Calcolo Scientifico e Modelli Matematici

Alla Ricerca Delle Cose Nascoste Attraverso le Cose Manifeste

6 – 8 Aprile 2022
Aula Convegni, CNR, Roma

Il comitato organizzatore:

Maurizio Falcone (Università di Roma La Sapienza)
Luciano Lopez (Università di Bari)
Carla Manni (Università di Roma "Tor Vergata")
Roberto Natalini (IAC-CNR, Roma)

Abstracts

High dimensional data integration using graphical models

Claudia Angelini (IAC-CNR, Napoli)

Data integration is one of the most challenging problems in high-dimensional statistics. This talk proposes the Gaussian Graphical Models as a framework for data integration. We assume to integrate several datasets sampled from multivariate Gaussian distributions with the same conditional independence structures but not the same precision matrix. First, we describe jewel 1.0 [1], a novel method that uses a node-wise penalized regression approach to estimate the common graph. In particular, jewel 1.0 uses a group Lasso penalty to simultaneously guarantee the resulting adjacency matrix's symmetry and the graphs' joint learning. We solve the minimization problem using the group descend algorithm and propose two procedures for estimating the regularization parameter. Second, we present the extension jewel 2.0 that can simultaneously infer common and case-specific graphs when we relax the assumptions to similar conditional independence structures between the datasets. Finally, we illustrate the performance of our methods through simulated and real data examples on gene regulatory networks.

Joint work with D. De Canditiis and A. Plaksienko.

[1] C. Angelini, D. De Canditiis, A. Plaksienko. Jewel: A Novel Method for Joint Estimation of Gaussian Graphical Models. *Mathematics*, 9:2105, 2021.

Numerical methods for piecewise Chebyshevian splines and applications

Carolina Beccari (Università di Bologna)

In approximation theory, the expression "spline space" refers to a space of functions defined piecewisely, with some prescribed regularity connection conditions between consecutive pieces. Whereas these "pieces" are usually assumed to be polynomials, the idea of considering more general functions has been investigated since the dawn of spline theory. In that direction, a crucial step consisted in replacing polynomial spaces by their most natural extensions, namely Extended Chebyshev (EC) spaces, which share with them the same bounds concerning the numbers of zeros. This large class of spaces offer more flexibility in approximating functions and datasets, for they inherently possess shape parameters. Classical examples of EC-spaces are all kernels of linear differential operators with constant coefficients on intervals of convenient lengths.

To take full advantage of these parameters, one can even consider splines with pieces taken from different EC-spaces, referred to as "piecewise Chebyshevian splines". This is the framework of the present talk. Of course the higher capabilities of this large class of splines come at a price. In this respect, we will tackle two prominent issues which stand on the way to practical applications. One is that not all piecewise Chebyshevian spline spaces have a B-spline basis and, even should this be the case, this basis may not be refinable. We shall thus discuss how to characterize the existence of refinable piecewise Chebyshevian B-spline bases through numerical procedures. As an additional issue, we shall discuss the practical problem of evaluating such piecewise Chebyshevian B-spline bases. We present a conceptually simple numerical method which ensures reasonable accuracy and compare it with existing ones. These results open the way to advantageously exploiting piecewise Chebyshevian splines in any application field where splines have been used so far. This will be illustrated considering both classical applications, such as interpolation and design, and some simple problems in isogeometric analysis.

Adaptive optimization methods using random models and examples from machine learning

Stefania Bellavia (Università di Firenze)

We discuss trust region and adaptive regularized methods using random models. The primary motivation for developing these methods is the need to solve optimization problems that arise in machine learning, which because of the enormous amounts of data involved in each computation of the function and gradient, usually require a stochastic optimization approach. The main issues that we address in this talk are the adaptive choice of step-size and of the the accuracy conditions that the models and function values have to satisfy. In particular we assume that our models satisfy some good quality conditions with some probability fixed, but can be arbitrarily bad otherwise. Both theoretical and computational results will be presented.

Forward-backward methods for convex and nonconvex optimization in imaging

Silvia Bonettini (Università di Modena e Reggio Emilia)

Several relevant problems in a variety of different fields, such as signal and image processing and machine learning, are formulated as optimization problems. The recent research leads such variational models to be more and more accurate and very challenging from the numerical and theoretical point of view. Indeed, the objective function to be minimized may include nonsmooth and nonconvex terms, which are difficult to handle by optimization methods. Thus, the research aims to develop new approaches which are required to have both reliable theoretical convergence properties and effective practical performances.

In this framework, forward-backward methods are a well established and valid numerical tool and they are largely employed to solve convex variational models. However, the theoretical analysis and the implementation of this kind of algorithms requires to be carefully restated when applied to optimization problems with no simple structure.

The aim of this talk is to present new convergence results about forward-backward methods, obtained under very general assumptions, and the corresponding applications to challenging imaging problems. Finally, one of the more interesting perspectives on this kind of methods will be illustrated, that is the possibility to use them in combination with machine/deep learning techniques in order to infer a reliable model for image reconstruction problems directly from the data.

Numerical computation of the basic reproduction number

Dimitri Breda (Università di Udine)

The twentieth century has witnessed the emergence of the basic reproduction number as a key player in assessing the growth of a population or the spread of a disease. Only in the nineties this quantity has been rigorously characterized as the spectral radius of a positive linear operator, promoting since then the use of increasingly realistic, yet more complicated, models. In this talk I would like to present some recent developments in the numerical approximation of this number, first illustrating a spectrally accurate discretization framework and then discussing its convergence. As an application I consider models of epidemics structured by individual traits as, e.g., age or immunity.

Neural Networks of ELM type for the numerical solution of PDEs with collocation

Francesco Calabrò (Università di Napoli Federico II)

In this talk, we present the construction of a collocation method with a Feedforward Neural Network (FNN) with a single hidden layer and sigmoidal transfer functions randomly generated, the so-called Extreme Learning Machines (ELM). Free parameters are only the external weights and in the proposed method these are fixed by imposing exactness on points via collocation. Because the exactness required involves a residual, these methods fall in the general framework of PINNs. In order to obtain accurate solutions, we underdeterminate the collocation equations. For linear PDEs, the weights are computed by a one-step least-square solution of the linear system. The least-square solution is capable of automatically selecting the important features, i.e. the functions in the space that are more influent for the solution. This leads to a one-shot automatic method and there is no need for adaptive procedures or tuning of the parameters as done when learning in other methods based on FNN.

We present results on elliptic problems both in the linear case and for the resolution and construction of bifurcation diagrams of nonlinear problems. For linear elliptic PDEs, in [1] we introduce the method and prove that ELMs can adapt "automatically" via Least Square and gain good accuracy also in steep gradient benchmark problems. In the case of nonlinear elliptic PDEs, in [2] we extend the method in order to deal with the nonlinearity and prove accuracy when computing tuning points of bifurcation diagrams. Burgers and Bratu's equations are taken as benchmark nonlinear problems.

[1] F. Calabrò, G. Fabiani, C. Siettos. Extreme learning machine collocation for the numerical solution of elliptic PDEs with sharp gradients. *Computer Methods in Applied Mechanics and Engineering*, 387:114188, 2021.

[2] G. Fabiani, F. Calabrò, L. Russo, L. Siettos. Numerical solution and bifurcation analysis of nonlinear partial differential equations with extreme learning machines. *J. Sci. Comput.* 89:44, 2021.

Vehicular and pedestrian traffic: optimization through digital twins

Emiliano Cristiani (IAC-CNR, Roma)

In this talk I present the results of two collaborations: the first one is with the company Autovie Venete, concessionaire of the highways in the north-east of Italy, with which we have created a digital twin of the road network to describe and predict the dynamics of cars and trucks. The second is with the Galleria Borghese museum in Rome, with which we have created a digital twin of the museum that simulates the paths followed by the visitors. The software was used to modify the ticketing strategy and visitor entrances, with the aim of maximizing the number of daily visitors under the numerous safety and historical-artistic constraints present in the museum.

AMG preconditioners for computational and data science at extreme scale

Pasqua D'Ambra (IAC-CNR, Napoli)

The challenge of exascale requires rethinking numerical algorithms and mathematical software for efficient exploitation of heterogeneous massively parallel supercomputers. I will present some activities aimed at developing highly scalable and robust sparse linear solvers for solving scientific and engineering applications with a huge number of degrees of freedom (dofs) [1, 2, 3, 4]. Main focus is on algorithmic advances and implementation aspects in the design of Algebraic MultiGrid (AMG) preconditioners based on aggregation, to be used in conjunction with Krylov-subspace projection methods, suitable to exploit high levels of parallelism of current petascale supercomputers. These activities are carried on within two ongoing European Projects: the Energy-oriented Center of Excellence (EoCoE-II) and the

EuroHPC TEXTAROSSA project, having the final aim to provide methods and tools for preparing scientific applications in facing and successfully grasping the near future exascale challenge. Beyond possible advances in base software technology to make available programming environments that tend to hide the details of the hardware, we still need to rethink and redesign numerical methods and applications, especially for irregular computations and memory-bound kernels, like sparse solvers. Algorithms that express a high level of data parallelism should be preferred to algorithms that induce data dependency even though, sometimes, the former may have worse convergence properties; extra computations are often well tolerated and balanced by a very efficient execution on multi/many-core architectures. Such is the case, for example, of some smoothers and coarsest solvers in AMG cycles or sub-optimal maximum weight matching algorithms employed in the setup of the AMG matrix hierarchy, which avoid intrinsically sequential computational kernels. Memory footprint, measured in terms of hierarchy complexity, is also a key issue in pursuing scalability in AMG preconditioners; balancing hierarchy complexity and convergence property of the final AMG is another main challenge in the current research on the topic. I will discuss the above issues while presenting a software framework for Parallel Sparse Computations (PSCToolkit [5]), which has recently been selected by EU Innovation Radar as Excellent Innovation and is under extension in the aformentioned projects. Results obtained with our algorithms and software, on some of the most powerful European supercomputers, for solving systems with tens of billions of dofs arising from scientific applications in the energy sector will be presented.

Joint work with a group of researchers affiliated at IAC-CNR in different forms.

[1] M. Bernaschi, P. D'Ambra, D. Pasquini. AMG based on compatible weighted matching on GPUs. *Parallel Computing*, 92, 2020.

[2] P. D'Ambra, F. Durastante, S. Filippone. AMG Preconditioners for Linear Solvers towards Extreme Scale. *SIAM Journal on Scientific Computing*, 43(5), 2021.

[3] D. Bertaccini, P. D'Ambra, F. Durastante, S. Filippone. Preconditioning Richards equations: spectral analysis and parallel solution at very large scale. Under revision.

[4] P. D'Ambra, F. Durastante, S. Filippone, L. Zikatanov. On the Quality of Matching-based Aggregates for Algebraic Coarsening of SPD Matrices in AMG. Under revision.

[5] P. D'Ambra, F. Durastante, S. Filippone. PSCToolkit Web page. Available at https://psctoolkit.github.io/

Controlling complex systems: challenges and opportunities

Mario Di Bernardo (Università di Napoli Federico II)

Network control systems are the subject of much ongoing research but what about very large-scale systems? From large flocks of minidrones or flying insects to cellular populations, finding a way to close the loop between the microscale, where agents live, and the macroscopic properties that typically need to be controlled is a crucial open challenge for network control. Controlling a system of interest requires being able to sense, compute and actuate. When complex systems are involved, addressing each of these ingredients requires finding new approaches. What and how many agents need to be controlled/sensed and at what scale is a question beyond the current state-of-the-art that requires a new holistic approach to modelling/analysing and controlling large scale network systems. In this talk I will give snapshots into some recent work from my group aimed at addressing the problem of combining concepts from network science, control theory and other disciplines for the solution of this class of problems. I will use some case studies from applications to motivate and illustrate the theoretical derivations giving an overview of the key challenges in the field and opportunities for further research.

Modelling the transmission of SARS-CoV-2 in the early phases of the COVID-19 pandemic

Ilaria Dorigatti (Imperial College London)

Italy was the first European country to be hit by COVID-19. On 21 February 2020, the first COVID-19 death was detected in the Italian municipality of Vo', a small town near Padua (Italy). Since then, in collaboration with the University of Padua, we implemented two sequential molecular swab surveys in the Vo' population (in February and March 2020) which were then followed by 3 serological surveys (in May and November 2020, and more recently in June 2021), to evaluate the population exposure to SARS-CoV-2, the extent of antibody waning and the effect of vaccination.

In this talk I will present the statistical analyses and mathematical models developed during the early phases of the pandemic to better understand the epidemiology of SARS-CoV-2, quantify the effectiveness of the interventions implemented at the time, and evaluate the role of testing going forward. I will discuss the importance of linking data from multiple sources, adopting an evidence-based approach, and how mathematical models are a useful tool to inform public health policy decisions against SARS-Cov-2 and other infectious diseases worldwide.

Smooth path planning for autonomous vehicles: perspectives from the theory of Pythagorean-hodograph curves

Carlotta Giannelli (Università di Firenze)

Pythagorean-hodograph (PH) curves provide distinctive advantages in planning curvilinear paths for autonomous vehicles of different kinds. The increasing exploitation of PH curves in this application setting often suggests and motivates new research directions for the development of basic theory and application algorithms. The talk provides an introduction to the key properties of PH curves which can be suitably exploited to design effective control strategies, and presents novel algorithms and exact constructions of particular interest in planning smooth PH spline paths.

Fractional calculus: from physics to mathematical models (and numerical simulations)

Roberto Garrappa (Università di Bari)

Fractional calculus (namely, the use of integrals and derivatives of non-integer order) is employed nowadays in a variety of models, mainly to introduce some memory effects and non-local dynamics. Although in several cases applications of fractional-order operators appear rather artificial, there are some situations in which it is the nature of the problem which suggests the use of the fractional calculus to better model physical phenomena. Starting from an application in physics of matter, namely the description of polarization processes in dielectrics showing anomalous behaviors, we will illustrate the way in which some models incorporating fractional-order derivatives are derived from physical properties and observed data; moreover, we will also discuss the way by which standard operators of fractional calculus can be further generalized to provide more accurate models. The main computational difficulties encountered in the simulation of these models will be also illustrated together with some tools for their efficient treatment.

Geometries on the cone of positive definite matrices and their relation to the power means

Bruno Iannazzo (Università di Perugia)

Endowing a space with a geometry may allow one to identify the hidden structure of an object, such as a dataset, belonging to that space. On the other hand, geometrical quantities such as geodesics and distances can be used to provide solutions to problems of averaging and clustering, respectively. We

introduce a new family of non-Euclidean geometries on the cone of positive definite matrices obtained from the Hessian of the power potential and provide explicit expressions for the related geodesics and distances. This generalizes in some sense the geometry obtained from the Hessian of the logarithmic potential, whose geodesic has been understood as the weighted geometric mean of two matrices. Indeed, the new geometries provide a definition of matrix power mean alternative to the existing ones. We discuss some properties of the proposed power mean and relate it with the geometric mean. Finally, we discuss how these geometries can be used to accelerate the convergence of optimization algorithms for the matrix geometric mean of several variables.

Stable approximation of Helmholtz solutions by evanescent plane waves

Andrea Moiola (Università di Pavia)

Solutions of the Helmholtz equation are known to be well approximated by superpositions of propagative plane waves. This observation is the foundation of successful Trefftz methods. However, when too many plane waves are used, the computation of the expansion is known to be numerically unstable. This effect is due to the presence of exponentially large coefficients in the expansion and can severely limit the efficiency of the approach.

We show that the Helmholtz solutions on a disk can be exactly represented by a continuous superposition of evanescent plane waves, generalizing the classical Herglotz representation. The density in this representation is uniformly bounded in a weighted Lebesgue norm, hence overcoming the instability observed with propagative plane waves. This allows the construction of suitable finite-dimensional sets of evanescent plane waves using sampling strategies in a parametric domain. Provided one uses sufficient oversampling and regularization, the resulting approximations are shown to be both controllably accurate and numerically stable, as supported by numerical evidence.

Joint work with E. Parolin (Pavia) and D. Huybrechs (KU Leuven).

Towards the computational design of smart nanocarriers

Annalisa Quaini (University of Houston)

Membrane fusion is a potentially efficient strategy for the delivery of macromolecular therapeutics into the cell cytoplasm. However, existing nanocarriers formulated to induce membrane fusion suffer from a key limitation: the high concentrations of fusogenic lipids needed to cross cellular membrane barriers lead to toxicity in vivo. To overcome this limitation, we are developing in silico models that will explore the use of membrane phase separation to achieve efficient membrane fusion with minimal concentrations of fusion-inducing lipids and therefore reduced toxicity. The models we consider are formulated in terms of partial differential equations posed on evolving surfaces. For the numerical solution, we use a fully Eulerian hybrid (finite difference in time and trace finite element in space) discretization method. The method avoids any triangulation of the surface and uses a surface-independent background mesh to discretize the problem. Thus, our method is capable of handling problems posed on implicitly defined surfaces and surfaces undergoing strong deformations and topological transitions.

Preserving exactly equilibrium solutions to obtain accurate off-equilibrium simulations

Semplice Matteo (Università dell'Insubria)

Systems of evolutionary balance laws possess a very important class of solutions that is composed by steady state solutions and many natural phenomena of interest are in fact small perturbations of these

equilibria. Tsunamis and Rayleigh-Taylor instabilities are well-known examples based respectively on the Saint-Venant and on the Euler equations.

In a numerical model, if the discretization of the spatial differential operator and of the source term of the balance law are chosen independently of each other, it may happen that the steady state solutions of the continous problem is not an exact solution of the discretized problem. In practice, initializing a computation with the discretization of an exact steady state, one would observe the emergence of spurious waves with size comparable to the discretization parameter. Thus, in a simulation of a small perturbation of a steady state, in order to distinguish if the waves observed represent real phenomena or are simply numerical artifacts, one should employ fine discretizations of a size which is often unaffordable and in any case disproportionate with the task at hand.

The solution is to construct so-called well-balanced schemes, for which, thanks to a careful coupled choice of the discretization of all terms, continous steady states are also steady states for the discrete problem. This schemes allow to compute accurate solutions for these small perturbation problems using a much coarser grid and thus with much less computational effort. We will present examples of such schemes, in a finite volume setting, of arbitary high order and illustrate them for the cases of the standard shallow water equations, the coupling of Euler gasdynamics and gravity, and finally a model of shallow water and rain presented at the 2018 edition of this same conference.

Joint work with G. Puppo, G. Visconti, C. Klingenberg, M. Castro-Diaz, C. Escalante and O. Lakkis.

Selection of the regularization parameter comes for free with sequential Monte Carlo samplers

Alberto Sorrentino (Università di Genova)

Sequential Monte Carlo samplers are powerful computational algorithms for sampling/approximating probability distributions of interest. They find natural applications in both non-linear inverse problems, and in linear inverse problems where sparse solutions are sought. In their classical formulation, SMC samplers are a class of iterative algorithms that sample from a tempering sequence of auxiliary distributions bridging between a simple distribution, often the prior, and the target distribution, i.e. the posterior distribution. Samples from intermediate auxiliary distributions are typically discarded, because they are only instrumental to reaching the target density. However, if the tempering sequence of distributions is defined wisely, the intermediate distributions become themselves alternative posterior distributions corresponding to a different value of a hyperparameter, e.g. the noise standard deviation/regularization parameter. This way, the hyperparameter is estimated for free, i.e at no additional computational cost, exploiting samples from the intermediate distributions.

A multi-fidelity method for uncertainty quantification in engineering problems

Lorenzo Tamellini (IMATI-CNR, Pavia)

Computer simulations, which are nowadays a fundamental tool in every field of science and engineering, need to be fed with parameters such as physical coefficients, initial states, geometries, etc. This information is however often plagued by uncertainty: values might be e.g. known only up to measurement errors, or be intrinsically random quantities (such as winds or rainfalls). Uncertainty Quantification (UQ) is the research field devoted to dealing efficiently with uncertainty in computations. UQ techniques typically require running simulations for several (carefully chosen) values of the input parameters, and computing statistics of the outputs of the simulations (mean, variance, ...), to provide decision-makers with quantitative information about the reliability of the predictions. It is easy to see how these techniques can quickly become very computationally expensive.

In recent years, multi-fidelity approaches have been devised to lower the computational burden: these techniques explore the bulk of the variability of the solution of the equation at hand by means of low-fidelity/low-cost simulations, and then correct the results by running a limited number of high-fidelity/high-cost simulations. They also provide the user a so-called "surrogate-model" of the system response, that can be used to approximate the outputs of the system without actually solving the underlying equations.

In this talk we illustrate a multi-fidelity method (the so-called multi-index stochastic collocation) and its application to a naval engineering problem.

[1] C. Piazzola, L. Tamellini, R. Pellegrini, R. Broglia, A. Serani, M. Diez. Comparing Multi-Index Stochastic Collocation and Multi-Fidelity Stochastic Radial Basis Functions for Forward Uncertainty Quantification of Ship Resistance. *Engineering with Computers*, 2022.

[2] J. Beck, L. Tamellini, R. Tempone. IGA-based Multi-Index Stochastic Collocation for random PDEs on arbitrary domains. *Computer Methods in Applied Mechanics and Engineering*, 2019.

Learning from network data with nonlinear eigenvectors

Francesco Tudisco (GSSI, L'Aquila)

Recent work in network science has shown that there is a great value in studying multiple interactions across an arbitrary number of components in a system. This is typically modeled via a hypergraph or a simplicial complex, where each edge (or simplex) may involve multiple nodes. In order to fully take into account for these higher-order interactions, models have been proposed based on so-called nonlinear Laplacians, in contrast with more standard linear mappings used to work out classical graph (pairwise) representations.

In this talk we present a nonlinear eigenvalue framework for incorporating higher-order interactions into network centrality measures. The proposed framework covers classical network coefficients such as matrix and tensor eigenvector centralities, but further allows for many interesting extensions. In particular, we show how this can be used to detect core and periphery structures in hypergraphs. The underlying object of study is a constrained nonlinear eigenvalue (or singular value) problem. By exploiting recent developments in nonlinear Perron-Frobenius theory, we can provide guarantees of existence and uniqueness for the network measures, which we can also efficiently compute via a nonlinear power method.

An introduction to the divergence-free Virtual Element Method with focus on the Oseen Equation

Giuseppe Vacca (Università di Bari)

The Virtual Element Method (VEM) is a technology introduced in [Beirão da Veiga, Brezzi, Cangiani, Manzini, Marini, Russo, 2012, M3AS] for the discretization of partial differential equations. The VEM can be interpreted as a novel approach that generalizes the classical Finite Element Method to arbitrary even non-convex element-geometry. By avoiding the explicit integration of the shape functions that span the discrete Galerkin space and introducing a novel construction of the associated stiffness matrix, the VEM acquires very interesting properties and advantages with respect to more standard Galerkin methods, yet still keeping the same coding complexity. The present talk is both an introduction to the divergence-free VEM, aiming at showing the main ideas of the method, and a brief look at some application to the Oseen equation.

In the first part part of the talk we will describe the basics of the divergence-free VEM of [Beirão da Veiga, Lovadina, Vacca, 2018] and the related advantages. In the second part we extend the previous approach to the Oseen problem, including a suitable stabilization procedure that guarantees robustness in the convection dominated case without disrupting the divergence-free property. The stabilization is inspired from [Ahmed, Barrenechea, Burman, Guzmán, Linke, Merdon, 2020] and includes local SUPG-like terms of the vorticity equation, internal jump terms for the velocity gradients, and an additional VEM stabilization. We derive theoretical convergence results that underline the robustness of the scheme in different regimes, including the convection dominated case.

Adaptive Virtual Element Method

Marco Verani (Politecnico di Milano)

The Virtual Element Method (VEM) is relatively new paradigm for the discretization of PDEs which allows for general polytopal meshes. This geometric flexibility is very useful in many engineering applications, in particular when adaptive mesh refinement is needed to enhance the quality of the approximate solution. In this respect, two crucial, but yet open, questions arise: (a) how to systematically refine general polytopes (and preserve geometric properties of the computational mesh)?; (b) how to design adaptive algorithms with provable convergence and optimal complexity properties?

In this talk, having in mind these two questions, we briefly review the state of the art of the research and discuss recent results on the study of the convergence and optimal complexity properties of an Adaptive Virtual Element Method (AVEM) for the solution of a second order elliptic problem in two dimensions. Finally, limitations and future developments of the presented results will be discussed.