Computational Learning for Model Reduction
Poster Session Abstracts
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Extended one-dimensional reduced model for blood flow within a stenotic artery
Yifan Wang, Texas Tech University

We introduce an adapted one-dimensional (1D) reduced model aimed at analyzing blood flow within stenosed arteries. Differing from the prevailing 1D AQ model, our approach incorporates the variable radius of the blood vessel. Our methodology begins with the non-dimensionalization of the Navier-Stokes equations for axially symmetric flow in cylindrical coordinates and then derives the extended 1D reduced model, by making additional adjustments to accommodate the effects of variable radii of the vessel along the longitudinal direction. Additionally, we propose a method to extract radial velocity information from the 1D results during post-processing, enabling the generation of two-dimensional (2D) velocity data. We validate our model by conducting numerical simulations of blood flow through stenotic arteries with varying severities, ranging from 23% to 50%. The results were compared to those from the established 1D model and a full three-dimensional (3D) simulation, highlighting the potential and importance of this model for arteries with variable radius.

Nonlinear model order reduction for parametric PDEs via contour integral methods
Mattia Manucci, University of Stuttgart

We discuss a projection model order reduction(MOR) method for a class of parametric linear evolution PDEs, which is based on the application of the Laplace transform. The main advantage of this approach is that the Laplace transform allows us to compute the solution directly at a given time instant. This can be done efficiently by approximating the contour integral associated with the inverse Laplace transform by a suitable quadrature formula. This feature is very important in terms of classical model order reduction methodologies. Differently from time stepping integrators (like Runge--Kutta methods), the use of the Laplace transform determines a significant reduction of the size of the reduced space. In this article, we propose two reduction methods; the first one is linear since it constructs a unique reduced space, based on the vectors representing the Laplace transform at the chosen quadrature points for different values of the parameters, and the second one is instead nonlinear since it constructs several reduced spaces, one at each quadrature node. This last approach is particularly well suited to a parallel computation approach, allowing a faster computation. We show the effectiveness of the method by some illustrative parabolic PDEs arising from finance.

Domain-decomposed method for Bayesian inverse problems
Zhihang Xu, University of Houston

This poster addresses Bayesian inverse problems involving PDEs, focusing on overcoming challenges of high computational cost and dimensionality. First, we propose a domain-decomposed method utilizing local KL expansions and Gaussian process regression to represent unknown parameters. This approach enables efficient and parallel subdomain inversions while resolving interface issues through an active learning Gaussian process regression algorithm and reconstructing the global field. Second, when the prior information is available only in the form of historical data, we introduce a domain-decomposed method based on variational autoencoders (VAEs) to construct local generative models, significantly reducing training complexity and dimensionality. Poisson image blending integrates the local results into a coherent global solution. Numerical experiments validate the proposed methods, demonstrating superior computational efficiency and stability in solving high-dimensional inverse problems.

Tensor Parametric Hamiltonian Operator Inference

Arjun Vijaywargiya, Sandia National Laboratories

This work presents a tensor-based approach to constructing data-driven reduced-order models corresponding to semi-discrete partial differential equations with canonical Hamiltonian structure. By expressing parameter-varying operators with affine dependence as contractions of a generalized parameter vector against a constant tensor, this method leverages the operator inference framework to capture parametric dependence in the learned reduced-order model via the solution to a convex, least-squares optimization problem. This leads to a simple and straightforward implementation which compactifies previous parametric operator inference approaches and directly extends to learning parametric operators with symmetry constraints\textemdash a key feature required for constructing structure-preserving surrogates of Hamiltonian systems. The proposed approach is demonstrated on both a (non-Hamiltonian) scalar heat equation with variable diffusion coefficient as well as a wave equation with variable wave speed.

Reduced Order modeling approach to imaging with waves

Jörn Zimmerling, Uppsala Universitet

We introduce a computationally inexpensive approach for imaging with an active array of sensors, which probe an unknown medium with a pulse and measure the resulting waves. The imaging function uses a data-driven estimate of the ”internal wave” originating from the vicinity of the imaging point and propagating to the sensors through the unknown medium. We explain how this estimate can be obtained using a reduced order model for the wave propagation.

Trajectorial-average in Nambu systems with application in plasma physics

Kun Huang, The University of Texas at Austin

We present a struture-preserving solver for particle-wave(electron-plasmon) interaction in magnetized plasmas. The solver combines a conservative LDG(local discontinuous Galerkin) scheme for the interaction part with a trajectorial averaging method for the Hamiltonian dynamics part. The trajectorial averaging method significantly reduces computational cost by taking advantage of the multiscale structure of this system. By introducing a novel concept "trajectroy bundle", we transform a continuous topological problem into a discrete graph theory problem. Numerical examples for a non-uniform magnetized plasma in an infinitely long symmetric cylinder is presented. It is verified that the connection-proportion algorithm allows to distinguish different trajectory bundles, and the proposed scheme rigorously preserves all the conservation laws.

Senior Research Scientist

Lei Jiang, SLB

Deep transient pressure testing, using a state-of-the-art formation testing platform, allows deeper investigation into a subsurface formation compared to previous wireline-conveyed testing techniques. Given the associated interaction of the pressure with more varied geological features, numerical reservoir models and simulation are generally required to capture the reservoir or formation heterogeneity that may be encountered during a test. However, the long computation time of such numerical simulation poses challenges for some critical interpretation tasks, such as model inversion. We propose a novel method for the parameter estimation in geologically complex reservoirs by conducting Bayesian inversion with surrogate models. To account for the geology complexity, we utilize surrogate models constructed through the Polynomial Chaos Expansion method, to serve as a substitute of the numerical simulators. It allows to simulate the pressure response in a timely manner while at the same time providing global sensitivity analysis for each uncertain parameter in the model. The Markov Chain Monte Carlo (MCMC) method is then employed with the surrogate models for conducting the Bayesian inversion with pressure transient measurements. Through our studies, we demonstrate that the adoption of surrogate models considerably reduces the computation time required, allowing the Bayesian inversion to be completed within minutes, which was unachievable with the numerical simulators. Furthermore, this new method offers accurate parameter estimations and provides posterior distributions of uncertain parameters, as well as unveiling correlations among the parameters for the interpretation of measurement. These capabilities were lacking in the current inversion process utilizing numerical simulators. Finally, the new method lends itself ideally to workflow automation for history matching, thus reducing the workload on petro-technical experts and addressing today's imperatives of faster and more cost-efficient field development.

Quadrature-based balanced truncation for LQO systems

Reetish Padhi, Virginia Tech

Quadrature-based balanced truncation (Quad-BT) is a non-intrusive, data-based balancing approach for linear (and bilinear) time invariant systems that computes reduced models purely from samples of the time-domain kernels and their derivatives. We present the extension of Quad-BT to linear systems with quadratic outputs and propose a QDEIM based selection procedure to select quadrature nodes to improve computational time of our algorithm.

Computational Advances in Optimal Control Space Reduction in Applications to Electrical Impedance Tomography for Early Cancer Detection

Vladislav Bukshtynov, University of Colorado Boulder

We propose a set of novel approaches combined in the fully developed computational framework EIT-OPT for the optimal reconstruction of binary-type images suitable for various models seen in biomedical applications. This framework enables accurate solutions to the inverse problem of cancer detection (IPCD) while applying the electrical impedance tomography (EIT) for detecting multiple cancer-affected regions of different sizes and different levels of complexity based on available (noisy) measurements. A new spatial partitioning methodology and efficient scheme for switching between fine and coarse scales allow higher variations in the geometry of reconstructed binary images with superior performance confirmed computationally on various models. The efficiency in computational speed and accuracy is achieved by combining the advantages of recently developed optimization methods that use sample solutions with customized geometry and control space reduction based on the samples' geometry and individual contributions paired with gradient-based techniques. A nominal number of input parameters makes the approaches simple for practical implementation in diverse settings and extendable to the broad range of problems in biomedical sciences, physics, geology, chemistry, etc.

Efficient Dynamic Image Reconstruction with Motion Estimation

Mirjeta Pasha, Virgina Tech

Large-scale dynamic inverse problems are typically ill-posed and suffer from complexity of the model constraints and large dimensionality of the parameters. A common approach to overcome ill-posedness is through regularization that aims to add constraints on the desired parameters in both space and temporal dimensions. In this work, we propose an efficient method that incorporates a model for the temporal dimension by estimating the motion of the objects alongside solving the regularized problem. In particular, we consider the optical flow model as part of the regularization that simultaneously estimates the motion and provides an approximation for the desired image sequence. To overcome high computational cost when processing massive scale problems, we combine our approach with a generalized Krylov subspace method that efficiently solves the problem on relatively small subspaces. Further, we explore subspace restarting and recycling to overcome limited memory constraints and preconditioning to accelerate convergence. The effectiveness of the prescribed approaches is illustrated through numerical experiments arising in dynamic computerized tomography and image deblurring applications. This is joint work with Toluwani Okuanola, Misha Kilmer, and Melina Freitag.

Parametric reduced order modeling for nonlocal PDEs

Yumeng Wang, Missouri University of Science and Technology

Many applications involve parametric nonlocal PDEs that need to be solved repeatedly for different parameter values. However, solving these PDEs even for a single parameter set can be challenging due to significant computational and storage costs. To address these challenges, we propose a convolutional neural network-based reduced-order modeling approach. Our method can predict solutions accurately for new parameters and significantly reduce computational costs. Extensive numerical experiments will be provided to demonstrate the performance of our method.

Parametric model reduction of mean-field and stochastic systems on the space of probability densities

Tobias Blickhan, New York University

We learn surrogate models for the population dynamics of physical systems featuring stochastic and mean-field effects and a dependence on physics parameters. By population dynamics we refer to the evolution of the ensemble of samples that represent the system as opposed to the trajectories of individual samples. Crucially, different sample dynamics can collectively give rise to the same population dynamics. We aim to exploit this redundancy to achieve a reduction of complexity in the model. Building on the Benamou-Brenier formula from optimal transport, we use a variational problem to infer parameter- and time-dependent gradient fields that represent approximations of the population dynamics. The inferred gradient fields can then be used to rapidly generate sample trajectories that mimic the dynamics of the physical system on a population level over varying physics parameters. We show that combining Monte Carlo sampling with higher-order quadrature rules is critical for accurately estimating the training objective from sample data and for stabilizing the training process. We demonstrate on Vlasov-Poisson instabilities as well as on high-dimensional particle and chaotic systems that our approach accurately predicts population dynamics over a wide range of parameters and outperforms state-of-the-art diffusion-based and flow-based models that simply condition on time and physics parameters.

A Dynamic Network Model for Thermally-Driven Reactive Transport Near Chemical Equilibrium via Spectral Decomposition

Binan Gu, Worcester Polytechnic Institute

Predicting the fluid, thermal, and solutal transport in an evolving complex network of pores requires a fundamental description of the transport processes and their coupling to the underlying reaction chemistry. To tackle the dynamics under various competing timescales (chemical, advective, thermal, and mass diffusive) and solution-coupled boundary conditions, we perform a small-amplitude perturbation analysis on the leading-order equations derived from an existing first-principle model [Tilley et al. 2021]. To characterize the dynamics on each edge (treated as a 1D interval) in a reduced order, we derive a spectral decomposition of temperature and species transport near chemical equilibrium and express the coupled pressure and pore radius evolution in terms of the spectral bases and forcings at adjacent vertices. By imposing flux conservation laws at network vertices via a weakly nonlinear analysis, we close the network model by describing the time evolution of temperature and species at interior vertices. This work introduces a general approach to pore network modeling with PDE dynamics near equilibrium and provides a firm analytical background for adaptation to nonlinear dynamics.

Lagrangian operator inference enhanced with structure-preserving machine learning for nonintrusive model reduction of mechanical systems

Harsh Sharma, UC San Diego

Complex mechanical systems often exhibit strongly nonlinear behavior due to the presence of nonlinearities in the energy dissipation mechanisms, material constitutive relationships, or geometric/connectivity mechanics. Numerical modeling of these systems leads to nonlinear full-order models that possess an underlying Lagrangian structure. This work proposes a Lagrangian operator inference method enhanced with structure-preserving machine learning to learn nonlinear reduced-order models (ROMs) of nonlinear mechanical systems. This two-step approach first learns the best-fit linear Lagrangian ROM via Lagrangian operator inference and then presents a structure-preserving machine learning method to learn nonlinearities in the reduced space. The proposed approach can learn a structure-preserving nonlinear ROM purely from data, unlike the existing operator inference approaches that require knowledge about the mathematical form of nonlinear terms. From a machine learning perspective, it accelerates the training of the structure-preserving neural network by providing an informed prior (i.e., the linear Lagrangian ROM structure), and it reduces the computational cost of the network training by operating on the reduced space. The numerical results demonstrate that the proposed approach yields generalizable nonlinear ROMs that exhibit bounded energy error, capture the nonlinear characteristics reliably, and provide accurate long-time predictions outside the training data regime.

Optimal Control of Maxwell's Equations

Yaw Owusu-Agyemang, George Mason University

Maxwell’s equations are an important modeling component in a variety of modern engineering applications, ranging from nanoscale optical devices to magnetic confinement fusion. Despite the significant advances in the mathematical analysis and numerical methods for the solution of Maxwell’s equations, little progress has been made in our understanding of optimal control and optimal design problems governed by Maxwell’s equations. This poster presents results on the mathematical and computational challenges associated with such optimization problems. A theoretical framework for the time-discrete forward problem is shown. Well-posedness of the optimization problem is then established by the direct method, and the first order necessary and sufficient optimality conditions are given. A physics-compatible finite element pair for electric and magnetic field is used, and the numerical results carried out with an advanced electromagnetic software MrHyDE (Sandia National Labs) are shown. Capabilities of the Rapid Optimization Library (ROL) are used to carry out large scale optimization and the results are also shown.

Learning Mechanical Systems From Data via Structured AAA Algorithms

Michael Ackermann, Virgina Tech

The modeling of physical systems from first principles typically results in dynamical systems with physical or differential structures. Data-driven modeling of complex dynamical systems has proven to be an important tool for creating models when the governing equations are unknown, however such data-driven models may not preserve the physical or differential structures. Based on our previous work on structured barycentric forms, we present a structured Adaptive Anderson-Antoulas (AAA) algorithm which constructs second-order dynamical systems from frequency domain measurements. We take special care in the treatment of the underlying nonlinear least-squares problem and provide a comparison of two solution methods.

Variational problems with gradient constraints: A priori and A posteriori error identities

Rohit Khandelwal, George Mason University

Nonsmooth variational problems are ubiquitous in science and engineering, for e.g., fracture modeling and contact mechanics. This poster presents a generic primal-dual framework to tackle these types of nonsmooth problems. Special attention is given to variational problems with gradient constraints. The key challenge here is how to project onto the constraint set both at the continuous and discrete levels. In fact, both a priori and a posteriori error analysis for such nonsmooth problems has remained open. In this poster, on the basis of a (Fenchel) duality theory at the continuous level, an a posteriori error identity for arbitrary conforming approximations of primal-dual formulations is derived. In addition, on the basis of a (Fenchel) duality theory at the discrete level, an a priori error identity for primal (Crouzeix–Raviart) and dual (Raviart–Thomas) formulations is established. The poster concludes by deriving the optimal a priori error decay rates.

Sensor Selection Using End-to-End Differentiable Networks with Application to Field Reconstruction

Sridhar Chellappa, Max Planck Institute for Dynamics of Complex Technical Systems

Reconstucting field variables based on partially observed data is an important problem arising in a number of practical applications such as climate science, fluid dynamics, nuclear engineering [1, 2, 3]. To achieve accurate approximations, two crucial aspects need to be considered: (a) choosing the optimal location for data sensors and (b) identifying a suitable model to map the measured data to the corresponding high-dimensional fields.

Existing approaches to address this challenge either adopt a linear model for reconstruction [1], leading to poor approximations or follow an ad-hoc (random) choice of sensor locations that fail to efficiently recover the true underlying field [2, 3]. In this contribution, we combine the functionalities of sensor selection and nonlinear reconstruction by proposing an end-to-end network that leads to improved reconstruction performance, while using fewer sensor measurements. Our approach leverages suitable sparsity constraints to achieve this. The proposed method iteratively learns (a) good sensor locations for the field reconstruction

via stochastic optimization and (b) the parameters of a neural network that will reconstruct the field from the sparsely measured data during the inference stage. We illustrate the benefits of the new approach on numerical examples arising in fluid dynamics and climate science.

Data-Driven Reduced Order Models For Radar Imaging In Multi-Scattering Environment

Mikhail Zaslavskiy, Southern Methodist University

We consider the inverse scattering problem with monostatic time-domain data. Keeping in mind the synthetic aperture radars applications, the data is assumed to be given by series of the single-input-single-output (SISO) channels corresponding to moving collocated sources and receivers. Interpolatory reduced-order models formulations we developed allow to learn the internal solutions using only data-driven Grammians of the time-domain snapshots. In particular, we construct internal solutions for each SISO channel separately and then merge them together via Lippmann-Schwinger integral equation. We also discuss how to improve the solution learning by enhancing the aperture via data completion that enables lifting of SISO data series to mulit-input-multi-output data. Numerical experiments illustrating the performance of our approach will be provided.