Mathematics of reduced order models

Poster Session Abstracts
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Context-aware model reduction for multifidelity importance sampling
Terrence Alsup, Courant Institute of Mathematical Sciences

Multifidelity methods leverage low-cost surrogate models to speed up computations and make occasional recourse to expensive high-fidelity models to establish accuracy guarantees. Because surrogate and high-fidelity models are used together, poor approximation by the surrogate models can be compensated with frequent recourse to high-fidelity models. Thus, there is a trade-off between investing computational resources to improve surrogate models and the frequency of making recourse to high-fidelity models; however, this trade-off is ignored by traditional model reduction methods that construct surrogate models that are meant to replace high-fidelity models rather than being used together with high-fidelity models. In this presentation, we consider multifidelity importance sampling and explicitly take into account the trade-off between improving the approximation quality of surrogate models for constructing biasing densities and the frequency of recourse to the high-fidelity models to estimate statistics. Given a total computational budget, an optimization problem determines how much of the budget to invest into constructing a surrogate model versus sampling the high-fidelity model with the objective to minimize the error of the estimator. Numerical examples demonstrate that optimal surrogate models have significantly lower fidelity than what typically is set as tolerance in traditional model reduction, leading to runtime speedups in our examples.

Model Order Reduction for Stochastic problems
Raed Blel, CERMICS

The aim of this work is to develop a new methodolgy, based on reduced basis techniques, in order to construct efficient control variates to reduce variance in Monte Carlo methods. More precisely, the aim of our work is to compute efficiently the expectation of a collection random variables of the form $g_\mu(Z)$, where Z is a given random variable, μ belongs to a set of parameter values $\mathcal P$, and for all $\mu \in \mathcal P$, g_μ is a smooth real-valued function. The control variates are constructed as linear combinations of a few numbers of, say n, of such functions, corresponding to n different values of the parameter μ. Greedy algorithms provide a practical and efficient way to select n almost-optimal values of the parameter, in the case where the variances of the different random variables at hand can be computed exactly. In this work, we study the effect of sampling on the theoretical convergence results of these greedy algorithms, and show that it is possible to adapt in a practical the number of samples of the variable Z to be used to compute approximate variances in order to guarantee, with high probability, that the rates of approximations given by greedy algorithms will be close to the decay of the Kolmogorov width of the set \{g\mu(Z), \quad \mu \in \mathcal P\}. Finally we present numerical tests on a simple case to illustrate the theoretical results.

Realizations of Port Hamiltonian systems
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Port-Hamiltonian systems have gained attention in recent years due to their interesting properties in energy-based modelling and control. They are particularly interesting for systems interconnection since networks of port-Hamiltonian systems also exhibit global port-Hamiltonian structure. In order to be able to benefit from this structure, one has to model the dynamical system in port-Hamiltonian form, i.e., its ""realization"" should satisfy the port-Hamiltonian formalism. We present realization methods for port-Hamitonian system that have minimal order. We focus on the construction of minimal realizations of linear time-invariant port-Hamiltonian systems. The goal is to be able to compute the port-Hamiltonian minimal realization directly from time (frequency) domain input/output data of the system.

Reduced Order Modeling of Electromagnetic Particle-in-Cell Kinetic Plasma Simulations
Julio de Lima Nicolini, Ohio State University

High-power microwave devices and other industrial applications can be modeled via plasmas and their interactions with electromagnetic fields; simulating the behavior such devices is one of motivations in developing computational methods for plasmas. However, fine computational meshing is required to capture complex problems, increasing the number of degrees of freedom that must be stored and updated in a numerical algorithm. Additionally, update equations require repeated costly matrix solvers or approximate methods for explicit update. A projection of the problem onto a smaller subspace (model order reduction) can be employed to reduce the number of degrees of freedom and overall computational costs, which we apply to our finite-element-based particle-in-cell algorithm. Our method is based on a formulation of Maxwell's equations using differential forms that allows for exact charge- and energy-conservation to be obtained for the first time on unstructured grids. The method is divided into four main steps: updating fields, gathering the fields at each particle location, updating particles, and scattering the current/charge information from the particles back to the mesh. To circumvent the large number of degrees of freedom required due to fine meshing in geometrically complex problems, as well as obviate the need for costly matrix solvers or approximate methods in the (implicit) field update equation, the field solver step is reduced via a projection into a reduced basis obtained from data extracted from a simulation run using the full algorithm. The resulting reduced-order field update is able to consistently evolve particle dynamics at lower computational cost.

Semi-Lagrangian Nodal Discontinuous Galerkin Method for the BGK Model: Accuracy and Stability Analysis
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DEWe consider the 1D1V BGK model, a simplified relaxation model for the Boltzmann equation, which describes the dynamic of gases in both hydrodynamic and rarefied regimes using a probability density function. We propose an asymptotic preserving (AP) and asymptotic accurate semi-Lagrangian (SL) method for the BGK model with a mass conservative nodal discontinuous Galerkin (DG) method for spatial discretization, and diagonally implicit Runge-Kutta (DIRK) method for temporal discretization of the stiff relaxation term along characteristics. A local maximum principle preserving limiter is added to avoid numerical oscillations in the transport step. The time stepping constraint is relaxed and much larger than that from an Eulerian framework with explicit treatment of the source term due to the SL and implicit nature of time discretization.

We perform accuracy analysis of the scheme in both kinetic and fluid regimes. A family of third order DIRK methods are developed based on one extra accuracy order condition in the fluid limit. Von Neumann analysis to a simplified two-velocity linear kinetic model is conducted to study the stability of DIRK methods in both regimes.

Extensive numerical tests are presented to verify the high order accuracy, conservation property of the proposed method for smooth test cases, and its AP performance on problems with shocks. Our future work includes the extension of the proposed algorithm to high dimensional model with more general boundary conditions.

Learning block-oriented nonlinear models of dynamical systems from data
Victor Gosea, Max Planck Institute, Magdeburg, Germany

We present a procedure for learning block-oriented models of dynamical systems from input-output data. This can be viewed as an extension of the classical Loewner framework for linear systems to block-oriented systems that comprise of linear time-invariant (LTI) system blocks and static nonlinear blocks. Such types of systems include Wiener or Hammerstein models, and many different types of cascaded interconnections (such as Hammerstein-Wiener models).

emgr -- EMpirical GRamian Framework
Christian Himpe, MPI Magdeburg

A wide range of industrial applications from control engineering, systems engineering, computational engineering or uncertainty quantification are addressed by mathematical system theory, including reduced order modeling. For linear systems, an essential tool for these tasks are system Gramian matrices. Yet, linear or linearized systems may not suffice to model and simulate dynamics of complex technical systems. So, for nonlinear or parametric systems, the data-driven empirical system Gramian matrices generalize linear methods, and the empirical Gramian framework - emgr - is an open-source software toolbox for their computation.

L1- and R2-based Reduced Over Collocation methods for parametrized nonlinear partial differential equations
Lijie Ji, UmassD/Shanghai Jiao Tong University

The onerous task of repeatedly resolving certain parametrized partial differential equations (pPDEs) in, e.g. the optimization context, makes it imperative to design vastly more efficient numerical solvers without sacrificing any accuracy. Reduced basis method (RBM) seeks a surrogate solution in a carefully-built subspace of the parameter-induced high fidelity solution manifold.
In this paper, we extend the empirical interpolation method (EIM) approach in the context of solving pPDEs resulting in the L1-based and R2-based reduced over collocation method (L1-ROC, R2-ROC).This new scheme is online efficient and immune from the efficiency degradation of EIM for nonlinear and nonaffine problems.

Dynamic Mode Decomposition--Accuracy Analysis and Construction of Reduced Order Modeling
Hannah Lu, Stanford University

Dynamic mode decomposition (DMD), within the family of singular-value decompositions (SVD), is a popular tool of data-driven regression. While multiple numerical tests demonstrated the power and efficiency of DMD in representing data (i.e., in the interpolation mode), applications of DMD as a predictive tool (i.e., in the extrapolation mode) are scarce. This is due, in part, to the lack of rigorous error estimators for DMD-based predictions. We provide a theoretical error estimator for DMD extrapolation of numerical solutions to linear and nonlinear parabolic equations. This error analysis allows one to monitor and control the errors associated with DMD-based temporal extrapolation of numerical solutions to parabolic differential equations. We use several computational experiments to verify the robustness of our error estimators and to compare the predictive ability of DMD with that of proper orthogonal decomposition (POD), another member of the SVD family. Our analysis demonstrates the importance of a proper selection of observables, as predicted by the Koopman operator theory. In all the tests considered, DMD outperformed POD in terms of efficiency due to its iteration-free feature. In some of these experiments, POD proved to be more accurate than DMD. This suggests that DMD is preferable for obtaining a fast prediction with slightly lower accuracy, while POD should be used if the accuracy is paramount.

System-theoretic Model Reduction with pyMOR
Petar Mlinarić, Max Planck Institute for Dynamics of Complex Technical Systems

We discuss model order reduction for control systems using pyMOR, a freely available software library of model order reduction algorithms implemented with the Python programming language. The initial focus of pyMOR was on reduced basis methods for parameterized partial differential equations. As such, it was designed to allow easy integration with existing open-source high-performance partial differential equation solvers, e.g., deal.II, DUNE, or FeniCS. In particular, all reduction algorithms in pyMOR are implemented generically via operations on well-defined vector array, operator, and model interface classes. This enables, for instance, the implementation of a generic Petrov-Galerkin projection method for a variety of input-state-output systems, e.g., second-order, time-delay, and bilinear systems. We discuss the pyMOR implementation of systems-theoretical model order reduction algorithms, e.g., balanced truncation and iterative rational Krylov algorithm, and present the partial differential equation

solver integration on several benchmark examples.

Reduced-Order Model Prediction of Kinetic Plasma Behavior Using Dynamic Mode Decomposition'.
Indranil Nayak, Ohio State University

Plasma simulations are very useful for analysis of high-power microwave and terahertz devices, ionosphere and magnetosphere phenomena, directed energy devices and a series of other applications. The electromagnetic particle-in-cell (EM-PIC) algorithm is a popular method for kinetic plasma simulation, however, one of its disadvantages is that the computation time is very high for large number of particles. We present a reduced order model based on Dynamic Mode Decomposition (DMD) for prediction of kinetic plasma behavior in future time. DMD is a data driven equation-free method for extracting dominant features of a complex dynamical system. It models the time evolution by finite approximation of the infinite-dimensional Koopman operator, which makes it applicable to non-linear dynamics as well. We analyze the case of a 2D electron beam propagation inside a perfect electric conductor (PEC) cavity in the presence of a transverse oscillating magnetic field. We discretize the spatial domain using irregular triangular grids and express Maxwell's equations in the language of differential forms. We run the charge-conserving finite-element time-domain (FETD) based EM-PIC simulation until certain time (harvesting limit) for collecting snapshots of degree of freedom (dof) of electric field on the mesh edges. We apply DMD on the collected data to extract DMD modes and corresponding eigenvalues for prediction of electric field (self-field) distribution in future time without the need of running the full-order simulation further.

Multifidelity Approximate Bayesian Computation
Thomas Prescott, University of Oxford

Multifidelity approximate Bayesian computation (MF-ABC) is a likelihood-free technique for parameter inference that exploits model approximations and low-fidelity simulations to significantly increase the speed of ABC algorithms. We integrate the multifidelity approach with the ABC sequential Monte Carlo (ABC-SMC) algorithm into a novel MF-ABC-SMC algorithm. We show that the improvements generated by each of ABC-SMC and MF-ABC to the efficiency of generating Monte Carlo samples and estimates from the ABC posterior are amplified when the two techniques are used together.

Lift & Learn: From nonlinear PDEs to low-dimensional polynomial models
Elizabeth Qian, MIT

We present Lift & Learn, a physics-informed method for learning analyzable low-dimensional models for large-scale dynamical systems governed by nonlinear partial differential equations (PDEs). The method exploits domain knowledge of a system's governing equations to identify a coordinate transformation in which the governing PDE has quadratic structure. This transformation is called a lifting map because it often adds auxiliary variables to the system state. Data in the new, lifted coordinates is obtained by first evaluating a model for the original nonlinear PDE and then applying the lifting map to the resulting simulation data. The proper orthogonal decomposition (POD) is used to reduce the high-dimensional lifted data by projecting the data onto its leading POD modes. Low-dimensional linear and quadratic matrix operators are fit to the lifted reduced data using a least-squares operator inference procedure, yielding an analyzable quadratic reduced model. Theoretical analysis shows that the learned model captures the system physics in the lifted coordinates at least as accurately as traditional intrusive model reduction approaches. This provides a bridge from our learned models to the interpretability and analyzability of traditional reduced models and makes the Lift & Learn models robust to changes in inputs. Numerical experiments on problems drawn from neuron and fluid modeling demonstrate the accuracy and robustness of the learned models.

Manifold Approximations via Transported Subspaces: Model reduction for transport-dominated problems
Donsub Rim, New York University

This work presents a method for constructing online-efficient reduced models of systems governed by parametrized nonlinear scalar conservation laws. The solution manifolds induced by transported-dominated problems such as hyperbolic conservation laws typically exhibit traveling structures, which means that traditional model reduction methods based on linear approximations are inefficient when applied to these problems. In contrast, the approach introduced in this work derives reduced approximations that are nonlinear by explicitly composing global transport dynamics with locally linear approximations of the solution manifolds. A time-stepping scheme evolves the nonlinear reduced models by transporting local approximation spaces along the characteristic curves of the governing equations. The proposed computational procedure allows an offline/online decomposition and is online efficient in the sense that the costs of time-stepping the nonlinear reduced models are independent of the number of degrees of freedom of the full model. Numerical experiments with transport through heterogeneous media and the Burgers' equation show orders of magnitude speedups of the proposed nonlinear reduced models based on transported subspaces compared to traditional linear reduced models and full models.

Coarse-graining of Overdamped Langevin Equations
Felix Ye, Johns Hopkins University

The overdamped Langevin equations have many applications in molecular dynamics. Due to the curse of dimensionality, the cost of simulating the full system is prohibitively expensive. Usually, the dynamics has the low-dimensional variable that could capture the quantities of interest, which is called {\it resolved variable}. We are interested in the dynamical property of the resolved variable, such as, the correlation and transition rates between metastable states. So it is important to develop an efficient and accurate coarse-graining model that reproduce the distribution and correlation correctly.

Data-driven Discovery of Emergent Behaviors
Ming Zhong, Johns Hopkins University

Agent-based systems are a ubiquitous modeling tool in many disciplines. We consider the fundamental problem of inferring interaction kernels from observations of agent-based collective dynamical systems exhibiting various kinds of emergent behaviors. As extension of [1], we provide extensive numerical evidence that the estimators provide faithful approximations to the interaction kernels, and provide accurate predictions for trajectories started at new initial conditions, both throughout the “training” time interval in which the observations were made, and often much beyond. We demonstrate these features on a number of prototypical systems. Our experiments also suggest that our estimated systems can display the same emergent behaviors of the observed systems. Finally, in the case of families of systems governed by a parameterized family of interaction kernels, we introduce novel estimators that estimate the parameterized family of kernels. We demonstrate this in the case of gravity, by learning both the “common component 1/r2” and the dependency on mass, without any a priori knowledge of either one.

[1] F. Lu, M. Zhong, S. Tang, M. Maggioni. Nonparametric inference of interaction laws in systems of agents from trajectory data, PNAS, 116 (3), 14424 - 14433, 2019.

Reduced order model approach to inverse scattering
Jörn Zimmerling, University of Michigan

Inverse scattering problems are inherently non-linear; nevertheless, many solution methods rely on linearization of the problem. In this contribution, we present a reduced order modeling approach to inverse scattering problems that allows us to mitigate this non-linearity. The key idea of our approach is to construct data-driven reduced-order models (ROMs) via time-domain Loewner inner products. Using a series of linear algebraic transforms allows an interpretation of the ROM as a coarse finite-difference discretization of the underlying PDE operator. As

such, it (approximately) inherits the straightforward dependence of the PDE on its coefficients. We now solve the inverse problem by minimizing the Frobenius distance between the observed ROM and a model ROM, rather than minimizing the mismatch between observed and modeled data, as most conventional methods do. This reformulation leads to fast convergence since the ROM approach mitigates the non linearity of the inverse scattering problem.