Second Congress of Greek Mathematicians – SCGM, Athens, July 4–8, 2022

Session Numerical Analysis & Scientific Computing: Programme

Wednesday (06/07/2022)

9:00-10:00	**Th. Sapsis** (Massachusetts Institute of Technology)
	Title: Likelihood-weighted active learning with application to Bayesian optimization, uncertainty quantification, and decision making in high dimensions
10:00-10:30	**K. Papafitsoros** (Weierstrass Institute Berlin)
	Title: Optimization with learning-informed nonsmooth differential equation constraints
10:30-11:00	**P. Perdikaris** (University of Pennsylvania)
	Title: *Learning the solution operator of parametric partial differential equations*

Thursday (07/07/2022)

9:00-9:30	**D. Giannakis** (New York University)
	Title: *Embedding classical dynamics in a quantum computer*
9:30-10:00	**Th. Katsaounis** (University of Crete & IACM/FORTH)
	Title: A relaxation scheme for the numerical approximation of the Schrödinger-Poisson system
10:00-10:30	**M. Kazolea** (INRIA, University of Bordeaux, CNRS)
	Title: *A hybrid FV/FE method for weakly dispersive highly nonlinear waves on unstructured meshes*
10:30-11:00	**Th. Papathanasiou** (Aston University)
	Title: A nonconforming finite element for ice shelf hydroelastic flexure

16:30-17:00	**K. Zygalakis** (University of Edinburgh)
	Title: *Lyapunov functions, convergence to equilibrium and applications to sampling and optimization*
17:00-17:30	**E. Kalligiannaki** (IACM/FORTH)
	Title: *Inference methods for stochastic differential equations and applications*
17:30-18:00	**G. Arambatzis** (ETH, Zürich)
	Title: *Multiscale simulations of complex systems by learning their effective dynamics*

18:30-19:00	**D. Noutsos** (University of Ioannina)
	Title: *Preconditioning techniques for Non-Symmetric Real Toeplitz Systems*
19:00-19:30	**F. Karakatsani** (University of Ioannina)
	Title: *TBA*
19:30-20:00	**E. Karatzas** (National Technical University of Athens)
	Title: *Advances in finite element computation and analysis of PDE systems within random geometries based on Embedded FEMs and applications*

Friday (08/07/2022)

9:00-10:00	**E. Gallopoulos** (University of Patras)
	Title: *TBA*
10:00-10:30	**G. Zouraris** (University of Crete)
	Title: *On the numerical approximation of partial differential equations with logarithmic non-linearity*
10:30-11:00	**D. Mitsoudis** (University of West Attica & IACM/FORTH)
	Title: *Imaging in three-dimensional waveguides with partial-aperture data*

Session Numerical Analysis & Scientific Computing: Abstracts & Titles

Georgios Arampatzis (ETH, Zürich)

Title: Multiscale simulations of complex systems by learning their effective dynamics

Abstract:
Predictive simulations of complex systems are essential for applications ranging from weather forecasting to drug design. The veracity of these predictions hinges on their capacity to capture effective system dynamics. Massively parallel simulations predict the system dynamics by resolving all spatiotemporal scales, often at a cost that prevents experimentation, while their findings may not allow for generalization. On the other hand, reduced-order models are fast but limited by the frequently adopted linearization of the system dynamics and the utilization of heuristic closures.

In this talk I will present a novel systematic framework that bridges large-scale simulations and reduced-order models to learn the effective dynamics of diverse, complex systems. The framework forms algorithmic alloys between nonlinear machine learning algorithms and the equation-free approach for modelling complex systems. Learning the effective dynamics deploys autoencoders to formulate a mapping between fine- and coarse-grained representations and evolves the latent space dynamics using recurrent neural networks. Learning the effective dynamics is applicable to systems ranging from chemistry to fluid mechanics and reduces the computational effort by up to two orders of magnitude while maintaining the prediction accuracy of the full system dynamics.

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Efstratios Gallopoulos (University of Patras)

Title & Abstract: TBA

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Dimitrios Giannakis (New York University)

Title: Embedding classical dynamics in a quantum computer

Abstract:
We present a framework for simulating a measure-preserving, ergodic dynamical system by a finite-dimensional quantum system amenable to implementation on a quantum computer. The framework is based on a quantum feature map for representing classical states by density operators on a reproducing kernel Hilbert space, H, of functions on classical state space. Simultaneously, a mapping is employed from classical observables into self-adjoint operators on H such that quantum mechanical expectation values are consistent with pointwise function evaluation. Meanwhile, quantum states and observables on H evolve under the action of a unitary group of Koopman operators in a consistent manner with classical dynamical evolution. The state of the quantum system is projected onto a finite-rank density operator on a 2^n-dimensional tensor product Hilbert space associated with n qubits. The finite-dimensional quantum system is factorized into tensor product form, enabling implementation through an n-channel quantum circuit with O(n) gates. Furthermore, the circuit features a quantum Fourier transform stage with O(n^2) gates, which makes predictions of observables possible by measurement in the standard computational basis. We illustrate our approach with quantum circuit simulations of low-dimensional dynamical systems, as well as actual experiments on the IBM Quantum System One.

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Evagelia Kalligiannaki (IACM/FORTH)

Title: Inference methods for stochastic differential equations and applications

Abstract:
Most problems we meet in science and engineering, finance, et al. have inherent and intrinsic uncertainty reflecting our knowledge and observation limitations. Thus, probabilistic modeling is necessary. We will present the application of stochastic differential equations in modeling complex molecular systems. Specifically, we look for reduced-order models effectively representing a fully detailed system. Our approach is data-driven, based on simulated or observed data. We will present inference methods we apply to learn parametrized stochastic differential equations for systems at stationary and transient states. Results in coarse-graining molecular systems will be presented.

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Fotini Karakatsani (University of Ioannina)

Title & Abstract: TBA

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Eftymios Karatzas (National Technical University of Athens)

Title: Advances in finite element computation and analysis of PDE systems within random geometries based on Embedded FEMs and applications.

Abstract:
We introduce and discuss some results related to unfitted finite element methods for partial differential equations with geometrically random deformations enhanced by level set descriptions and a fixed background geometry. An efficient model order reduction technique is proposed to integrate the embedded boundary finite element methods. Results are validated numerically. This methodology which extracts an unfitted mesh Nitsche finite element method in reduced order proper orthogonal decomposition method is based on a background mesh and PDE systems are examined. This approach achievements are twofold. Firstly, we reduce much computational effort since the unfitted mesh method allows us to avoid remeshing when updating the parametric domain. Secondly, the proposed reduced order model technique gives implementation advantage considering geometrical randomness. Computations are even exploited more efficiently since mesh is computed once and the transformation of each geometry to a reference geometry is not required. These combined advantages allow to solve many PDE problems more efficiently, and to provide the capability to find solutions in cases that could not be resolved in the past.

Acknowledgments. This work has received funding from the Hellenic Foundation for Research and Innovation (HFRI) and the General Secretariat for Research and Technology (GSRT), under grant agreement No[1115], and the ”First Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment” grant 3270 and the FSE-European Social Fund-HEaD “Higher Education and Development” SISSA operazione 1, Regione Autonoma Friuli-Venezia.

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Theodoros Katsaounis (University of Crete & IACM/FORTH)

Title: A relaxation scheme for the numerical approximation of the Schrödinger-Poisson system

Abstract:
We introduce a new second order in time relaxation scheme for approximating solutions of the Schrödinger-Poisson system. More specifically, we use the Crank-Nicolson scheme as a time stepping mechanism, the standard conforming finite element method for the spatial discretization whilst the nonlinearity is handled by means of a relaxation approach. We prove that discrete versions of the system's conservation laws, mass and energy, hold and we conclude by presenting some numerical experiments, including an example from cosmology, that demonstrate the effectiveness and robustness of the new scheme.

This is a joint work with: A. Athanassoulis, I. Kyza and S. Metcalfe.
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Maria Kazolea (INRIA, University of Bordeaux, CNRS)

Title: A hybrid FV/FE method for weakly dispersive highly nonlinear waves on unstructured meshes

Abstract:
We study a hybrid approach combining a Finite Volume (FV) and Finite Element (FE) method to solve a fully nonlinear and weakly-dispersive depth averaged wave propagation model. The FV method is used to solve the underlying hyperbolic shallow water system, while a standard P1 finite element method is used to solve the elliptic system associated to the dispersive correction. We study the impact of several numerical aspects: the impact of the reconstruction used in the hyperbolic phase; the representation of the FV data in the FE method used in the elliptic phase and their impact on the theoretical accuracy of the method; the well-posedness of the overall method. Concerning the elliptic step, the original problem is usually better suited for an approximation in H(div) spaces. However, it has been shown that perturbed problems involving similar operators with a small Laplace perturbation are well behaved in H^1. We show, based on both heuristic and strong numerical evidence, that numerical dissipation plays a major role in stabilizing the coupled method, and not only providing convergent results, but also providing the expected convergence rates. The numerical scheme is tested on standard benchmarks using unstructured grids with sizes comparable or coarser than those usually proposed in literature.
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Dimitrios Mitsoudis (University of West Attica & IACM/FORTH)

Title: Imaging in three-dimensional waveguides with partial-aperture data

Abstract:
We consider the problem of imaging extended reflectors in three-dimensional cylindrical, locally-perturbed acoustic waveguides using a planar array that is parallel to the waveguide's cross-section. We consider two cases, as far as the waveguide geometry is concerned: the infinite waveguide, which allows waves to travel infinitely in both directions in range and the terminating waveguide, where, we assume that there is an additional boundary on the one side of the waveguide, and consequently waves are only allowed to propagate infinitely on the other side. Our data is the multiple-frequency array response matrix. To form an image we back-propagate a projection of the data on the propagating modes in the waveguide. The projection operator is adequately defined for any array aperture size and shape that covers fully or partially the waveguide cross-section. Its definition hinges upon constructing a finite-

dimensional subspace of functions that are orthogonal along both the array and the waveguide cross-section and exhibit maximum fractional concentration of energy in the array aperture. The properties of the imaging method are analyzed theoretically and its effectiveness is assessed by numerical experiments for scatterers and arrays of varying shape and size.

This is joint work with Symeon Papadimitropoulos (Tel-Aviv University) and Chrysoula Tsogka (University of California).

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Dimitrios Noutsos (University of Ioannina)

Title: Preconditioning techniques for Non-Symmetric Real Toeplitz Systems

Abstract:

In this presentation we discuss on preconditioning techniques for the solution of nxn non-symmetric real Toeplitz systems $T_n(f\ )x = b$. The proposed preconditioner is derived under a combination of a band Toeplitz and a circulant matrix. We give details for the construction of the proposed preconditioner, for two cases: First, when the generating function f is known a priori and second, when the generating function is not known. We study the cluster of the eigenvalues, as well as of the singular values, of the preconditioned system and prove the efficiency of the Preconditioned Generalized Minimal Residual method (PGMRES) and the Preconditioned Conjugate Gradient method of Normal Equations (PCGN) for both cases. For the second case, a further analysis is given to estimate the generating function f by the entries of T_n. The efficiency of the proposed preconditioning techniques is shown in demonstrating numerical examples.

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Kostas Papafitsoros (Weierstrass Institute Berlin)

Title: Optimization with learning-informed nonsmooth differential equation constraints

Abstract:

In this talk, we will discuss a family of optimization problems that are constrained by differential equations with constituents which are only accessible through data-driven techniques. We particularly focus on the case where these components are machine-learned and substituted by artificial neural networks resulting in learning-informed differential equations. Initially we will motivate the framework with an application from the area of quantitative magnetic resonance imaging, where neural networks are employed to approximate the underlying physical processes (Bloch equations) that are used for the computation of quantitative maps of tissue dependent values of relevant biophysical parameters (e.g. relaxation times T1 and T2). We will then proceed to a detailed study of the optimal control of semilinear partial differential equations where neural networks aim to approximate an unknown nonlinearity in the PDE. We are

particularly interested in the case where the networks are nonsmooth, due to ReLU (Rectified Linear Unit) being the underlying activation function. Existence and uniqueness of the state equation are shown, and continuity as well as directional differentiability properties of the corresponding control-to-state map are established. Based on approximation capabilities of the pertinent networks, we address fundamental questions regarding approximating properties of the learning-informed control-to-state map and the solution of the corresponding optimal control problem. Finally, several stationarity conditions are derived based on different notions of generalized differentiability.

This is joint work with Guozhi Dong and Michael Hintermüller from Weierstrass Institute Berlin (WIAS).
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Theodosios Papathanasiou (Aston University)

Title: A nonconforming finite element for ice shelf hydroelastic flexure

Abstract:
The action of oceanic waves on ice shelves can cause hydroelastic flexural oscillations leading to rift generation and propagation, therefore contributing to calving events and other disintegration phenomena. Infragravity waves in particular can induce significant hydroelastic flexure on major Antarctic ice shelves, such as the Ross Ice Shelf. Considering long period waves, e.g. infragravity, and the large horizontal span of major Antarctic ice shelves, a model based on the linearised Shallow Water Equations and the Kirchhoff–Love theory for slender plates is appropriate for hydroelastic flexure studies. In this setting, a nonconforming Finite Element for ice shelf modal analysis is proposed. The aim is to identify resonant frequencies and eigenstates of hydrorelastic flexure. The finite element combines Specht's shape functions for plate bending with a linear triangle for the velocity potential approximation. A priori error estimates for the associated eigenvalue problem are derived and convergence characteristics are verified through several numerical tests. A specific case study, focusing on the Larsen C Ice Shelf, is considered. Modal analysis for this case study reveals that the fundamental eigenfrequency and lower order harmonics can be very accurately approximated using the eigenfrequencies of a water basin with adjusted bathymetry, ignoring thus the flexural effect of the ice shelf. However, this is not the case for the associated eigenfunctions since ice shelf flexure influences heavily the modal shapes and nodal lines.
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Paris Perdikaris (University of Pennsylvania)

Title: Learning the solution operator of parametric partial differential equations

Abstract:
Partial differential equations (PDEs) play a central role in the mathematical analysis and modeling of complex dynamic processes across all corners of science and engineering. Their solution often requires laborious analytical or computational tools, associated with a cost that is markedly amplified when different scenarios need to be investigated, for example, corresponding to different initial or boundary conditions, different inputs, etc. In this talk we will discuss the potential of neural operators – a class of methods for supervised learning in function spaces – in learning the solution operator of arbitrary PDEs, even in the absence of any paired input-output training data. We illustrate the effectiveness of such methods in rapidly predicting the solution of various types of parametric PDEs up to three orders of magnitude faster compared to conventional numerical solvers, setting a previously unexplored paradigm for modeling and simulation of nonlinear and nonequilibrium processes in science and engineering.
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Themistoklis Sapsis (Massachusetts Institute of Technology)

Title: Likelihood-weighted active learning with application to Bayesian optimization, uncertainty quantification, and decision making in high dimensions

Abstract:
Analysis of physical and engineering systems is characterized by unique computational challenges associated with high dimensionality of parameter spaces, large cost of simulations or experiments, as well as existence of uncertainty. For a wide range of these problems the goal is to either quantify uncertainty and compute risk for critical events, optimize parameters or control strategies, and/or making decisions. Bayesian active learning provides a flexible framework for performing these tasks. However, Bayesian calculations are often prohibitively expensive in terms of the required simulations or experiments, even in the active learning setting. In this talk we introduce a new class of acquisition functions that utilize a likelihood-weighted ratio that accounts for the importance of the output relative to the input. This ratio acts essentially as a probabilistic sampling weight and guides the sampling algorithm towards regions of the input space where the objective function assumes abnormal values, resulting in significant savings of computational or experimental resources needed for convergence. We show that the adopted acquisition functions can be rigorously derived as the asymptotic limit of an optimal acquisition function that has a minimax form over a functional space. Subsequently, we demonstrate their favorable properties compared to standard methods on benchmark functions commonly used in the optimization community as well as real world applications involving turbulence, fluid-structure interaction problems and optimal sensor placement.

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Georgios Zouraris (University of Crete)

Title: On the numerical approximation of partial differential equations with logarithmic non-linearity

Abstract:
We consider an initial and Dirichlet boundary value problem for the logarithmic Schrödinger equation or the logarithmic heat equation over a two dimensional rectangular domain.

We construct approximations of the solution to the problem using a standard second order finite difference method for space discretization along with a time discretization method, with or without regularizing the logarithmic term.

The corresponding convergence analysis yields almost optimal order a priori error estimates in various discrete norms.

Joint work with: P. Paraschis (NTUA)

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Konstantinos Zygalakis (University of Edinburgh)

Title: Lyapunov functions, convergence to equilibrium and applications to sampling and optimization

Abstract:
Lyapunov functions play a central role in examining the stability of (stochastic) dynamical systems. In this talk we will study the properties of Lyapunov functions connected to some (stochastic) differential equations which are central to construction of optimization and sampling algorithms. In particular, using a control theoretical formulation of these equations, we will utilise a set of linear matrix inequalities (applicable in the case of strongly convex potentials) which allow us to deduce their long-time properties as well as deducing the behaviour of a number of popular optimization and sampling algorithms.