimates. In this talk we will present some recent work on kernel greedy interpolation, which is an adaptive approximation technique where sample points are chosen to optimize some desired criterion. We present error estimates that show that these methods are optimal when approximating functions in certain Sobolev spaces, and may even achieve a dimension-independent error decay. Moreover, we will discuss some applications of these techniques for the construction of surrogate models of complex simulations, where in particular we will highlight the possibility to enforce energy and momentum conservation in the models.