

RAMSES: Reduced order models; Approximation theory, Machine Learning; Surrogates, Emulators and Simulators

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BOOK OF ABSTRACTS



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INVITED SPEAKER LIST

Jan S Hesthaven

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Title: Nonintrusive reduced order models using physics informed neural networks

Abstract: In this talk, we discuss the use of artificial feedforward neural networks to enable the development of fast and accurate nonintrusive models for complex problems. We demonstrate that this approach offers substantial flexibility and robustness for general nonlinear problems and enables the development of fast reduced order models for complex applications. We also discuss how to use residual based neural networks in which knowledge of the governing equations is built into the network and show that this has advantages both for training and for the overall accuracy of the model.

Time permitting, we finally discuss the use of reduced order models in the context of prediction, i.e. to estimate solutions in regions of the parameter beyond that of the initial training. With an emphasis on the Mori-Zwansig formulation for time-dependent problems, we discuss how to accurately account for the effect of the unresolved and truncated scales on the long term dynamics and show that accounting for these through a memory term significantly improves the predictive accuracy of the reduced order model.

Miguel A. Bessa

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Title: Adaptive Self-consistent Clustering Analysis: addressing the elephant in the room

Abstract: Analysis and design of materials can be significantly empowered by machine learning when large enough databases can be generated, as highlighted in our previous work. Yet, fast and accurate predictions of materials undergoing highly localized plasticity, damage and fracture phenomena have remained unattainable. This talk discusses how a new adaptive clustering machine learning model addresses this long standing challenge and opens avenues to the data-driven design and analysis of complex heterogeneous materials.

Harbir Antil

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Title: Optimization Based Deep Neural Networks with Applications

Abstract: This talk will introduce novel optimization based deep neural networks (DNNs). In particular, DNNs with memory, which helps to overcome the vanishing gradient challenge, will be considered. The talk will also explore reducing the computational complexity of DNNs by introducing a bias ordering. Approximation properties of the DNNs will also be discussed. If time permits, a risk-averse framework for these DNNs will also be presented.

These proposed DNNs will be shown to be excellent surrogates to parameterized partial differential equations (PDEs), Bayesian inverse problems, data assimilation problems, with multiple advantages over the traditional approaches. The DNNs will also be applied to chemically reacting flows problems. The latter requires solving a system of stiff ODEs and fluid flow equations. These are highly challenging problems, for instance, for combustion the number of reactions could be significant (over 100) and due to the large CPU requirements of chemical reactions (over 95%) a large number of flow and combustion problems are presently beyond the capabilities of even the largest supercomputers.

George Em Karniadakis

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Title: A comprehensive and fair comparison of two neural operators (with practical extensions) based on FAIR data

Abstract: Neural operators can learn nonlinear mappings between function spaces and offer a new simulation paradigm for real-time prediction of complex dynamics for realistic diverse applications as well as for system identification in science and engineering. Herein, we investigate the performance of two neural operators, and we develop new practical extensions that will make them more accurate and robust and importantly more suitable for industrial-complexity applications. The first neural operator, DeepONet, was published in 2019, and the second one, named Fourier Neural Operator or FNO, was published in 2020. In order to compare FNO with DeepONet for realistic setups, we develop several extensions of FNO that can deal with complex geometric domains as well as mappings where the input and output function spaces are of different dimensions. We also endow DeepONet with special features that provide inductive bias and accelerate training, and we present

a faster implementation of DeepONet with cost comparable to the computational cost of FNO. We consider 16 different benchmarks to demonstrate the relative performance of the two neural operators, including instability wave analysis in hypersonic boundary layers, prediction of the vorticity field of a flapping airfoil, porous media simulations in complex-geometry domains, etc. The performance of DeepONet and FNO is comparable for relatively simple settings, but for complex geometries and especially noisy data, the performance of FNO deteriorates greatly. For example, for the instability wave analysis with only 0.1% noise added to the input data, the error of FNO increases 10000 times making it inappropriate for such important applications, while there is hardly any effect of such noise on the DeepONet. We also compare theoretically the two neural operators and obtain similar error estimates for DeepONet and FNO under the same regularity assumptions.

Qiang Du

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Title: Linear Multistep Methods for Learning Dynamics

Abstract: Numerical integration of a given dynamic system can be viewed as a forward problem with the learning of unknown dynamics from available state observations as an inverse problem. The latter has been around in various settings such as model reductions of multiscale processes. It has received particular attention recently in the data-driven modeling via deep/machine learning. The solution of both forward and inverse problems forms the loop of informative and intelligent scientific computing. A naturally related question is whether a good numerical integrator for discretizing prescribed dynamics is also good for discovering unknown dynamics. This lecture presents a study in the context of linear multistep methods.

Rachel Ward

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Title: The power of random matrix computations in forecasting nonlinear dynamical systems

Abstract: Making predictions from snapshots of an unknown nonlinear dynamical system is an important problem in science and engineering. It is becoming

increasingly clear that tools from machine learning such as kernel methods, sparse approximation, and randomized embeddings, have significant potential in the design of more efficient and robust algorithms for prediction. We review two recent approaches to data-driven forecasting where inspirations from machine learning have made a clear and theoretically justified impact: sparse identification of nonlinear systems and streaming kernel analog forecasting.

Yvon Maday

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Title: How to turn phenomenological models into predictive ones

Abstract: The use of accurate mathematical models to understand, predict, control natural phenomenon is not always possible either by lack of understanding, lack of knowledge, lack of time .. In these cases, as indicated by eg Tony Patera "Back-of-the-Envelope Calculations" are often proposed involving simple phenomenological models to understand the basic mechanisms of the phenomenon. In such simple models, parameters allow to fit the model and understand the sequence of certain steps that describe roughly the analysis. In this presentation, we shall present some approaches that allow improve the accuracy of such models and even, in certain cases, allow make them predictive.

Francesco Rizzi

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Title: For projection-based ROMs, is a "large" (POD) subspace always an enemy? Sometimes, it can be your friend...

Abstract: Surrogate models aim to replace expensive high-fidelity models with a lower-cost, lower-fidelity counterpart. To be useful, surrogate models should meet accuracy, certification and speed requirements. Accuracy ensures that the surrogate produces a sufficiently small error in target quantities of interest. The maximum acceptable error is typically defined by the user and is problem dependent. Certification ensures that the error (and its bounds) introduced by the surrogate can be properly quantified and characterized. Speed ensures that the surrogate evaluates much more rapidly than the full-order model, and, in general, there is a tradeoff between speed and accuracy.

Projection-based reduced-order models (pROMs) are a class of surrogate models that rely on a projection process to reduce the number of degrees of freedom in the high-fidelity model. The key feature of pROMs is that they apply a projection process directly to the equations governing the high-fidelity model, thus enabling stronger guarantees. A common denominator of most previous works on pROMs has been to find the smallest approximation space (e.g., number of POD modes) suitable for the target problem. This has been motivated by the idea that "a smaller subspace is preferable".

In this talk, I am going to argue that a large subspace is (sometimes) not only necessary for accuracy, but it can also play in your favor computationally. Specifically, I will focus on linear time-invariant (LTI) systems, for which pROMs can be considered very mature in terms of methodological and theoretical development. I will discuss various aspects to ground my statement, and finally show a numerical demonstration based on the simulation of elastic seismic shear waves in an axisymmetric domain.

Yue Yu

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Title: Learning Nonlocal Operator for Heterogeneous Material Modeling

Abstract: Constitutive modeling based on the continuum mechanics theory has been a classical approach for modeling the mechanical responses of materials. However, when constitutive laws are unknown or when defects and/or high degrees of heterogeneity present, these classical models may become inaccurate. In this work, we propose to use data-driven modeling which directly utilizes high-fidelity simulation and/or experimental data on displacement fields, to predict a material's response without the necessity of using conventional constitutive models. Specifically, the material response is modeled by learning maps between loading conditions and its resultant displacement fields, so that the network is a surrogate for a solution operator. To model the material heterogeneity, the nonlocal kernel network (NKN) is employed, which is resolution-independent and naturally embeds the material micromechanical properties and defects in the integrand. We demonstrate the performance of our method for a number of examples, including hyperelastic, anisotropic and brittle materials. As an application, we employ the proposed approach to learn glove and biotissue material models directly from experimental measurements, and show that the learnt nonlocal solution operators

substantially outperform conventional constitutive models in predicting complex material responses.

Habib N. Najm

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Title: Surrogate models and physics constraints in atomistic modeling

Abstract: Atomistic computations rely on efficient and accurate representations of the potential energy surface (PES) of atomic/molecular systems. Every point on the PES of such a system provides the potential energy for a particular geometrical arrangement of the atoms, while its negative gradient provides the forces on the constituent atoms. The evaluation of potential energy and its gradient is generally done using quantum chemical (QC) computations, which are typically expensive. As a result, PES-surrogate models, calibrated with QC computational data, are universally relied upon in applications. A key requirement for these surrogates is that they satisfy physical constraints, aside from fitting the data. In fact, the PES of an N-atom system is a function of $3N-6$ atomic coordinates, given the invariance of potential energy with solid body translations and/or rotations of the system. These, and other invariances, such as permutational invariance whereby swapping locations of two identical atoms do not change the system properties, are crucial for the effectiveness of a PES surrogate. In this talk, I will discuss a range of PES surrogate constructions, including recent developments with neural network surrogates, highlighting both input features and functional forms, with a particular focus on the means of enforcement of necessary invariances. I will also present illustrations of their use in chemical and material science problems.

Giovanni Stabile

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Title: Hybrid reduced order models for coupled heat transfer problems

Abstract: In this talk we will review recent advances in hybrid reduced order models for coupled heat transfer problems. Particularly, a parametric, hybrid reduced order method based on the Proper Orthogonal Decomposition with both Galerkin projection and interpolation based on Radial Basis Functions method is presented. The method is tested on a turbulent non-isothermal mixing case, a common flow arrangement found in many industrial applications such as nuclear reactor cooling systems. The reduced order model is derived from the 3D unsteady,

incompressible Navier–Stokes equations weakly coupled with the energy equation. For high Reynolds numbers, the eddy viscosity and eddy diffusivity are incorporated into the Reduced Order Model with a Proper Orthogonal Decomposition (nested and standard) with Interpolation (PODI), where the interpolation is performed using Radial Basis Functions. In particular the methodology has been tested with the $k - \omega$ SST turbulence model.

Benjamin Peherstorfer

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Title: Nonlinear model reduction for transport-dominated problems

Abstract: Solution manifolds induced by transport-dominated problems such as hyperbolic conservation laws typically exhibit nonlinear structures. This means that traditional model reduction methods based on linear approximations in subspaces are inefficient when applied to these problems. This presentation discusses model reduction methods for constructing nonlinear reduced models that seek approximations on manifolds, rather than in subspaces, and so lead to efficient dimensionality reduction even for transport-dominated problems. First, we will discuss an online adaptive approach that exploits locality in space and time to efficiently adapt piecewise linear approximations of the solution manifolds. Second, we present an approach that derives reduced approximations that are nonlinear by explicitly composing global transport dynamics with locally linear approximations of the solution manifolds. The compositions can be interpreted as one-hidden-layer neural networks. Numerical results demonstrate that the proposed approaches achieve speedups even for problems where traditional, linear reduced models are more expensive to solve than the high-dimensional, full model.

Federico Pichi

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Title: An overview on bifurcating phenomena for parametrized PDEs: reduced order models and applications

Abstract: This work is concerned with the analysis and the development of efficient Reduced Order Models (ROMs) for the numerical investigation of complex bifurcating phenomena held by nonlinear parametrized Partial Differential Equations (PDEs). Indeed, the reconstruction of the bifurcation diagrams, which highlight the singularities of the equations and the possible coexisting states,

requires a huge computational effort, especially in the multi-parameter context. To overcome this issue, we developed a reduced order branch-wise algorithm for the efficient investigation of such complex behaviour, with a focus on the stability properties of the solutions. Examples of applications range from Continuum Mechanics to Quantum Mechanics, passing through Fluid Dynamics. In particular we studied the Von Kármán equations for buckling plates, the Gross-Pitaevskii equations in Bose-Einstein condensates, the Hyperelastic models for bending beams and the Navier-Stokes model for the channel flow. Several issues and questions arise when dealing with the approximation and the reduction of bifurcating phenomena, we addressed them by considering new models and emerging methodologies. Among them: (i) we proposed and discussed different Optimal Control Problems (OCPs) to steer the bifurcating behaviour towards desired states; (ii) we explored the multi-physics bifurcating scenario with nonlinear elasticity based Fluid-Structure Interaction (FSI) problem; and (iii) we exploited a Neural Network approach based on the Proper Orthogonal Decomposition (POD-NN) to develop a reduced manifold based bifurcation diagram.

C. Carstensen

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Title: Half a century of Crouzeix-Raviart finite elements

Abstract: Invented in 1973 for any polynomial degree to solve the Stokes equations with piecewise divergence-free velocities, the Crouzeix-Raviart finite elements allowed various applications to nonlinear PDE over the years. In their lowest-order version, they compete with conforming schemes in elasticity and the Bingham flow. But, most unexpectedly, they allow guaranteed lower eigenvalue bounds for the Laplacian and guaranteed lower energy bounds in convex minimization; they even overcome the Lavrentiev phenomenon.

The presentation discusses contributions to the aforementioned model problems from the speaker's group and former students. The circle through all those topics will be closed with remarks on the very beginning of the Crouzeix-Raviart finite element history: Crouzeix-Raviart triangular elements are inf-sup stable for any polynomial degree provided the mesh has interior vertices. This answers a conjecture of M. Crouzeix and R. Falk after three decades.

The time restrictions permit any discussion of a medius analysis, as addressed e.g. in an overview paper by S. Brenner, or of companion operators. Only minimal

comments on the a posteriori error control and the mathematics of adaptive mesh-refining algorithms might be expected.

Elisabeth Ullmann

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Title: Rare event estimation with PDE-based models

Abstract: The estimation of the probability of rare events is an important task in reliability and risk assessment of critical societal systems, for example, groundwater flow and transport, and engineering structures. In this talk we consider rare events that are expressed in terms of a limit state function which depends on the solution of a partial differential equation (PDE). We present recent progress on mathematical and computational aspects of this problem: (1) the impact of the PDE approximation error on the failure probability estimate, and (2) the use of the Ensemble Kalman Filter for the estimation of failure probabilities. This is joint work with Fabian Wagner (TUM), Iason Papaioannou (TUM) and Jonas Latz (Heriot-Watt University).

Suncica Canic

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Title: Fluid-poroelastic structure interaction motivated by the design of a bioartificial pancreas

Abstract: In this talk we present a complex, multi-scale model, and a recent well-posedness result in the area of fluid-poroelastic structure interaction, which have helped the design of a first implantable bioartificial pancreas without the need for immunosuppressant therapy. We show global existence of a weak solution to a fluid-structure interaction (FSI) problem between the flow of an incompressible, viscous fluid, modeled by the time-dependent Stokes equations, and a multi-layered poroelastic medium consisting of a thin poroelastic plate and a thick poroelastic medium modeled by a Biot model. This is the first global (weak) solution existence result in the context of poroelastic FSI. Numerical simulations of the underlying problem showing optimal design of a bioartificial pancreas, will be presented. This is a joint work with bioengineer Shuvo Roy (UCSF), and mathematicians Yifan Wang (UCI), Lorena Bociu (NCSU), Boris Muha (University of Zagreb), and Justin Webster (University of Maryland, Baltimore County).

Oliver Dunbar

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Title: Accelerating Parameter Learning Within An Idealized Climate Model

Abstract: Current state-of-the-art climate models produce uncertain predictions, but they are typically ill-equipped to quantify this uncertainty, evidenced by apparent variability of forecasts from competing models. The source of the uncertainty is from necessary simplified physical schemes used to represent small-scale dynamics or poorly understood physics. These schemes depend upon parameters that are calibrated (often by hand) to fit data, though there may be a wide distribution of parameters that feasibly produce a given piece of (noisy) data. In climate models, the range of parameters appearing in convection and turbulent schemes dominate the uncertainty of resulting decadal predictions; it is therefore essential to quantify it for robust prediction. This task is far more computationally intensive than parameter calibration (optimization), and historically has been out of reach of climate models.

We solve a suitable Bayesian inverse problem, which aims to learn the parameter distribution from judiciously chosen time-averaged statistical data. We do this successfully by applying the Calibrate-Emulate-Sample (CES) methodology. CES is based on three steps: a first calibration step, takes the climate model as a black box input, and is well adapted to derivative-free optimization in high performance computing architectures; a second Emulation step, automates, smooths, and accelerates calculation of the black box climate model by several orders of magnitude, using Gaussian processes (a machine learning tool); a final Sampling step uses standard methods from computational statistics applied to the accelerated model to obtain a data-informed posterior distribution for parameters. I will demonstrate this work within an idealized aquaplanet general circulation model, showing how parametric uncertainty quantification on the closure parameters for convection, can provide robust predictions of climate quantities. I shall also touch on other uses of parametric uncertainty, such as directing experimental design choices.

Clayton Webster

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Title: Learning high-dimensional systems from data by nonlinear sparse approximation

Abstract: This talk will focus on nonlinear approaches to sparse approximation of complex functions in high dimensions. Of particular interest is the parameterized PDE setting, where the target function is smooth, characterized by a rapidly decaying orthonormal expansion, whose most important terms are captured by a lower (or downward closed) set. By exploiting this fact, we will present and analyze several procedures for exactly reconstructing a set of (jointly) sparse vectors, from incomplete measurements, in particular:

- weighted l_1 minimization procedure for compressed sensing, with a precise choice of weights, for overcoming the curse of dimensionality;
- mixed-norm based regularization that simultaneously reconstructs parameterized PDEs solutions over both physical and parametric domains; and
- a class of null space conditions for sparse reconstruction by virtue of nonconvex, non-separable minimizations.

Such approaches will enable the reconstruction of the entire high-dimensional solution map, with accuracy comparable to the best approximation, while utilizing an optimal number of samples. Numerical examples are provided to support the theoretical results and demonstrate the computational efficiency of the described compressed sensing methods.

Antonio Huerta

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Title: A priori and a posteriori separated solutions of parametrized incompressible flow problems

Abstract: Reduced order models are commonly employed to solve parametric problems and to devise inexpensive response surfaces to evaluate quantities of interest in real-time. This is especially interesting in the context of design and optimization cycles in which multiple queries of the same problem need to be solved for different setups (e.g., material parameters, boundary conditions, geometric configurations, ...). The proper generalized decomposition (PGD) framework is employed to construct separated solutions, explicitly depending on the parameters of interest for the problem. This talk reviews some recent contributions involving a priori and a posteriori PGD algorithms for the solution of parametrized incompressible flow problems, from microfluidics to viscous laminar and turbulent flows. The performance of a priori PGD and sampling-based a posteriori PGD is compared in terms of accuracy and computational cost for the simulation of Stokes flows in geometrically parametrized domains. This problem is

particularly challenging as the geometric parameters affect both the solution manifold and the computational spatial domain. Moreover, in order to make the a priori PGD strategy appealing for industrial applications, a non-intrusive approach exploiting OpenFOAM native solver for incompressible flows is devised for viscous laminar and turbulent Navier-Stokes equations coupled with the Spalart-Allmaras model. Numerical experiments spanning geometrically parametrised devices in microfluidics and parametrised flow control problems in internal and external aerodynamics will be presented to demonstrate the potentiality of the discussed methods.

Amanda Howard

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Title: Two multifidelity approaches for machine learning

Abstract: In this talk, I will discuss two approaches to multifidelity machine learning: physics informed Gaussian process regression and multifidelity Deep Operator Networks (DeepONets.) In both cases, there is a need for fast and accurate models using only limited high fidelity data. In the Physics-informed CoKriging (CoPhIK) machine learning method we use a fast, but inaccurate physics-based model to constrain Gaussian process regression trained on a small amount of high fidelity experimental data. We demonstrate that the CoPhIK model shows good agreement with experimental results and significant improvements over existing physics-based models. We show that the proposed model is robust as it is not sensitive to the input parameters in the physics-based model. Additionally, we will discuss multifidelity DeepONets, with the ability to train operators using low fidelity noisy or low resolution data and a small amount of high fidelity data. Our approaches allow for accurate models when training with data alone is infeasible.

Simona Perotto

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Title: Advanced techniques for new challenges in structural topology optimization

Abstract: This presentation focuses on advanced numerical techniques to address topology optimization, both from a modeling and an algorithmic perspective.

We enhance standard methods for the optimization of structures at the macro- as well as at the micro-scale.

To this end, we exploit SIMPATY algorithm, a new procedure for the design of free-form structures, which couples a standard density-based method with anisotropic mesh adaptation.

The resulting layouts are characterized by very sharp and smooth void/material interfaces, thus limiting any post-processing before the manufacturing phase.

Additionally, SIMPATY structures exhibit good mechanical performances, such as, e.g., lightness and stiffness.

The same topology optimization strategy is employed to design new metamaterials which enjoy target macroscopic mechanical properties. In such a context we resort to inverse homogenization based on topology optimization.

Then, to improve the computational performances of standard topology optimization algorithms, we propose a new method based on model reduction. We adopt the offline/online POD paradigm to predict a layout, which is then improved by SIMPATY algorithm in the spirit of a predictor/corrector approach.

Finally, we will highlight some recent developments, with a focus on the main future perspectives.

POSTER PRESENTER ABSTRACTS

Willy Haik (room 1)

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Title: A real-time variational data assimilation method with model bias identification and correction

Abstract: Real-time monitoring on a physical system by means of a model-based digital twin may be difficult if occurring phenomena are multiphysics and multiscale. A main difficulty comes from the numerical complexity which is associated to an expensive computation hardly compatible with real-time. To overcome this issue, the high-fidelity parameterized physical model may be simplified which adds a model bias. All those errors affect the effectiveness of numerical diagnostics and predictions and need to be corrected with assimilation techniques on observation data. Therefore, the monitoring of a process occurs in two stages: (1) the state estimation at the acquisition time which may be associated with an identification of the set of unknown parameters of the parametrized model and an update state which enriches the model; (2) a state prediction for future time steps with the updated model.

The present study is mainly devoted to perform the state estimation using an extension, for time dependent problems, of the Parameterized Background Data-Weak (PBDW) method introduced in [2]. This method is a non-intrusive, reduced basis and in-situ data assimilation framework for physical systems modeled by parametrized Partial Differential Equations initially designed for steady-state problems. The key idea of the formulation is to seek an approximation to the true field employing projection-by-data, with a first contribution from a background estimate computed from a reduced order method (ROM) enhanced on-the-fly, and a second contribution from an update state informed by the experimental observations (correction of model bias). Further research works [3, 1] developed an extension to deal with noisy data and a nonlinear framework. Moreover, a priori error analysis was conducted by providing a bound on the state error. In the present work, the state prediction for future time steps is also performed from an evaluation of the updated model and an extrapolation of the time function from the tensor-based decomposition (SVD) on prior updates. Numerical experiments are conducted on a thermal conduction problem in the context of heating on a Printed Circuit Board (PCB) with different cases of model

bias: a bias on heat source, a biased boundary condition and an error on the constitutive equation. These numerical experiments show that the method significantly reduces the online computational time while providing relevant state evaluations and predictions. We thus illustrate the considerable improvement in prediction provided by the hybrid integration of a best-knowledge model and experimental observations.

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- [2] Y. Maday, A. T. Patera, J. D. Penn, and M. Yano. A parameterized-background data-weak approach to variational data assimilation: formulation, analysis, and application to acoustics. *International Journal for Numerical Methods in Engineering* , 102(5):933965, 2015.
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Jeffrey Kuan (room 2)

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Title: A stochastic fluid-structure interaction problem describing Stokes flow interacting with a membrane

Abstract: We present a recent well-posedness result for a stochastic fluid-structure interaction model. We study a fully coupled stochastic fluid-structure interaction problem, with linear coupling between Stokes flow and an elastic structure modeled by the wave equation, and stochastic noise in time acting on the structure. Such stochasticity is of interest in applications of fluid-structure interaction, in which there is random noise present which may affect the dynamics and statistics of the full system. We construct a solution by using a new splitting method for stochastic fluid-structure interaction, and probabilistic methods. To the best of our knowledge, this is the first result on well-posedness for fully coupled stochastic fluid-structure interaction. This is joint work with Sunčica Čanić (UC Berkeley).

Sascha Ranftl (room 3)

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Title: On the uncertainty of the surrogate – a Bayesian estimate

Abstract: Surrogate models are commonly chosen and deemed trustworthy, or not trustworthy, based on a variety of measures and diagnostics, before being used for uncertainty propagation or sensitivity analysis. A limitation of this binary view is: i) if the surrogate is not trustworthy, it is obsolete; ii) if the surrogate is trustworthy, then the contribution of the uncertainty of the surrogate itself to the inferential uncertainty on the quantity of interest (QoI) is neglected, as was discussed e.g. by [1] for Polynomial Chaos Expansions. Here, we seek to quantify trustworthiness beyond this binary judgement, and so introduce the surrogate’s trustworthiness, or rather uncertainty, as a continuous, unknown variable. Then, we can also investigate the additional inferential uncertainty caused by the uncertainty of the surrogate itself.

For a generalized linear surrogate model, i.e. linear in the surrogate parameters, and a Student-t likelihood for the simulation data, we find closed forms for the Bayesian estimates for the surrogate’s uncertainty [3]. From this follow semi-closed forms for the uncertainty of the QoI, where terms are identified as input-parametric uncertainty and inferential uncertainty, i.e. the later being caused by the uncertainty of the surrogate itself. The special cases of Polynomial Chaos Expansions or Gaussian Process Regression are discussed. Lastly, we demonstrate a numerical example where surrogate uncertainties are in part negligible and in part non-negligible [2].

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Philip Edel (room 4)

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Title: A heuristic a posteriori error indicator for reduced basis approximations to unconditionally stable parameterized PDEs

Abstract: Rigorous a posteriori error analysis of reduced basis approximations to affinely parametrized partial differential equations classically relies on the construction of lower bounds for the inf-sup stability constant. Despite efficient methods such as the Successive Constraints Method [2, 1], a significant amount of large-scale generalized eigenvalue problems must still be solved in the process, which can lead to prohibitive computational costs.

In this work, we propose heuristic a posteriori error indicators for both the reduced basis absolute and relative approximation errors. The proposed methodology is very efficient and does not require solving any large-scale generalized eigenvalue problems. However, the scope is restricted to a specific framework; namely, the parametrized partial differential equation must be unconditionally well-posed (i.e., there must be no "resonant" parameters) and the inf-sup stability constant must not depend too significantly on the parameters. We provide a criterion for detecting whether a given parametrized partial differential equation fits – or does not fit – this framework.

We show an example in electromagnetism, with a wavenumber-parametrized radiating antenna problem and an example in an aeroacoustic flow problem, with parametrized impedance boundary conditions. In both examples, the proposed heuristic performs very well.

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Margarita Chasapi (room 5)

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Title: Reduced ordered modelling for parametric multi-patch isogeometric analysis

Abstract: This contribution deals with reduced basis methods for IsoGeometric Analysis (IGA) in the context of parametrized partial differential equations. The introduction of IGA [1] enables a unified simulation framework based on a single geometry representation for both design and analysis. The coupling of reduced basis methods with IGA has been motivated in particular by their combined capabilities for geometric design and solution of parametrized geometries [2]. In most applications, the geometry is modelled with multiple patches in IGA [3]. Based on an existing component-based reduced basis method [4], we show a reduced order procedure for coupling multiple patches in a parametrized setting, where multiple evaluations are performed for a given set of physical and geometrical parameters. We consider the case where adjacent patches are conforming. At the interface a static condensation procedure is employed, whereas in the interior a reduced basis (RB) approximation enables an efficient offline-online decomposition. The full order model over which we set up the RB formulation is based on NURBS approximation, whereas the reduced basis construction relies on a certified greedy-based approach. In case of parametrized geometries, a suitable Empirical Interpolation Method (EIM) [5] enables to recover an affine parametric dependence. We illustrate the approach by considering linear elliptic partial differential equations as model problems. Numerical examples provide insight and preliminary results on the procedure.

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Gabriel F. Barros (room 6)

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Title: Enhancing Dynamic Mode Decomposition Data Pipeline

Abstract: Dynamic Mode Decomposition (DMD) is an equation-free data-driven method that has attracted considerable attention recently. DMD can easily identify coherent spatio-temporal structures in data and provide

reasonably accurate predictions for certain problems. Also, DMD has been used in a wide range of applications, from control systems to surrogate models. It is well known that data quality is directly related to the performance of a machine learning model. In this study, we focus on an enhanced data pipeline in Python for DMD. We automate the extraction and assembly of snapshots obtained from numerical simulations on standard finite element method libraries, such as LibMesh, FreeFem++, and FEniCS. The input consists

of snapshots stored in HDF5 or VTK files and PNG images, while the output is a NumPy 2D array that can be coupled to any standard DMD engine (for instance, PyDMD). Our framework also decompresses lossless and lossy compressed snapshots and enables data streaming

instead of batches for real-time analysis. We present our results in two CFD applications: the reconstruction of a bubble rising and a particle-laden flow simulation. For the first example, we generate PNG files for each snapshot, and DMD is evaluated incrementally

for each file added to the directory. For the second example, the snapshots are stored on HDF5 files, compressed to reduce disk storage, and decompressed for

processing. For both simulations, we consider LibMesh as our finite element framework.

Mattia Manucci (room 7)

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Title: Contour Integral Methods and Reduced Basis for parametric dynamical problems

Abstract: We discuss a reduced basis method for linear evolution PDEs, which is based on the application of the Laplace transform. The main advantage of this approach consists in the fact that, differently from time stepping methods, like Runge-Kutta integrators, the Laplace transform allows to compute the solution directly at a given instant, which can be done by approximating the contour integral associated to the inverse Laplace transform by a suitable quadrature formula. In terms of the reduced basis methodology, this determines a significant improvement in the reduction phase, like the one based on the classical proper orthogonal decomposition (POD), since the number of vectors to which the decomposition applies is drastically reduced as it does not contain all intermediate solutions generated along an integration grid by a time stepping method. We show by some illustrative parabolic PDEs arising from finance the effectiveness of the method and also provide some evidence that the method we propose, when applied to a simple advection equation, does not suffer the problem of slow decay of singular values which instead affects methods based on time integration of the Cauchy problem.

Raul Bravo (room 8)

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Title: A local POD-HROM framework for fast and accurate numerical simulations

Abstract: One of the classical techniques to construct reduced order models ROM is the proper orthogonal decomposition POD, which employs a linear subspace to approximate the curved submanifold over which the solution evolves.

POD has demonstrated to efficiently provide low-dimensional surrogates for the original high-dimensional systems. However, using a single linear subspace for the approximation can result in large ROMs. The aim of this work is to present a reduced-order model framework which utilizes an unsupervised learning technique based on the concept of local PCA in order to construct a set of linear

subspaces tailored for the approximation of specific sections of the solution manifold, resulting in smaller and faster ROMs.

In detail, the hyper-reduction technique employed for dealing with the nonlinear term is an adapted version of the ECM algorithm presented in [1], and later refined in [2], which exploits the local bases to reduce the number of selected HROM elements. Moreover, we propose a procedure to construct the bases which is less prompt to overfitting the training data, compared to the commonly used approaches. The benefits of the application of such a methodology is demonstrated using realistic geometries in the FEM software KratosMultiphysics [3].

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Title : A computational method for model reduction in index-2 dynamical systems for Stokes equations

Abstract : Our goal is to describe a Krylov based projection method in order to reduce high-order dynamical systems. We focus on differential algebraic equations (DAEs) of index-2 that arise from spatial discretization of Stokes equations. An efficient algorithm based on a projection technique onto an extended block Krylov subspace that appropriately allows us to construct a reduced order system is described. Numerical results are provided to confirm the performance of the derived method compared with other known ones.

Bernardo Ferreira (room 10)

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Title: Clustering adaptivity towards fast and accurate modeling of localized phenomena

Abstract: The recent paradigm coined Integrated Computational Materials Engineering (ICME) provides a framework to design materials and structures that meet high-performance criteria and fulfill safety standards at reduced development costs.

This framework integrates horizontal process-structure-property-performance relationships with vertical multi-scale process-structure and structure-property modeling over different scales. However, the true engineering applicability of such a computational framework demands the ability to perform accurate and efficient predictions of the material multi-scale behavior. Despite the high accuracy of the direct numerical simulation (DNS) methodologies, such as the Finite Element Method, the associated computational cost becomes prohibitive when dealing with multiple coupled scales, modeling complex material systems, or building reliable material response databases.

The recent family of clustering-based reduced-order models (CROMs) [1, 2] addresses this challenge by providing an appropriate balance between accuracy and computational cost. These methods rely on unsupervised machine learning clustering algorithms to perform a significant material model compression and have shown promising results in the multi-scale modeling of heterogeneous materials. Nonetheless, so far, the training-stage material clustering has remained constant through the actual problem solution, i.e., CROMs lack the required adaptivity throughout a general deformation path. This precludes their ability to accurately predict the onset and propagation of highly localized history-dependent phenomena such as plastic strain localization, damage and fracture.

In this context, we propose an Adaptive Clustering-based Reduced-Order Modeling (ACROM) framework [3] that enables the material clustering of any CROM to evolve dynamically throughout the actual equilibrium problem solution. The coined Adaptive Self-Consistent Clustering Analysis (ASCA) [3], the adaptive counterpart of the Self-Consistent Clustering Analysis (SCA) method [1], is shown to efficiently capture highly localized plastic yielding by ensuring an optimum clustering refinement on regions exhibiting steeper field gradients. This novel approach is believed to open important avenues in computational material design and sets the stage to explore adaptivity in the context of clustering-based reduced-order modeling.

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Title: Nanomechanical web-like resonator with ultralow dissipation found by Bayesian optimization

Abstract: Designing nanomechanical resonators with quality factors above a billion at hundreds of kHz has remained elusive due to bending losses at the clamping region. Yet, such resonators would achieve unprecedented force sensitivities and signal-to-noise ratios required for exotic applications such as dark matter sensing, extreme sensing of magnetic or electric fields, and other quantum optomechanical experiments. Inspired by nature and guided by machine learning, we explored a new web-like resonator concept and found a unique flexible hinge soft clamping mechanism that increased the quality factor significantly. It was found by searching beam-like structures' lower-order general vibration modes, overcoming the scarcity of data by Bayesian optimization. We fabricated a 3 mm optimized web-like resonator and measured a quality factor surpassing 1.8 billion around 130 kHz at room temperature. These figures of merit can only be seen in state-of-the-art cantilevers for atomic force microscopy when they are at cryogenic conditions. This work demonstrates that data-scarce machine learning and optimization algorithms can play a key role in discovering new geometries and exploring new physics in quantum optomechanical devices.

Joshua Hudson (room 12)

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Title: Detecting stiffness in ResNets inspired by Neural ODEs

Abstract: Neural ODEs (NODEs) emerge as the limit of Residual Neural Networks (ResNets) as the number of layers tends to infinity. For this reason, studying NODEs can provide insights into the role of depth in network architecture. In addition, differential equations are well-studied: many mathematical insights are available

that can be applied to NODEs to better understand the behavior of neural networks, improve their generalization, and develop more efficient training algorithms.

In the spirit of using NODEs as conduits for intuition from differential equations, we examine the role of stiffness as a means of regularization for ResNets. First, we give a motivational example describing stiffness for differential equations. Then, we describe a heuristic for quantifying the stiffness of a ResNet architecture encountered over an input sample, which can then be used as a penalty during training as a novel means of regularization.

Wayne Isaac Tan Uy (room 13)

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Title: Establishing trust in models learned from data via non-intrusive model reduction with operator inference and re-projection

Abstract: Learning dynamical-system models from data is a fundamental task that is often the first step in simulating physical systems if governing equations are unknown; however, establishing guarantees about the generalization of the learned models remains challenging. We contribute an approach that recovers from data the very same low-dimensional models that are obtained via projection of the governing equations onto low-dimensional spaces in classical model reduction. The key ingredient is sampling data that represent Markovian dynamics in low-dimensional spaces rather than dynamics in high-dimensional spaces. The recovery guarantee acts as a bridge between learning dynamical-system models from data and classical model reduction techniques. In particular, it enables carrying over the rich theory about stability, generalization and error bounds of classical reduced models to low-dimensional models learned from data. Building on the recovery guarantee, we (1) derive computable (a posteriori) generalization bounds for predictions made with the learned models and (2) propose a design-of-experiments scheme to reduce prediction errors due to noise in training data. Thus, our approach establishes trust in the learned models by providing certificates and guarantees that are essential for safely making high-consequence decisions from data in, e.g., engineering and medical applications.

Davide Calabrò (room 14)

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Title: "A deep learning approach for detection and localization of leaf diseases"

Abstract: Disease detection in plants has recently become a crucial point for achieving a more sustainable agriculture, which is needed to satisfy the ever-increasing demands for food in the coming decades. An early detection of the disease enables a timely intervention to prevent the disease from spreading to the rest of the plant and, thereafter, to the entire crop. Moreover, a precise disease localization allows to confine the use of pesticides and other chemical treatments to small strategically selected areas of the plant.

We developed a leaf disease detection method based on deep learning. An autoencoder is trained only on images of healthy leaves to learn the typical features of a disease-free leaf. This training allows the autoencoder to accurately reconstruct only images of healthy leaves as an output, regardless of the health condition of the input image. The mismatch between input and output images delivers the segmentation of the anomalies on the leaf, which in turn can be used to classify whether the leaf provided as an input is healthy or not.

Unlike classic supervised deep-learning methods, the proposed procedure is characterized by two advantages: (i) it does not need images whose anomalies have previously been segmented, and (ii) it does not require an a priori knowledge about the type of disease that may affect the leaf.

We compared the proposed approach with a leaf-segmentation based state-of-the-art method, on two datasets. Experimental results show that our method outperforms the competitor in terms of Area Under Curve (AUC) score.

Yiming Fan (room 15)

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Title: Bayesian Nonlocal Operator Regression (BNOR): Towards the Characterization of Uncertainty in Heterogeneous Materials

Abstract: We consider the problem of modeling heterogeneous materials where small-scale dynamics and interactions affect the global behavior; these situations are ubiquitous in engineering and scientific applications. The material's microstructure, properties, interfacial conditions, and operating environments cause variability in the material's response; hence it is often non-practical, if not impossible, to provide quantitative characterization for each sample. This fact calls for a stochastic modeling of the variability and characterization of the material responses through uncertainty quantification.

The goal of this work is to develop a Bayesian framework to characterize the uncertainty of material response when using a nonlocal, homogenized model to

describe wave propagation through heterogeneous, disordered materials. Our approach is based on the nonlocal operator regression (NOR) technique, where a nonlocal homogenized model is learnt and is proved to reproduce wave propagation on distances that are much larger than the size of the microstructure, and Bayesian inference. Specifically, we use a MCMC method to predict the probability distribution of the nonlocal constitutive law that embeds the material's properties. As an application, we consider the wave propagation problem in a heterogeneous bar with randomly generated microstructure layers. In particular, we apply the proposed approach to model the stress wave propagation and provide a characterization of the uncertainty in the material microstructure. With several numerical tests, we illustrate the effectiveness of our approach in predicting the posterior distribution of the optimal nonlocal model.

Mamikon Gulian (room 16)

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Title: Partition of unity networks: deep hp-approximation

Abstract: Approximation theorists have established best-in-class optimal approximation rates of deep neural networks by utilizing their ability to simultaneously emulate partitions of unity and monomials. Motivated by this, we propose partition of unity networks (POUnets) which incorporate these elements directly into the architecture. Classification architectures of the type used to learn probability measures are used to build a meshfree partition of space, while polynomial spaces with learnable coefficients are associated to each partition. The resulting hp-element-like approximation allows use of a fast least-squares optimizer, and the resulting architecture size need not scale exponentially with spatial dimension, breaking the curse of dimensionality. An abstract approximation result establishes desirable properties to guide network design. Numerical results for two choices of architecture demonstrate that POUnets yield hp-convergence for smooth functions and consistently outperform MLPs for piecewise polynomial functions with large numbers of discontinuities.

Angela Monti (room 17)

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Title: A POD-DEIM correction approach for coupled PDE problems with Turing pattern formation

Abstract: We are interested in the approximation of the so-called Turing patterns that are spatially non-homogeneous stationary solutions of reaction-diffusion systems of partial differential equations (RD-PDE). The computational challenges in the numerical approximation of Turing patterns are related to: i) long time integration to identify the final pattern as an asymptotic solution of the PDE system; ii) a large and finely discretized spatial domain to recognize the pattern structure [3].

For these reasons, we apply reduced order methods (ROM) to obtain a low-dimensional model that preserves the essential features of the RD-PDE system. In particular, when we deal with coupled RD-PDE problems in presence of Turing solutions, POD (Proper Orthogonal Decomposition) [4] shows an unstable error decay over the dimension of the reduced model.

To overcome this instability, by following the approach in [1], we propose a POD-Galerkin version with a correction term. To further improve the accuracy of the reduced model, we apply the Discrete Empirical Interpolation Method (DEIM, [2]) to the correction term.

Numerical results show the accuracy and efficiency of the proposed method for the Schnakenberg model, prototype of RD system with Turing pattern formation, and for the DIB electrodeposition RD system for battery modelling [3,5].

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Title: Data-driven learning of Reynolds stress tensor using nonlocal models

Abstract: The Reynolds-averaged Navier-Stokes (RANS) equations are well-known for their efficiency in simulating turbulent flows but require a model for the nonlinear Reynolds stress tensor to close the system of equations. While closures are traditionally obtained via introduction of transport models involving local differential operators, recent work has suggested that nonlocal interactions are important to correctly treat turbulent statistics. To this end, a machine learning framework is pursued to discover nonlocal closures from data.

This work presents a data-driven approach to learn a nonlocal model for the Reynolds stress tensor from high-fidelity direct numerical simulation datasets. In this approach, the Reynolds stress tensor is modeled as an integral operator acting over a finite range of lengthscales, and therefore is capable of capturing important aspects of the small-scale anisotropic behavior in turbulent flows. To obtain a nonlocal stress tensor that efficiently and accurately captures turbulent behavior, we propose an optimization-based operator regression approach where the residual of the RANS equations is minimized to calibrate the RANS closure to direct numerical simulation (DNS) data. Different nonlocal kernels are investigated and the resulting accuracy of optimal Reynolds stress closures are demonstrated for fully-developed internal flows.

Pierre Jacquet (room 19)

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Title: Fluid flow data assimilation from reduced order models and sparse measurements

Abstract: Monitoring a patient's cardiovascular disorder can be burdensome, expensive and lead to stressful examinations that can perturb the patient's state. Cardiovascular system digital twins allow to complete medical analyses by limiting the intrusive examinations. However, these simulations are expensive and hardly the expertise of the medical profession.

Reduced Order Models (ROM) and data assimilation can overcome these difficulties and offer extremely-fast analysis tools. On the one hand, pure data-driven fluid dynamics models (e.g., pure machine learning) may not be accurate or robust enough. On the other hand, pure physics-based model simulations (e.g. LES, RANS)

are often too slow for real-time applications and might miss some important spatio-temporal scale information. ROM are hence a good trade-off (see e.g. [1] for haemodynamic applications). In particular, the Proper Orthogonal Decomposition (POD)–Galerkin method relies on physical equations while constraining the solution to live in a small subspace learned from data.

Another challenging requirement for model–measurement coupling is the dynamical model’s accuracy quantification at the specific measurement locations. The “dynamics under location uncertainty” is a stochastic fluid mechanics framework designed for this purpose [2]. Thus, several model simulations are run in parallel, covering all the possible future states of the system, and at the end of the pipeline, with each observation a non-linear data assimilation scheme corrects the error on-the-fly.

This reduced data assimilation procedure has been applied to a 3-dimensional cylinder wake flow at Reynolds number 300 [3]. Without initial condition information, our on-line data assimilation technique simulates the stochastic low-dimensional model and assimilates measurements on-the-fly. As a benchmark, the same procedure was done with a reduced order model with optimally fitted eddy viscosity and additive noise, and our method surpasses its flow estimation capabilities. Our methodology is now implemented on the OpenFOAM-based ROM library ITHACA-FV [4]. We are now considering the hyper-reduction (DEIM [5]) of non-polynomial terms appearing in turbulence models (e.g., LES). Therefore, this technology allows us to consider more turbulent phenomena and raises the prospect of wind energy and aeronautical applications.

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Francesco Romor (room 20)

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Title: Nonlinear manifold ROM with Convolutional Autoencoders and Reduced Over-Collocation method.

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

Ivan Prusak (room 21)

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Title: A reduced order model for the optimisation-based domain decomposition algorithm for the incompressible Navier-Stokes equations

Abstract: In the last few decades, there has been an explosion in the numerical analysis for Computational Fluid Dynamics, and many different methods have been proposed to solve Navier-Stokes equations numerically. Nevertheless, there is still an immense need to reduce the computational costs of the simulations. Domain Decomposition Methods and Reduced-order models are ones of such techniques. The former allows splitting the solves to usually much more computational simulations (due to solving problems of much smaller scales and usually with much simpler geometry) and the latter is an effective tool in the reducing cost of simulation of time-dependent and/or parametrised problem. In our work we tried to combine both approaches. In particular, we consider an optimisation-based

domain-decomposition algorithm for the incompressible Navier–Stokes equations and propose a reduced-order model for the resulting optimal control problem. The reduced-order model for the optimisation is based on Proper Orthogonal Decomposition technique and the presented methodology is tested on the stationary backward-facing step fluid dynamics test case. The simulations showed great performance in the sense of drastically reducing both the dimension of the resulting optimisation and the number of iterations of the optimisation algorithm.

Anna Ivagnes (room 22)

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Title: Data enhanced reduced order methods for turbulent flows

Abstract: The focus of the talk is on reduced order models (ROMs) applied to the study of turbulent flows. To ensure a low ROM computational cost, relatively few basis functions are usually considered to build the model. However, when a marginally-resolved modal regime is adopted, the number of modes is enough to capture the underlying dynamics of the system, but the standard Galerkin-ROM yields inaccurate results. In order to improve the results in terms of velocity and pressure accuracy, the ROM approach is combined with data-driven techniques.

Specifically, we propose the first pressure-based data-driven variational multiscale ROM, in which the available data are used to construct correction/closure terms for both the momentum and the continuity equations.

These terms are aimed at reintroducing the contribution of the neglected modes in the reduced equations, and are computed by solving an optimization problem between the exact correction term and a postulated ansatz chosen to model it.

The case study considered in our numerical investigation is the two-dimensional flow past a circular cylinder and two different approaches for the velocity–pressure coupling are used. In the first one, additional supremizer modes are added to the velocity POD space to ensure the fulfillment of the inf-sup condition. In the second approach, the continuity equation is replaced by the pressure Poisson equation, leading to the formulation of novel pressure correction terms.

The techniques we discuss yield significantly more accurate results than the standard ROM and, more importantly, than the original data-driven variational multiscale ROM (i.e., without pressure components).

In particular, our numerical results show that adding the correction/closure term in the momentum equation significantly improves both the velocity and the pressure approximations. On the other hand, adding the novel pressure

correction/closure terms only improves the pressure approximation, leading to a better reconstruction of important engineering quantities, such as lift and drag.

Laura Meneghetti (room 23)

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Title: Reduced Convolutional Neural Networks for image recognition in professional appliances.

Abstract: In the last decades artificial intelligence became a popular tool, increasingly exploited in several scientific and engineering fields such as computer vision, natural language processing, robotics, and speech recognition. The continuous demand for application to more complex tasks has forced the architectures to go deep, leading also to an increasing number of parameters that needed to be calibrated during the training phase. Therefore, the employment of deep neural networks, such as Convolutional Neural Networks, in industries opened several computational issues since these architectures have usually to operate in embedded systems with limited hardware [3]. The resulting memory constraints have led to the creation of a reduction strategy for the development of a reduced version of an Artificial Neural Network and in particular of a Convolutional Neural Network.

In our work [4] we propose an extension of [1] for dimensionality reduction of CNNs, exploring both the active subspace (AS) property and the proper orthogonal decomposition (POD) technique. The reduced network is obtained by splitting the original one in two different nets connected by the reduction method: the first one obtained by retaining a certain number of layers of the original CNN and a second one that deals with the classification of the features extracted by the previous part. We then present the numerical results obtained by applying such method to the problem of image recognition, using as test datasets CIFAR-10 and an application-specific one. In particular we compare the final outcome of the original CNN in exam (VGG-16 [2]) with that of its reduced version in terms of final accuracy, memory allocation, speed of the procedure.

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RAMSES: Reduced order models; Approximation theory, Machine Learning; Surrogates, Emulators and Simulators

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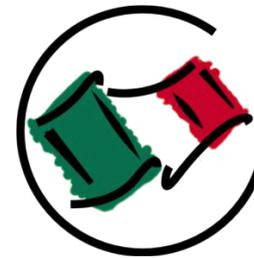
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