The Mathematics of Scientific Machine Learning and Digital Twins

November 20–24, 2025

International School of Mathematics "G. Stampacchia", Erice, Italy

Organizers:

Harbir Antil — Center for Mathematics and Artificial Intelligence (CMAI), George Mason University, USA[1]

Enrique Zuazua — FAU Center for Mathematics of Data (MoD), Erlangen–Nürnberg, Germany[2]

Overview. This workshop brings together experts at the interface of *computational and applied mathematics*, *machine learning*, and *scientific computing*, with a special focus on the mathematical foundations of emerging *Digital Twin* technologies. The program combines concise research presentations with extended discussion periods, fostering collaboration and exchange of ideas across disciplines.

Website: `https://cmai.gmu.edu/scimldt/`

[1] `https://cmai.gmu.edu`
[2] `https://mod.fau.eu`

Attendees

1. Alcalde, Albert – Erlangen-Nuernberg, Germany
2. Antil, Harbir – George Mason University
3. Antonietti, Paola – Polytechnic University of Milan, Italy
4. Arceci, Francesca – MOX, Department of Mathematics, Politecnico di Milano
5. Biccari, Umberto – University of Deusto, Spain
6. Bungert, Leon – University of Würzburg, Germany
7. Buttazzo, Giuseppe – Università di Pisa
8. Cannarsa, Piermarco – University of Rome, Italy
9. Despres, Bruno – Sorbonne University, France
10. Giesselmann, Jan – Technical University of Darmstadt, Germany
11. Ghattas, Omar – The University of Texas Austin, USA
12. Gomes, Diogo – KAUST, Saudi Arabia
13. Gomez, Marcella – University of California, Santa Cruz
14. Fernandez, Daniel – Erlangen-Nuernberg, Germany
15. Hayat, Amaury – École des Ponts ParisTech, France
16. Hintermüller, Michael – WIAS, Berlin, Germany
17. Hu, Weiwei – University of Georgia, USA
18. Kaltenbach, Alex – TU Berlin
19. Kobeleva, Xenia – Ruhr University Bochum, Germany
20. Lazar, Martin – University of Dubrovnik, Croatia
21. Leugering, Guenther – Germany
22. Li, Ziqian – Erlangen-Nuernberg, Germany
23. Liu, Kang – Université Bourgogne Europe, France
24. Lopez Montero, Daniel – Erlangen-Nuernberg, Germany
25. De Nitti, Nicola – EPFL, Switzerland
26. Penk, Dominik – Schaeffler Technologies AG & Co. KG, Germany
27. Reich, Sebastian – University of Potsdam, Germany
28. Rozza, Gianluigi – SISSA
29. Schreiber, Tatjana – Albert-Ludwigs-Universität Freiburg
30. Venturi, Daniele – University of California, Santa Cruz
31. Wang, Ziqi – Erlangen-Nuernberg, Germany
32. Zhang, Yaoyu – Shanghai Jiao Tong University, China
33. Zunino, Paolo – Politecnico di Milano, Italy
34. Zuazua, Enrique – Erlangen-Nuernberg, Germany

Schedule [3]

Thursday, November 20, 2025

8:40AM - 8:45AM	Welcome address by the Center Directors
8:45AM - 9:00AM	Welcome address by the Organizers: Harbir Antil and Enrique Zuazua
9:00AM - 10:30AM	Session 1 (Plenary Talks) Günter Leugering (FAU Erlangen-Nürnberg and SSC) Paola F. Antonietti (Politecnico di Milano) Dominik Penk (Schaeffler Technologies AG & Co. KG)
10:30AM - 11:00AM	Coffee
11:00AM - 12:30PM	Session 2 (Plenary Talks) Gianluigi Rozza (SISSA) Bruno Despres (Sorbonne Universite) Weiwei Hu (University of Georgia)
12:30PM - 2:30PM	Lunch
2:30PM - 4:00PM	Session 3 (Early Career Talks) Daniel Montero Lopez (FAU, Erlangen-Nürnberg) Ziqi Wang (FAU, Erlangen-Nürnberg) Ziqian Li (FAU, Erlangen-Nürnberg)
4:00PM - 4:30PM	Coffee
4:30PM - 5:30PM	Karen Willcox (UT Austin) – **recording**

[3] Each **talk** will be 20-minutes followed by a moderated panel discussion of 30 minutes.

Friday, November 21, 2025

9:00AM - 10:30AM	Session 4 (Plenary Talks)
	Xenia Kobeleva (Ruhr University Bochum, Germany)
	Paolo Zunino (Politecnico di Milano)
	Leon Bungert (University of Würzburg)
10:30AM - 11:00AM	Coffee
11:00AM - 12:30PM	Session 5 (Plenary Talks)
	Diogo Gomes (King Abdullah University of Science and Technology)
	Francesca Arceci (Politecnico di Milano)
	Piermarco Cannarsa (University of Rome Tor Vergata)
12:30PM - 2:30PM	Lunch
2:30PM - 4:00PM	Session 6 (Plenary Talks)
	Jan Giesselmann (Technical University of Darmstadt)
	Umberto Biccari (University of Deusto)
	Enrique Zuazua (FAU, Erlangen-Nürnberg)
4:00PM - 4:30PM	Coffee
4:30PM - 6:00PM	Session 7 (Plenary Talks)
	Michael Hintermüller (WIAS, Berlin)
	Martin Lazar (University of Dubrovnik)
	De Nitti, Nicola

Saturday, November 22, 2025

9:00AM - 10:30AM	Session 8 (Plenary Talks)
	Sebastian Reich (University of Potsdam)
	Yaoyu Zhang (Shanghai Jiao Tong University)
	Harbir Antil (George Mason)
10:30AM -	Social trip to ....

Sunday, November 23, 2025

9:00AM - 10:30AM	Session 9 (Plenary Talks)
	Giuseppe Buttazzo (University of Pisa)
	Amaury Hayat (Ecole des Ponts ParisTech)
	Alex Kaltenbach (TU Berlin)
10:30AM - 11:00AM	Coffee
11:00AM - 12:30PM	Session 10 (Early Career Talks)
	Tatjana Schreiber (Albert-Ludwigs-Universität Freiburg)
	Daniel Fernandez (FAU, Erlangen)
	Albert Alcalde (FAU, Erlangen)
12:30PM - 2:30PM	Lunch
2:30PM -	**Free afternoon but Conference Dinner at Night**

Monday, November 24, 2025

9:00AM - 10:30AM	Session 11 (Plenary Talks)
	Kang Liu (Université Bourgogne Europe)
	Marcella Gomez (UC Santa Cruz)
	Omar Ghattas (The University of Texas Austin)
10:30AM - 12:00PM	Discussion and Conclusion
12:00PM - 2:00PM	Lunch

Titles and Abstracts

Time-Delayed Transformers for Nonlinear Modeling of Physical Dynamics

Alcalde, Albert

Erlangen-Nürnberg, Germany

We introduce the time-delayed transformer (TD-TF), a simplified transformer architecture tailored for data-driven modeling of temporal dynamics in physical systems. Building on formal connections to time-delayed dynamic mode decomposition (TD-DMD), we show that a single self-attention layer with feed-forward mappings can be interpreted as a nonlinear extension of TD-DMD, where adaptive attention weights replace fixed linear coefficients, and feature mappings introduce nonlinear observables. This formulation bridges transformer-based sequence modeling with classical operator-theoretic approaches rooted in time-delay embeddings. Through numerical experiments on systems of increasing dynamical complexity, we demonstrate that TD-TF retains the efficiency of TD-DMD while improving predictive accuracy in nonlinear and chaotic regimes. These results indicate that adding structured time-delay mechanisms to transformer models can improve interpretability and physical consistency in data-driven modeling of dynamical systems.

Digital Twins: A PDE–Constrained Optimization Perspective

Antil, Harbir

George Mason University, USA

Digital Twins (DTs) are adaptive, real-time virtual replicas of physical systems that integrate physics-based models, sensor data, and intelligent decision-making. At their core, DTs can be rigorously framed within PDE–constrained optimization (PDECO). This talk develops a unified PDECO framework for state estimation and control, leveraging adjoint-based methods in both deterministic and stochastic settings. To address the challenges of infinite-dimensional, large-scale optimization, novel function space based algorithms are discussed. Applications span a wide range of domains, including structural and biomedical systems—from bridges and dams to aneurysm modeling, optimal insulation, electromagnetic cloaking, light bending, and neuromorphic imaging. Together, these examples highlight a pathway toward predictive, adaptive, and trustworthy Digital Twins.

Machine Learning Enhanced Polytopal Finite Element Methods

Antonietti, Paola

Polytechnic University of Milan, Italy

In this talk, we discuss the integration Machine Learning (ML) techniques into polytopal Finite Element Methods to enhance their accuracy and flexibility while addressing the complexities encountered in practical applications such as computational neuroscience. We present innovative ML-driven mesh agglomeration strategies in polytopal Finite Element Methods. We introduce novel algorithms based on Graph Neural Networks to process the connectivity graph of mesh elements and the physical properties of the model under analysis simultaneously, thereby agglomerating mesh elements and ensuring the generation of high-quality agglomerated grids. The resulting agglomerated meshes can be employed to reduce the computational burden while maintaining a detailed representation of the geometry and to construct efficient geometric Multigrid solvers, demonstrating significant improvements in computational efficiency. In the second part of the talk, we present a novel method based on deep learning to accelerate the convergence of Algebraic Multigrid (AMG) techniques. Specifically, ANNs are trained to predict the optimal strong connection parameter that governs the sequence of coarsened matrix problems within the AMG algorithm, thereby effectively reducing the time to a solution. We examine diverse differential problems and discretisation schemes to validate the proposed methodologies, including Virtual Element Methods (VEMs) and polytopal Discontinuous Galerkin (PolyDG) methods.

Digital Twins in Computational Oncology: Probabilistic Formulation of Personalized Risk Assessment

Arceci, Francesca[1], Vitullo, Piermario[1], Dionisi, Benedetta[2], Rancati, Tiziana[2], Zunino, Paolo[1,2]

[1]*Politecnico di Milano;* [2]*CMON Lab, Data Science Unit, Fondazione IRCCS Istituto Nazionale dei Tumori*

Digital twins in oncology aim to provide patient-specific models that integrate multi-source clinical, biological, and treatment data to support prediction, decision-making, and long-term risk monitoring. To establish a rigorous methodological foundation for such systems, we propose a probabilistic formalization of personalized risk assessment that is naturally expressed through probabilistic graphical models and dynamic Bayesian networks, which allow modular representation of risk, support heterogeneous and missing data, and provide a formal basis for both predictive and causal inference. We demonstrate the application of this methodology in predicting severe late toxicity after breast cancer radiotherapy.

Deep Operator Networks in Control Theory: Concepts and Applications

Biccari, Umberto

University of Deusto, Spain

Deep Operator Networks (DeepONets) provide a powerful framework for learning nonlinear operators from data. Unlike conventional neural networks, which approximate functions, DeepONets approximate mappings between function spaces, allowing them to capture complex relationships governed by differential equations. This operator-learning capability makes them particularly suitable for digital twin technology, where fast, data-driven surrogates of physical systems are required for prediction, monitoring, and control. In this talk, we will introduce the DeepONet architecture and its universal approximation property, which guarantees its ability to learn general nonlinear operators under suitable assumptions. We will discuss how this property underpins the use of DeepONets as digital twins for dynamical systems and control applications. The presentation will include two illustrative examples: a classical LQR control and a more challenging case of backstepping stabilization for a stochastic system. Beyond these applications, I will provide a critical comparison with alternative operator learning approaches, highlighting both the strengths and limitations of DeepONets in terms of scalability, data efficiency, and generalization. Together, these elements aim to position DeepONets within the broader landscape of operator learning and control-oriented digital twin design.

Graph-based Learning

Bungert, Leon

University of Würzburg, Germany

Despite the omnipresence of deep learning, in many application scenarios (e.g. when labeled data is scarce) it pays off to utilize graph representations of the data to solve the learning task at hand. Most of these models are supported by strong mathematical theory.
In this talk we review unsupervised and semi-supervised learning models involving weighted graphs. These models typically involve certain partial differential equations on graphs. We revisit spectral clustering and its convex relaxation involving the eigenvalue problem for the graph Laplacian. Then we shall discuss semi-supervised learning with (nonlinear) graph Laplace and Poisson equations and review new results on their large data limits.

Optimal Sampling for Linear Control Systems

Buttazzo, Giuseppe

Università di Pisa, Italy

In digital control systems, the state is sampled at given sampling instants and the control is kept constant between two consecutive instant. The choice of sampling instants is crucial in order to perform an optimal control and to govern efficiently the system. By optimal sampling problem we mean the selection of sampling instants and control inputs, such that a given function of the state and input is minimized. We consider a linear quadratic control problem and we discuss several sampling methods; we also propose a new quantization-based sampling strategy that is capable of achieving near-optimal cost. This new strategy is shown to be optimal in several situations.

Singularities in Dynamic Programming: A Paradise of Choices, a Nightmare for Numerics

Cannarsa, Piermarco

University of Rome, Italy

Dynamic Programming in optimal control relies on the analysis of the Hamilton-Jacobi-Bellman (HJB) equation—a fully nonlinear partial differential equation whose solutions are typically nonsmooth. Points of non-differentiability often correspond to the existence of multiple optimal trajectories, whereas differentiability reflects a unique optimal choice. While this multiplicity can be seen as an advantage—offering fallback options or a "Plan B, C, D..."—it presents serious challenges for numerical approximation. This talk will place these ideas in a rigorous mathematical framework, highlighting key results on the formation and propagation of gradient singularities (or shocks) and their implications for both theory and computation.

Differentiability Properties of Non-smooth Functions Used in Neural Networks

Despres, Bruno

Sorbonne University, France

Non smooth functions (like ReLU or maxpool) are more and more common in the design of functions in Neural Networks and Machine Learning. A mathematical question is to determine a functional framework for the associated algebra. I will show that the Murat-Trombetti Theorem is a powerful answer and it provides a natural answers to many practical questions arising in the field.

A Principled Perspective on Neural PDE Solvers: From Coercivity to Condensation

Fernandez, Daniel

FAU, Erlangen, Germany

Neural PDE solvers often lack a basic theoretical guarantee: the training objective need not admit a minimizer. We trace this well-posedness gap to a structural lack of coercivity of the loss functional. Focusing on radial basis function (RBF) architectures, we rigorously characterize the parameter blow-up mechanism and its connection to the well-known condensation phenomenon in neural networks. Guided by this analysis, we introduce a principled penalization that restores coercivity as an alternative to the classical Tikhonov regularization. Numerical experiments across representative elliptic PDEs corroborate our theoretical findings

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Data Assimilation for Gas Flows on Networks

Giesselmann, Jan

Technical University of Darmstadt, Germany

We consider the construction and analysis of observers for gas networks. The observer system is (nearly) a copy of the original system which, in our case, is governed by the barotropic Euler equations. The observer receives measurements of certain point values of the original system and uses them as boundary conditions. In this talk we will address two specific questions:

1) Suppose measurements are given at every boundary node of the network, how many internal measurement points are needed – and where should they be located – so that we can guarantee that the state of the observer system approximates the original system state for long times.

2) What happens if the observer system uses a different set of PDEs than the original system? We will show that if the two PDE systems are similar (in a sense that we will make precise) then the state of the observer will end up in a neighborhood of the original system state whose size is proportional to the difference between the two systems.

This is joint work with M. Gugat (Erlangen) and T. Kunkel and V. Kumar (Darmstadt)

Real Time High Fidelity Bayesian Inversion, Prediction, and OED for Large Scale LTI Systems, with Application to Tsunami Early Warning

Ghattas, Omar

The University of Texas at Austin, USA

Efforts are underway to instrument subduction zones with seafloor acoustic pressure sensors to provide tsunami early warning. Our goal is to create a physics-based early-warning system that employs this pressure data, along with the 3D coupled acoustic–gravity wave equations forward model, to infer the earthquake-induced spatiotemporal seafloor motion in real time. The Bayesian solution of this inverse problem then provides the seafloor forcing to forward propagate the tsunamis toward populated areas along coastlines and issue forecasts with quantified uncertainties. We apply this framework to the Cascadia subduction zone, which has been assigned a 37% probability of a magnitude 8.2+ earthquake in the next 50 years.
Solution of a single forward problem alone entails severe computational costs stemming from the need to resolve ocean acoustic waves in a subduction zone of length 1000 km and width 200 km. A single forward problem requires 1 hour on a supercomputer. The Bayesian inverse problem, with a billion uncertain parameters, formally requires hundreds of thousands of such forward and adjoint wave propagations; thus real time inference appears to be intractable. We propose a novel approach to enable accurate solution of the inverse and prediction problems in real time on a GPU cluster. The key is to exploit the structure of the parameter-to-observable map, namely that it is a time shift-invariant operator and upon discretization can be recast as a block Toeplitz matrix, permitting FFT diagonalization and fast GPU implementation. We discuss the Bayesian formulation and real time GPU solution, and demonstrate that tsunami inverse problems with $O(10^9)$ parameters can be solved exactly in a fraction of a second. This fast Bayesian inversion capability is then exploited to solve the optimal experimental design problem of placement of seafloor pressure sensors to maximize expected information gain. The methodological framework directly extends to any source inversion problem governed by linear time-invariant dynamics.
This work is joint with Sreeram Venkat (UT Austin), Stefan Henneking (UT Austin), and Alice Gabriel (UCSD).

A Banach Space Approach to Mean-Field Games via Monotonicity

Gomes, Diogo
KAUST, Saudi Arabia

Mean-Field Games (MFGs) model strategic interactions in large populations across fields such as economics, finance, and social dynamics. Establishing the existence of solutions traditionally involves specialized techniques with limited applicability. This talk introduces a unified Banach space framework utilizing monotone operator theory to establish existence results for stationary MFGs under general growth conditions, including congestion models. Our approach employs p-Laplacian regularizers, enabling strong and weak solution formulations via variational inequalities and Minty's method. Crucially, we derive ϵ-independent estimates simplifying convergence analysis compared to traditional Hilbert space methods. This approach also benefits numerical implementations by using simpler regularizations.

Combining Deep Learning Models and Reinforcement Learning to Drive Wound Healing Outcomes

Gomez, Marcella
University of California, Santa Cruz, USA

Precision medicine optimizes a treatment strategy for maximum efficiency or therapeutic benefit for a given individual. Due to system size and complexity, data-driven methods need to be explored to develop multi-dimensional quantifiable indicators tracking systemic changes for real-time decision making. In this work I discuss how bioelectronic devices enhanced with deep learning can help facilitate real-time sensing and actuation for automated decisions in treatment for wound healing for both quantifying and tracking state progression and accelerating wound closure. We combine a deep learning model that maps high-dimensional states to a latent space. A linear model is learned for the evolution of the latent space and leveraged to guide a reinforcement learning algorithm that outputs a custom treatment strategy for electric field and drug application.

How Can Machine Learning Help Mathematicians?

Hayat, Amaury

École des Ponts ParisTech, France

The advent of artificial intelligence raises an important question: Can AI assist mathematicians in solving open problems in mathematics? This talk explores this question from multiple perspectives. We will explore how different types of AI models can be trained to provide valuable insights into mathematical questions and recent progress in the field of automated theorem proving.

A Neural Network Approach to Learning Solutions of a Class of Elliptic Variational Inequalities

Hintermüller, Michael

WIAS, Berlin, Germany

We discuss a weak adversarial approach to solving obstacle problems using neural networks. By employing (generalised) regularised gap functions and their properties we rewrite the obstacle problem (which is an elliptic variational inequality) as a minmax problem, providing a natural formulation amenable to learning. Our approach, in contrast to much of the literature, does not require the elliptic operator to be symmetric. We provide an error analysis for suitable discretisations of the continuous problem, estimating in particular the approximation and statistical errors. Parametrising the solution and test function as neural networks, we apply a modified gradient descent ascent algorithm to treat the problem and conclude the talk with various examples and experiments. Our solution algorithm is in particular able to easily handle obstacle problems that feature biactivity (or lack of strict complementarity), a situation that poses difficulty for traditional numerical methods.

Cellular Flow Control Design for Mixing Based on the Least Action Principle

Hu, Weiwei

University of Georgia, USA

We consider a novel approach for the enhancement of fluid mixing via pure stirring strategies building upon the Least Action Principle (LAP) for incompressible flows.
The LAP is formally analogous to the Benamou–Brenier formulation of optimal transport, but imposes an incompressibility constraint. Our objective is to find a velocity field generated by Hamiltonian flows that minimizes the kinetic energy while ensuring that the initial scalar distribution reaches a prescribed degree of mixedness by a finite time.

Analysis and Numerical Approximation of an Optimal Thermal Insulation Problem: The Heat Conduction Case

Kaltenbach, Alex

Technical University of Berlin, Germany

In this talk, we address the analysis and numerical approximation of a non-local and non-smooth convex minimization problem arising in the optimal thermal insulation of thermally conducting bodies, where the major mode of heat transfer is heat conduction. The goal is to determine the optimal boundary distribution $\mathtt{d} : \partial\Omega \to [0, +\infty)$ of a given total amount $m > 0$ of insulating material on the boundary of a thermally conducting body given via a polyhedral Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$. The resulting optimization problem emerges as the Γ-limit of a class of extended "thin insulation" models (in the sense of G. Buttazzo), leading to a non-local and non-smooth convex formulation.
To cope with the non-local and non-smooth character of the problem, we employ a duality-based approach: the Fenchel dual problem admits a quadratic programming structure that can be efficiently solved via a primal–dual active set strategy, interpreted as a semismooth Newton method. Finally, the primal solution is recovered from the discrete dual solution using an inverse generalized Marini formula.

Digital Twins of the Brain - A Perfect Case Study for Interdisciplinary Collaboration

Kobeleva, Xenia

Ruhr University Bochum, Germany

In clinical neurology, demographic changes and increases in diagnostic complexity coupled with limited financial resources call for novel AI-driven technologies such as digital twins. In this talk I will review some relevant barriers for translation of digital twins into the clinical realm, while stressing the potential of interdisciplinary collaboration between mathematics and medicine.

Be greedy and Learn: Efficient and Certified Algorithms for Parametrized Optimal Control Problems

Lazar, Martin

University of Dubrovnik, Croatia

We consider a family of parametrized linear equations and provide their online-efficient solutions by combining greedy reduced basis methods and machine learning algorithms. To this end, we first run the offline part of the greedy control algorithm, which builds a reduced basis for the manifold of solutions. Afterwards, we apply machine learning surrogates to accelerate the online evaluation of the reduced model. The error estimates proven for the greedy procedure are further transferred to the machine learning models and thus allow for efficient a posteriori error certification. The method is applied to parametrized linear-quadratic optimal control problems, accompanied by numerical examples that show the tremendous potential of the proposed methodology.
The talk is based on a joint work with Hendrik Kleikamp and Cesare Molinari.

Space–Time Domain Decomposition for 1-D Wave Equations on Networks with PINN Surrogates

Leugering, Guenther

Erlangen-Nürnberg, Germany

We investigate space and time domain decomposition methods and their numerical realizations for 1-D wave equations on networks with a particular emphasis on PINN surrogates in part of the network.

Deep Neural ODE Operator Networks for PDEs

Li, Ziqian

Erlangen-Nürnberg, Germany

We introduce a deep neural ordinary differential equation (ODE) operator-learning framework, termed NODE-ONet. The approach uses an encoder–decoder architecture with three components: an encoder that spatially discretises input functions, a neural ODE that captures latent temporal dynamics, and a decoder that reconstructs solutions in physical space. We propose physics-encoded neural ODEs to incorporate PDE-specific structure. These designs reduce model complexity and improve numerical efficiency, robustness, applicability, and generalisation. Owing to its flexibility to accommodate diverse encoders/decoders and to generalise across related families of PDEs, NODE-ONet provides a scalable, physics-aware tool for scientific machine learning.

Inverse Problem of Heat Equation and Diffusion Model

Liu, Kang

Université Bourgogne Europe, France

In this presentation, we address a classical ill-posed inverse problem: the identification of the initial source in the heat equation. We then establish a connection between this inverse problem and generative diffusion models. Next, we examine the well-posedness of diffusion models and analyze their asymptotic behavior. Finally, drawing on energy estimates for the backward Fokker–Planck equation, we provide theoretical justification for certain loss function designs used in the training process.

Kernel Methods and Machine Learning

Lopez Montero, Daniel

Erlangen-Nürnberg, Germany

We explore the paradigm of learning dynamical systems using kernel methods and examine their relationship with other machine learning frameworks. We study several key aspects, including universal approximation, the representer theorem, interpretability, and scalability. Experimentally, we compare our approach with the well-established NeuralODE model.

Optimal Transport of Measures via Autonomous Vector Fields

De Nitti, Nicola

Università di Pisa, Italy

We study the problem of transporting one probability measure to another via an autonomous velocity field. We rely on tools from the theory of optimal transport. In one space-dimension, we solve a linear homogeneous functional equation to construct a suitable autonomous vector field that realizes the (unique) monotone transport map as the time-1 map of its flow. Generically, this vector field can be chosen to be Lipschitz continuous. We then use Sudakov's disintegration approach to deal with the multidimensional case by reducing it to a family of one-dimensional problems.

This talk is based on a joint work with Xavier Fernández-Real.

ASAP – Automated Simulation Abstraction Pipeline

Penk, Dominik

Schaeffler Technologies AG & Co. KG, Germany

Neural network-based surrogate models for mechanical simulations offer many benefits such as improved computational speed and effective intellectual property protection. However, these models often face skepticism from expert users who question the reliability of the simulation results. Additionally, there is a technical challenge of data scarcity, which arises from the time-consuming and costly process of generating synthetic training data. In this talk, we present a practical implementation pipeline designed to address both concerns. We enhance trust in the simulation outcomes by providing quality estimates and insights into the proximity of new data to previously seen datasets. To mitigate the data scarcity challenge, we employ a gradient-aware training approach that maximizes learning efficiency even with limited data availability. Our pipeline is demonstrated with simulations of a suite of bearing models, where additional data scarcity mitigation is achieved through fine-tuning techniques.

McKean–Pontryagin Minimum Principle for Stochastic Optimal Control

Reich, Sebastian

University of Potsdam, Germany

The talk outlines a novel extension of the classical Pontryagin minimum (maximum) principle to stochastic optimal control problems. Contrary to the well-known stochastic Pontryagin minimum principle involving forward–backward stochastic differential equations, the proposed formulation is deterministic and of mean-field type. The Hamiltonian structure of the proposed Pontryagin minimum principle is achieved via the introduction of an appropriate gauge variable. The gauge freedom can be used to decouple the forward and reverse time equations, hence simplifying the solution of the underlying boundary value problem. We also consider infinite-horizon discounted-cost optimal control problems. In this case, the mean-field formulation allows converting the computation of the desired optimal control law into solving a pair of forward mean-field ordinary differential equations.

Enhancing CFD Simulation with Reduced Order Methods and Scientific Machine Learning

Rozza, Gianluigi
SISSA, Italy

Partial differential equations (PDEs) are invaluable tools for modeling complex physical phenomena. However, only a limited number of PDEs can be solved analytically, leaving the majority of them requiring computationally expensive numerical approximations. To address this challenge, reduced order models (ROMs) have emerged as a promising field in computational sciences, offering efficient computational tools for real-time simulations. In recent years, deep learning techniques have played a pivotal role in advancing efficient ROM methods with exceptional generalisation capabilities and reduced computational costs, especially for parametric settings and turbulent flows.
In this talk we explore how classical ROM techniques can be elevated through the integration of some deep learning models. We will introduce hybrid approaches, which consider both physics-based and purely data-driven techniques, as well as aggregated ones, where the model is built as a combination of different pre-trained models. Examples will deal with parametric flows in presence of compressibility as well as turbulence.

Learning Adaptive Step Sizes for the Harmonic Map Heat Flow

Schreiber, Tatjana
Albert-Ludwigs-Universität Freiburg, Germany

Selecting an appropriate step size is crucial for the efficiency and stability of iterative solvers for partial differential equations. Traditional strategies such as Armijo or Golden-Section line searches ensure stability, but they often come with high computational costs. In this presentation, we propose using supervised learning to select the step size in harmonic map heat flow. Therefore, we train a neural network to predict step sizes based on state features encoding energy, residual and curvature information. Safeguards ensure energy monotonicity and numerical stability. We analyse which state feature information influences the predicted step size.

A Potential Game Framework for Incentive Design in Federated Learning

Wang, Ziqi

Erlangen-Nürnberg, Germany

Federated learning (FL) enables collaborative model training across distributed clients without centralizing data. While traditional FL assumes that a central server assigns training strategies to clients, a game-theoretic perspective allows clients to choose their own participation levels. To analyze these interactions, we introduce a potential game framework in which each client's payoff depends on their individual effort and the server's reward, the latter modulated by a tunable reward factor and influenced by the collective efforts of all clients. We prove the existence of Nash equilibria (NEs) in this setting and further explore conditions for uniqueness in stationary cases. Notably, we identify a critical reward factor at which clients' efforts increase sharply. Extensive experiments on various datasets and model architectures show that incorporating equilibrium-based client behavior significantly improves model performance and validates the proposed reward mechanism.

Condensation Sheds Light on the Mathematical Foundation of Deep Neural Networks

Zhang, Yaoyu
Shanghai Jiao Tong University, China

Condensation (also known as quantization, clustering, or alignment) is a widely observed phenomenon where neurons in the same layer tend to align with one another during the nonlinear training of deep neural networks (DNNs). It is a key characteristic of the feature learning process of neural networks. In recent years, to advance the mathematical understanding of condensation, we uncover structures regarding the dynamical regime, loss landscape and generalization for deep neural networks, based on which a novel theoretical framework emerges. This presentation will cover these findings in detail. First, I will present results regarding the dynamical regime identification of condensation at the infinite-width limit, where small initialization is crucial. Then, I will discuss the mechanism of condensation at the initial training stage and the global loss landscape structure underlying condensation in later training stages, highlighting the prevalence of condensed critical points and global minimizers. Finally, I will present results on the quantification of condensation and its generalization advantage, which includes a novel estimate of sample complexity in the best-possible scenario. These results underscore the effectiveness of the phenomenological approach to understanding DNNs, paving a way for further developing deep learning theory.

Scientific Machine Learning for Computational Oncology: From Reduced Order Modeling to Patient-Specific Models

Vitullo, Piermario; Dimola, Nunzio; Zunino, Paolo
Politecnico di Milano, Italy

The integration of scientific machine learning with model order reduction techniques offers powerful tools for addressing the complexity and multiscale nature of physiological systems in oncology. In this talk, we explore how deep learning-based reduced order models enable efficient and accurate approximations of high-dimensional parametric PDEs, particularly in microvascular and tissue models. These methods are crucial for simulating oxygen delivery, drug transport, and tissue perfusion in realistic anatomical domains under clinical constraints. We further discuss their application in developing digital twins of the tumor microenvironment for decision-making in radiotherapy.

Hybrid-Cooperative Learning for PDEs

Zuazua, Enrique

Erlangen-Nürnberg, Germany

In this talk, we present Hybrid-Cooperative (HYCO) learning, a novel strategy for constructing mathematical models of physical systems that unites physics-based modeling with machine learning. Traditional approaches are often polarized: data-driven neural networks can capture patterns but struggle with physical consistency, while high-fidelity PDE-based models ensure accuracy but are computationally demanding. HYCO bridges these paradigms by embedding them in a cooperative, game-theoretic framework that exploits their complementary strengths. By merging empirical patterns extracted from data with the structural knowledge encoded in physical laws, HYCO delivers robust and interpretable models of complex phenomena. Numerical experiments show that HYCO outperforms both purely data-driven and purely physics-based methods, particularly in regimes with sparse, noisy, or localized data, highlighting its potential as a next-generation tool for scientific computing. This talk is based on joint work with L. Liverani and T. Steynberg.

Practical Notes

1. **Arrival and departure:** Free taxis from Palermo and Trapani airports are provided on Nov 19 (arrival day) and on Nov 25 (departure day). Please note that no scientific talks are scheduled on these days.

2. **Taxi and hotel reservation:** In order to arrange taxi and reserve hotel for you (and accompanying person), the Center needs arrival times and flights numbers of all the participants. Please update the google form that was circulated around.

   You are also welcome to send this information via email: `hantil@gmu.edu`

3. **Payment:** 150 Euros per night (including hotel and food). Additional 75 Euros for any accompanying person. Payment options:

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