Weizhu BAO

Modeling, analysis and simulation for degenerate dipolar quantum gas

In this talk, I will present our recent work on mathematical models, asymptotic analysis and numerical simulation for degenerate dipolar quantum gas. As preparatory steps, I begin with the three-dimensional Gross-Pitaevskii equation with a long-range dipolar interaction potential which is used to model the degenerate dipolar quantum gas and reformulate it as a Gross-Pitaevskii-Poisson type system by decoupling the two-body dipolar interaction potential which is highly singular into short-range (or local) and long-range interactions (or repulsive and attractive interactions). Based on this new mathematical formulation, we prove rigorously existence and uniqueness as well as nonexistence of the ground states, and discuss the existence of global weak solution and finite time blowup of the dynamics in different parameter regimes of dipolar quantum gas. In addition, a backward Euler sine pseudospectral method is presented for computing the ground states and a time-splitting sine pseudospectral method is proposed for computing the dynamics of dipolar BECs. Due to the adoption of new mathematical formulation, our new numerical methods avoid evaluating integrals with high singularity and thus they are more efficient and accurate than those numerical methods currently used in the literatures for solving the problem. In addition, new mathematical formulations in two-dimensions and one dimension for dipolar quantum gas are obtained when the external trapping potential is highly confined in one or two directions. Numerical results are presented to confirm our analytical results and demonstrate the efficiency and accuracy of our numerical methods. Some interesting physical phenomena are discussed too.

Zhenning CAI

Linear regularized 13-moment equations for rarefied gas dynamics

We develop the regularized 13-moment (R13) equations in the linear regime for rarefied gas dynamics with general collision models. The equations are modeled by a novel model reduction method that generalizes the classical Chapman-Enskog expansion. Applying this method to the Boltzmann equation, which is a six-dimensional time-dependent equation, we can derive a reduced model with only 13 three-dimensional equations up to the super-Burnett order. The validity of our model is verified by benchmark examples for the one-dimensional channel flows.

Tomas CHACON REBOLLO

Mathematics-based and physics-based Reduced Basis solution of LES Smagorinsky turbulence models.

Abstract: In this talk we address the ROM solution of turbulent flows through the reduction of LES turbulence models. On one hand, we build certified reduced basis for the Smagorinsky turbulence model based upon mathematics-based a priori error estimates. We present some application of this method, in particular to the solution of thermal flow with both physical and geometrical parameters and to the thermal comfort optimization of cloisters. On another hand, we build reduced basis for the same model by means of a physics-based a priori error estimator, that measures the distance of a trial solution w.r.t. the theoretical $k^{-5/3}$ spectrum of turbulence in statistical equilibrium. We present some applications of this method to academic turbulent flows with well-developed inertial spectrum.

Xiaoli CHEN
Learning reduced stochastic dynamical systems and application in polymer dynamics

In this talk, I will discuss how to use machine learning methods to learn the stochastic problem. To begin, I will introduce how to use stochastic OnsagerNet to learn closure dynamical systems. We propose a general machine learning approach to construct reduced models for noisy, dissipative dynamics based on the Onsager principle for non-equilibrium systems. Then I will demonstrate our method by modelling the folding and unfolding of a long polymer chain in an external field - a classical problem in polymer rheology - though our model is suitable for the description of a wide array of complex, dissipative dynamical systems arising in scientific and technological applications.

Francisco CHINESTA
Physics-Based and Data-Driven Hybrid Modelling for Decision-making in Critical Urban Systems

Critical systems, as for example civil and industrial infrastructures, transport networks, multi-agent systems, grids, … and more generally complex systems of systems, need for efficient diagnosis and prognosis procedures, able to encompass rapidity and accuracy, to make the right decision at the right moment.
Existing paradigms exhibit limitations for addressing such a challenging scenario. Models based on physics and existing knowledge, fail to address large systems, exhibiting rich and complex behaviors and involving a noticeable degree of uncertainty with different origins, of epistemic nature, due to fluctuating behaviors and variability, and because of human intervention.
On the other hand, the alternative route based on the exclusive use of collected data also fails because of the fact that, in many cases, data is not abundant enough. Critical large infrastructures are not equipped of millions of sensors.
Thus, allying these two worlds could be an opportunity: the one of the physics manipulated by adequate methods of applied mathematics, and the one of the data, manipulated at its turn by machine learning and artificial intelligence techniques (physics informed). Within this hybrid framework, one expects reducing the amount of needed data, transforming the big-data paradigm into a smarter one.

Eric CHUNG
A robust two-level overlapping preconditioner for Darcy flow in high-contrast media

In this talk, we present a two-level overlapping domain decomposition preconditioner for solving linear algebraic systems obtained from simulating Darcy flow in high-contrast media. Our preconditioner starts at a mixed finite element method for discretizing the partial differential equation by Darcy's law with the no-flux boundary condition and is then followed by a velocity elimination technique to yield a linear algebraic system with only unknowns of pressure. Then, our main objective is to design a robust and efficient domain decomposition preconditioner for this system, which is accomplished by engineering a multiscale coarse space that is capable of characterizing high-contrast features of the permeability field. A generalized eigenvalue problem is solved in each non-overlapping coarse element in a communication- free manner to form the global solver, which are accompanied by local solvers originated from additive Schwarz methods but with a non-Galerkin discretization to derive the two-level preconditioner. We provide a rigorous analysis indicating that the condition number of the preconditioned system could be bounded above with several assumptions. Extensive numerical experiments with various types of three-dimensional high-contrast models are exhibited. In particular, we study the robustness against the contrast of the media as well as the influences of numbers of eigenfunctions, oversampling sizes, and subdomain partitions on the efficiency of the proposed preconditioner. Besides, strong and weak scalability performances are also examined. The work is partially supported by the Hong Kong RGC General Research Fund (Projects: 14305222 and 14304021).

Elías CUETO

Thermodynamics of learning physical phenomena

Thermodynamics could be seen as an expression of physics at a high epistemic level. As such, its potential as an inductive bias to help machine learning procedures attain accurate and credible predictions has been recently realized in many fields. We review how thermodynamics provides helpful insights in the learning process. At the same time, we study the influence of aspects such as the scale at which a given phenomenon is to be described, the choice of relevant variables for this description or the different techniques available for the learning process.

We review how thermodynamics can be considered as a high epistemic level inductive bias for techniques of machine learning physical phenomena. Starting with methods imposing conservation laws (particularly, in Hamiltonian or Lagrangian settings) we analyze how the principles of thermodynamics can also be used advantageously for dissipative phenomena. Beginning with methods that simply relax the requirements of conservation and/or equivariance, we see how thermodynamic formalisms can be developed that ensure by construction, either in soft or hard ways, the fulfillment of the principles of thermodynamics: conservation of energy in closed systems and non-negative entropy production. In any case, the main advantage of these approaches is that the resulting accuracy of these methods is considerably improved, or otherwise, the amount of necessary data is drastically minimized.

My Ha DAO

Reduced Order Modelling (ROM) and Physics-Informed Neural Nets (PINN): Research and Application

With the (re-) emergence of Artificial Intelligence (AI) and its successful applications recently, the needs of fast modelling tools for design optimization and digital twining in engineering applications have been becoming a focus in numerical modelling and simulation. Unlike traditional AI applications such as language and image processing, engineering applications require solutions with not only accuracy but also reliability and interpretability. Data availability is also a bottleneck in engineering applications, but on the other hands, we do know the underlying physics often in forms of the governing equations. Making use of the underlying physics and the power of data-mining methods, we can build good models that could serve our needs.

In this talk, I will share our developments of the ROM and PINN methods with a focus on practical applications. The developments range from incorporation of numerical approximation in standard PINNs to breakdown of a large system into components in ROM with an application on offshore wind turbine, and adaptation of ROM-based Operator Inference on a real-world data of ocean wave propagation.

Chenyu DONG
Predictability analysis of weather and climate on reduced manifolds

Climate of earth is widely known as a multi-scale, highly nonlinear and chaotic system, and numerical models describing them are extremely expensive computationally. In order to reduce the computation cost and have a better understanding of the underlying physical processes, many data-driven dimensionality reduction methods have been proposed to capture coherent modes of variability from the latest high quality reanalysis data in recent years. Despite extensive research focused on the explainability of the spatial patterns, the predictability of the temporal component is not well studied. In this research, we proposed a fully data-driven predictability analysis framework for weather and climate on reduced manifolds. This framework employs both model-free and model-based predictability analysis for different reduced spaces obtained by Proper Orthogonal Decomposition(POD), Spectral Proper Orthogonal Decomposition(SPOD) and Latent Dirichlet Allocation(LDA). This research also studies how climate drivers will impact the predictability of specific patterns or modes and whether there is a connection between high-impact extreme events and the predictability of specific modes.

Traian ILIESCU
Regularized Reduced Order Models (Reg-ROMs) for Turbulent Flows

Over the past decade, several closure and stabilization strategies have been developed to tackle the ROM inaccuracy in the convection-dominated, under-resolved regime, i.e., when the number of degrees of freedom is too small to capture the complex underlying dynamics. In this talk, I will survey regularized reduced order models (Reg-ROMs), which are simple, modular stabilizations that employ ROM spatial filtering of various terms in the Navier-Stokes equations (NSE) to alleviate the spurious numerical oscillations generally produced by standard ROMs in the convection-dominated, under-resolved regime. I will focus on two different types of Reg-ROM strategies: (i) the evolve-filter-relax ROM (EFR-ROM), which first filters an intermediate velocity approximation, and then relaxes it; and (ii) the Leray-ROM (L-ROM), which filters the convective term in the NSE. Throughout my talk, I will highlight the impact made by ROM spatial filtering on the Reg-ROM development. Specifically, I will talk about the two main types of ROM spatial filters: (i) the ROM differential filter; and (ii) the ROM projection. I will also propose two novel higher-order ROM differential filters. An important role played in ROM spatial filters and Reg-ROMs is the ROM lengthscale. In my talk, I will put forth a novel ROM lengthscale, which is constructed by leveraging energy balancing arguments. I emphasize that this novel energy-based lengthscale is fundamentally different from the standard ROM lengthscale introduced decades ago, which is based on simple dimensional arguments. Finally, I will illustrate the success achieved by ROM spatial filters and Reg-ROMs in under-resolved numerical simulations of the flow past a cylinder and turbulent channel flow.

Throughout my talk, I will discuss numerical analysis results proved for the Reg-ROMs that we proposed, including fundamental properties, e.g., stability, convergence, and parameter scalings. I will also present some of the challenges and open questions in the development of rigorous numerical analysis foundations for ROM closures and stabilizations.

This talk should be accessible to a wide audience, including students and postdocs.

Qianxiao LI
Learning parametric Koopman operators for prediction, identification and control

Koopman operator analysis is a popular method for data-driven analysis of nonlinear dynamical systems. For high-dimensional systems, however, its numerical computation is a challenging problem. In this talk, we discuss machine-learning aided construction of Koopman invariant subspaces and the associated projected Koopman operators for parametric dynamical systems. We present several applications in dynamics prediction, parameter identification and optimal control.

Bo LIN
Computing Committor Functions for the Study of Rare Events Using Deep Learning

The committor function is a central object of study in understanding transitions between metastable states in complex systems. However, computing the committor function for realistic systems at low temperatures is a challenging task due to the curse of dimensionality and the scarcity of transition data. In this talk, I will introduce the deep learning based methods that overcome these issues and achieve good performance on complex benchmark problems with rough energy landscapes or in high dimensions. These methods utilize efficient sampling techniques and provide an alternative practical way for studying rare transition events between metastable states in complex, high dimensional systems.

Jun LIU
Modeling and optimization of soft robotic with model order reduction technique through a Graph Neural Network (GNN) encoder

The Graph Neural Network (GNN) has gained popularity in recent years for its ability to capture graph data structures. It has demonstrated its strength in both node and graph level predictions by introducing the node connectivity information. This capability has inspired us to employ GNN in the numerical simulation field, where finite element (FE) meshes are naturally graph structures. In this work, we explore the powerful capabilities of GNNs and its variance to extract knowledge from FE meshes to analyze the mechanical behavior of a dielectric elastomer actuator (DEA), reducing the complex multi-physics electromechanics problem to a low-dimensional latent space. Compared to the conventional linear POD-based method, this approach offers a more general way for model order reduction and can potentially capture properties in the nonlinear manifold. Moreover, it can handle various mesh structures and remains robust against modifications in geometry and mesh. This technique enables us to predict the physical response of the DEA given an FEM mesh structure and perform design optimization based on model predictions to achieve optimal actuation distance while considering design constraints. We demonstrate this method brings benefits to solve optimization tasks for soft robotic design involving large deformation and complex physics.

Romit MAULIK
Multiscale Graph Neural Network Autoencoders for Interpretable Scientific Machine Learning

We develop a novel graph neural network (GNN) autoencoder with demonstrations on complex fluid flow applications. For interpretability, the GNN autoencoder uses an adaptive reduction procedure which performs flowfield-conditioned node sampling and sensor identification, and produces interpretable latent graph representations tailored to the flowfield reconstruction task.

These latent representations allow the user to (a) visualize where in physical space a given latent graph is active, and (b) interpret the time-evolution of the latent graph connectivity in accordance with the time-evolution of unsteady flow features (e.g. recirculation zones, shear layers) in the domain. For unstructured mesh compatibility, the autoencoding architecture utilizes a series of multi-scale message passing (MMP) layers, which model information exchange among node neighborhoods at various length-scales. The MMP layer, which augments standard single-scale message passing with learnable coarsening operations, allows the decoder to more efficiently reconstruct the flowfield from the latent representations. Analysis of latent graphs produced by the autoencoder for various model settings are conducted using unstructured snapshot data sourced from large-eddy simulations in a backward-facing step (BFS) flow configuration at high Reynolds numbers.

Matthias Heinkenschloss
<u>Certified Optimization with Reduced Order Models</u>

This talk presents recent advances in trust-region and line-search based optimization approaches for the optimization of expensive large-scale optimization problems using reduced order models (ROMs). The fundamental idea is to approximate computationally expensive evaluations of objective and constraint functions and their derivatives by inexpensive ROMs. To ensure convergence, the optimization algorithms adjust accuracy requirements on the ROM generated objective and constraint functions and their derivatives at the current optimization iterate as needed based on the progress of the optimization, allowing coarse, computationally inexpensive ROMs as much as possible. The trust-region approaches are implementable when only asymptotic ROM error bounds are available. To amortize the cost of ROM construction as much as possible during the optimization, the algorithms compute new iterates incorporating ROM error bounds to explore the design space more fully. This talk presents the optimization algorithms and their convergence results. Moreover, integration of ROM construction into the optimization algorithms is discussed. Numerical examples illustrate speed-ups achieved by the ROM based optimization algorithms.

Gianmarco MENGALDO
<u>Data-driven slow earthquake dynamics</u>

Friction is a complex phenomenon. This can be seen, for example, in laboratory experiments where stick-slip motion of various kind (i.e., slow and fast instabilities) can be produced when adapting the normal stress applied to the system. Similarly, natural earthquakes also produce complex stick-slip behaviour. A first challenge in the description of friction comes from the potentially high number of degrees of freedom (dofs) involved in the description of the dynamics of the sliding surfaces. Nonetheless, it was shown that friction can be described with a reduced number of dofs or variables of the dynamics. These may include the shear stress, the relative sliding slip rate, and one or more variables that describe the state of the contact of the sliding surfaces. We investigate the possibility to extract directly from the data the governing equations of friction starting from a simplified synthetic example. We further study the laboratory data with the Hankel Alternative View Of Koopman (HAVOK) theory, a method rooted in dynamical system theory that leverages data driven techniques and produces a Reduced Order Model (ROM) to reconstruct a shadow of the attractor of a system from observational data. We finally compare the results obtained for the laboratory experiments with Cascadia slow earthquakes.

Federico PICHI
A convolutional graph neural network approach to model order reduction for parametrized PDEs

The development of efficient reduced order models (ROMs) from a deep learning perspective enables users to overcome the limitations of traditional approaches. Convolutional autoencoder structures gained popularity in the ROM community as an extension to linear compression procedures [K. Lee and K. Carlberg. Model reduction of dynamical systems on nonlinear manifolds using deep convolutional autoencoders. JCP, 2020] and [S. Fresca, L. Dede, and A. Manzoni. A comprehensive deep learning-based approach to reduced order modeling of nonlinear time-dependent parametrized PDEs. JSC, 2021]. One drawback of these approaches is the lack of geometrical information when dealing with complex domains defined on unstructured meshes. The present work proposes a framework for nonlinear model order reduction based on Graph Convolutional Autoencoders (GCA) to exploit emergent patterns in different physical problems, including those that show a bifurcating behavior [F. Pichi, B. Moya, and J. S. Hesthaven. A graph convolutional autoencoder approach to model order reduction for parametrized PDEs. 2023]. Our methodology extracts the latent space's evolution while introducing geometric priors, and possibly alleviates the learning process through up- and down-sampling operations. We show the capability of this novel architecture w.r.t. classical benchmarks and non-uniqueness phenomena.

Annalisa QUAINI
Reduced Order Modeling and LES filtering

We will discuss the development of reduced order models (ROMs) for the incompressible Navier-Stokes equations (NSE) and the quasi-geostrophic equations (QGE). The commonality between these sets of equations is that in certain regimes (i.e., large Reynold number for the NSE and QGE and large Rossby number for the QGE) they require very fine meshes to compute accurate solutions. To circumvent this need, we adopt nonlinear filter stabilization as an efficient Large Eddy Simulation technique. For the realization of this stabilization, we combine a three-step algorithm called Evolve-Filter-Relax (EFR) with a computationally efficient finite volume method for both the NSE and the QGE.
The main novelty of our ROM for the NSE lies in the use within the EFR algorithm of a nonlinear, deconvolution-based indicator function that identifies the regions of the domain where the flow needs regularization. The ROM we propose is a hybrid projection/data-driven strategy: a classical Proper Orthogonal Decomposition Galerkin projection approach for the reconstruction of the velocity and the pressure fields and a data-driven reduction method to approximate the indicator function used by the nonlinear differential filter. This data-driven technique is based on interpolation with Radial Basis Functions.
The EFR approach is used as a regularization for ROMs for the QGE to increase the accuracy when the Proper Orthogonal Decomposition modes retained to construct the reduced basis are insufficient to describe the system dynamics.
For both sets of equations, the accuracy of the ROMs is assessed through several benchmark tests.

Gianluigi ROZZA
Reduced Order Modelling in Computational Fluid Dynamics: state of the art, challenges and perspectives

We provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD).

Efficient parametrisations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: (i) a better use of stable high fidelity methods, to enhance the quality of the reduced model too, also in presence of bifurcations and loss of uniqueness of the solution itself, (ii) capability to incorporate turbulence models and to increase the Reynolds number; (iii) more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; (iv) the improvements of the certification of accuracy, established on residual based error bounds, and of the stability factors, as well as (v) the guarantee of the stability of the approximation with proper space enrichments. All the previous aspects are quite relevant -- and often challenging -- in CFD problems to focus on real time simulations for complex parametric industrial, environmental and biomedical flow problems, or even in a control flow setting with data assimilation and uncertainty quantification. Some model problems will be illustrated by focusing on few benchmark study cases, for example on simple fluid-structure interaction problems and on shape optimisation, applied to some industrial and environmental problems of interest.

Wil SCHILDERS

The importance of MOR in the age of HPC and AI

Model order reduction (MOR) is a flourishing field of research since more than 2 decades, and many fantastic results have been obtained. MOR is also an important aspect of today's research in science and technology, fitting with the adagio ''think twice, compute once'', as it can substantially reduce energy consumption while still obtaining accurate results. This is extremely important in the current age of high performance computing, but also related to the field of artificial intelligence and machine learning. The novel field of scientific machine learning aims to combine methods from scientific computing with those in machine learning, leading to very interesting challenges. For example, how to reduce dynamic neural networks and predict the topology of such networks rather than using the commonly used guesswork.
In this talk, we will address both aspects of modern MOR: on the one hand significantly reducing computational efforts, on the other hand relations of MOR with machine learning. Regarding the latter, we will show how state space models can be transformed to dynamic neural networks and how properties of the system matrix determine the topology of the network. These are exciting times for computational scientists, and especially for researchers working in the MOR area!

Giovanni STABILE

Non-Linear Manifold projection reduced order models for parametric partial differential equations with efficient hyper-reduction

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 nonlinear approximation techniques such as 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 regimes characterized by an abundance of data. Not to mention that none of the knowledge on the physics of the model is exploited during the predictive phase. In this talk, in order to overcome these weaknesses, we implement a variant of the nonlinear manifold method introduced in previous works with hyper-reduction achieved through reduced over-collocation and teacher-student training of a reduced decoder. We test the methodology on test cases with increasing levels of complexity and compare the results we would obtain with a purely data-driven method for which the dynamics is approximated in time with a long-short-term memory network. The presented work is in collaboration with F. Romor and G. Rozza.

Maria STRAZZULLO

Model order reduction for parametric optimal control problems: overview and applications

Optimal control governed by parametric partial differential equations (PDEs) is a mathematical tool of great interest in many scientific and industrial fields. The main goal of optimal control is to steer the classical solution of a system toward a more advantageous state.
Despite its undeniable usefulness in applied research, the computational complexity of the optimization problem still limits its applicability.
Indeed, standard discretization techniques might lead to prohibitive computational costs. This issue is even more pronounced in time-dependent and nonlinear frameworks.
The talk focuses on various techniques to deal with this issue using model order reduction. First, we present some algorithms showing how reduced order methods are a useful strategy for optimal control problems, testing them on many PDEs (time-dependent and nonlinear equations in space-time formulation).
The second part of the talk describes how we can exploit reduced control approaches in several scientific fields under the applied viewpoint, such as bifurcating phenomena, uncertainty quantification, geophysics, and numerical stabilization.

Marco Tezzele

Recent advances in parameter space reduction

We present data-driven reduced order models with a focus on reduction in parameter space to fight the curse of dimensionality. We focus on extensions of the linear active subspaces (AS) technique: a kernel version exploiting an intermediate mapping to a higher dimensional space, and a local approach in which a clustering induced by a global active subspace is used for regression and classification tasks. We also show how to integrate parameter space reduction methods within a multi-fidelity nonlinear autoregressive scheme to improve the approximation accuracy of high-dimensional functions. Finally, we present applications in shape optimization using AS into the genetic algorithm to enhance the convergence during the minimization of high-dimensional quantities of interest. These methods are also applied to solve large scale structural optimization tasks in naval engineering.

Xin TONG

Likelihood informed subspace

The likelihood-informed subspace (LIS) method offers a viable route to reducing the dimensionality of high-dimensional probability distributions arising in Bayesian inference. LIS identifies an intrinsic low-dimensional linear subspace where the target distribution differs the most from some tractable reference distribution. Such a subspace can be identified using the leading eigenvectors of a Gram matrix of the gradient of the log-likelihood function. We will establish mathematical error bound for such method and discuss its relationship with Monte Carlo Methods.

Alessandro VENEZIANI
<u>Model Order Reduction in Cardiovascular Clinical Problems: A Case-Study Introduction</u>

While the role of computational modeling in understanding cardiovascular diseases has been highlighted for different applications and pathologies, the impact on the clinical routine is still limited. The main reasons, related to the intrinsic complexity of the problems to consider when dealing with living systems, must be identified in the high computational costs associated with the solution of inverse problems – the problems we need to solve to optimize devices and surgical procedures. For instance, the Total Cavopulmonary Connection is a complex pediatric surgery intended to buy time for newborns affected by Hypoplastic Left Ventricle waiting for a heart transplant. While there is evidence that the shape left by the surgeons has a major impact on the long-term conditions of the patient, a rigorous identification of the optimal condition was prevented by the high computational costs of the mathematical procedure. Reduced Order Models open a completely different perspective also in this field. The significant shortening of the computational costs enables the use of scientific computing not only for a general understanding but also for a patient-specific optimization of therapies, bringing the concept of precision personalized medicine to an unprecedent level. This case-study presentation will present some current and future challenges. We will discuss the comparison and the interplay between “classical” reduced models and other – more data-driven – forms of surrogate modeling.

Karen Veroy-Grepl
<u>Model Order Reduction in the Multi-Scale Materials Setting</u>

Two-scale simulations are often employed to analyze the effect of the microstructure on a component’s macroscopic properties. Understanding these structure–property relations is essential in the optimal design of materials, or to enable (for example) estimation of microstructure parameters through macroscale measurements. However, these two-scale simulations are typically computationally expensive and infeasible in multi-query contexts such as optimization and inverse problems. To make such analyses amenable, the microscopic simulations can be replaced by inexpensive, parametric surrogate models. In this talk, we (1) present some recent work on a non-intrusive reduced basis method to construct inexpensive surrogates for parametrized microscale problems, and (2) highlight difficulties for model order reductino presented by highly nonlinear constitutive relations in multi-scale problems in mechanics.