Cross Interpolation for Solving High-Dimensional Dynamical Systems on Low-Rank Tensor Manifolds

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Abstract

We present a novel tensor interpolation algorithm for the time integration of nonlinear tensor differential equations (TDEs) on the tensor train and Tucker tensor low-rank manifolds, which are the building blocks of many tensor network decompositions. This work builds upon our previous work presented last year (Donello et al., Proceedings of the Royal Society A, Vol. 479, 2023) on solving nonlinear matrix differential equations on low-rank matrix manifolds using CUR decompositions. The methodology we present offers multiple advantages: (i) It delivers near-optimal computational savings both in terms of memory and floating-point operations by leveraging cross algorithms based on the discrete empirical interpolation method to strategically sample sparse entries of the time-discrete TDEs to advance the solution in low-rank form. (ii) Numerical demonstrations show that the time integration is robust in the presence of small singular values. (iii) High-order explicit Runge-Kutta time integration schemes are developed. (iv) The algorithm is easy to implement, as it requires the evaluation of the full-order model at strategically selected entries and does not use tangent space projections, whose efficient implementation is intrusive. We demonstrate the efficiency of the presented algorithm for several test cases, including a nonlinear 100-dimensional TDE for the evolution of a tensor of size $70^{100} \approx 3.2 \times 10^{184}$ and a stochastic advection-diffusion-reaction equation with a tensor of size 4.7×10^9.

Data-Rich Multi-Fidelity Methods for Aerospace Vehicle Design

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Abstract

Two topics are described in this year's review. First, we further explore acceleration of CFD analysis via ML initialization, here considering ML-predicted wakes. An improved bluff-body flow initialization is efficiently obtained through the recursive use of CNN as applied to the wake region, providing over an order of magnitude speedup, a significant improvement over initializations limited to nearfield ML-predictions. Second, we compute the low-dimensional latent space associated with a minimum-compliance optimized structural topology and find latent-space clustering associated with changes in structural topology. Accuracy of reconstructed topologies is quantified and the variation of topological coherence on latent space coordinates assessed. The compact latent space is sufficient to identify unconstrained optima outside the training set and provides a pathway for highly efficient online, physics-based, stress-constrained optimization. For both topics, generalization of the procedures to appropriate arrays of design variables needs to be examined.

Interpolating many-electron wave functions through chemical space

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Abstract

It has been an exciting time in the field of quantum many-body problems, with new methods emerging for interacting electrons and their potential impact on fields such materials science or drug discovery – not least because of advances in the use of quantum computers and machine learning parameterizations. We have been contributing in this grant to this effort, bringing together the fields of tensor factorizations and neural network quantum states. However, as we push to higher accuracy in demanding problems, we have been aware that the field is increasingly disconnected from problems that take place on the timescales of atomic (rather than electronic) motion. This is because propagating atoms in time along with the explicit electronic structure entails a prohibitive number of electronic structure calculations. We will present our recent work to straddle this gap, with a surprisingly effective interpolation scheme, allowing efficient inference of the many-body electronic wave function through chemical space, and coupling this to the explicit motion of the atoms. We will show how this has enabled the advances in high-accuracy electronic structure to be coupled to molecular dynamics with unprecedented accuracy, for the first time enabling molecules to move on the *exact* potential energy surface, as provided by state-of-the-art tensor network or machine learning inspired many-electron states. This opens up advances in electronic structure to study realistic chemical reactions and photochemistry, and we will consider the dynamics of the Zundel cation, and the evolution of hydrogenic systems as our first investigations in this direction.

Optimal control of conditional processes: old and new.

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Abstract

In this talk, we consider the conditional control problem introduced by P.L. Lions in his lectures at the College de France in November 2016. As originally stated, the problem does not fit in the usual categories of control problems considered in the literature, so its solution requires new ideas, if not new technology. In his lectures, Lions emphasized some of the major differences with the analysis of classical stochastic optimal control problems and in so doing, raised the question of the possible differences between the value functions resulting from optimization over the class of Markovian controls as opposed to the general family of open loop controls. While the equality of these values is accepted as a "folk theorem" in the classical theory of stochastic control, optimizing an objective function whose values strongly depend upon the past history of the controlled trajectories of the system is a strong argument in favor of differences between the optimization results over these two different classes of control processes. The goal of the talk is to elucidate this quandary and provide elements of response to Lions' original conjecture, both in the case of "soft killing" (R.C. - Lauriere - Lions, Illinois Journal of Math) and in the case of hard killing for which together with D. Lacker ,we proved a new conditional mimicking theorem.

Multi-scale invariant models leading to new understanding of ductile damage

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Most of the efforts in modeling ductile damage concern materials for which the matrix irreversible behavior depends only on J_2, the second-invariant of the stress deviator (von Mises-type behavior). On the other hand, the experimental evidence suggests that for most metallic materials the plastic deformation depends on both J2, and J3, the third-invariant of the stress deviator. In this talk, we report results of a theoretical and numerical study that reveal the effects of the matrix sensitivity to J3 on the void evolution and strength of porous ductile materials. Moreover, we show that this sensitivity to J3 is tied to macroscopic plastic properties, namely the ratio between the tensile and shear yield strength, τ_Y/σ_T . It is shown that under axisymmetric loadings at fixed triaxiality, irrespective of the sign of J3, the lower is the τ_Y/σ_T ratio the greater is the rate of void growth or collapse, the rate of softening or compaction, and the change in the inter-void ligament along the direction of the minimum applied stress. For materials with $\tau_Y/\sigma_T < 1/\sqrt{3}$ the rate of void growth is faster for loadings such that $J3 > 0$ than for loadings where $J3 < 0$; the lower is the ratio τ_Y/σ_T , the more pronounced is the influence of the loading path on void growth. For loadings at fixed triaxiality such that $J3 = 0$, it is shown that materials with $\tau_Y/\sigma_T < 1/\sqrt{3}$ exhibit faster void growth and respectively collapse than under axisymmetric loadings, the opposite being true for materials with $\tau_Y/\sigma_T > 1/\sqrt{3}$. These findings may guide selection of materials such as to either promote or reduce the rate at which damage accumulates for a given loading.

Ambiguity-aware Artificial Intelligence via Statistical Inference

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Abstract

In this talk, we will introduce our YIP award titled "Ambiguity-aware Artificial Intelligence via Statistical Inference". Recent successes of machine learning (ML) and artificial intelligence (AI) in computer vision and natural language processing have garnered a great deal of attention. At the same time, ML and AI systems are built for straightforward prediction tasks by design, and struggle to handle ambiguity and uncertainty. Empirical evidence shows that such methods often fail in ambiguous situations. In this project, we aim to develop innovative mathematical methods and algorithms to help machine learning systems better deal with ambiguity. We will adapt tools from statistical inference (e.g., calibration, confidence intervals, prediction sets) to modern machine learning and artificial intelligence scenarios.

Bi-fidelity Optimization and Failure Probability Estimation

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Abstract

Reduced order, lower-fidelity, or surrogate models have shown great promise in reducing the cost of uncertainty quantification, reduced order modeling, and optimization of complex engineering systems, while producing comparable accuracy to high-fidelity models. We present two new developments regarding the use of lower-fidelity models for optimization and failure probability estimation. In the first part of the talk, we introduce a novel surrogate-adjusted line search algorithm that utilizes reduced-order or surrogate models to approximate the optimal step size in a gradient free optimization scheme. We provide a comprehensive theoretical analysis of the surrogate-adjusted line search algorithm, which includes a rigorous convergence analysis and a discussion on the trade-offs between the number of iterations and the accuracy of surrogate construction required for optimal step size adjustment. In the second part of the talk, we introduce an importance-sampling-based estimator, termed the Langevin bi-fidelity importance sampling (L-BF-IS) estimator for (failure) probability estimation. This estimator uses score-function-based sampling algorithms to generate new samples from a newly designed biasing distribution to substantially reduce the mean square error of the failure probability estimate. We demonstrate that L-BF-IS exhibits remarkable performance, particularly in situations with extremely high-dimensional (≥ 100) input space and limited high-fidelity evaluations. This is based on joint work with Nuojin Cheng and Stephen Becker from CU Boulder.

A Robust Multi-Physics Design Analysis and Optimization Framework for Hypersonic Systems Grounded in Rigorous Model Reduction

Charbel Farhat and Juan Alonso, Stanford University
Graham Candler and Maziar Hemati, the University of Minnesota
Matthias Heinkenschloss, Rice University
and Matthew Zahr, the University of Notre Dame

The development of hypersonic systems must overcome many physics, engineering, and computational challenges, including management of extreme heating; engineering of materials that withstand the consequences of such heat; design of control laws that enable maneuverability with high level of precision; and development of design optimization methods based on predictive and yet affordable numerical simulations. This complex problem is compounded by limited ground test facilities and segregated design and analysis tools. Its solution requires the right blend of tests and analyses. In this MURI effort, we proposed to overcome the computational challenges associated with this problem by developing an innovative, computationally tractable framework for tightly coupled multi-physics design analysis and optimization (MDAO) of hypersonic systems, under uncertainty.

For the last two years and a half, we have been building on recent advances in computational engineering sciences of relevance to hypersonic flight. We have achieved tight coupling between interacting physics by connecting the differential equations governing aerodynamics, structural dynamics, heat transfer. and flight control via most-appropriate transmission conditions, then discretizing these conditions by provably stable and accurate methods. To enable an exploration of the entire design space that is not possible with subsystem-by-subsystem approaches, we are simultaneously parameterizing the vehicle's trajectory, shape, material properties, and control law. We are achieving computational tractability by grounding our framework for tightly coupled MDAO under model-form and parametric uncertainties in surrogate modeling; developing methods for adaptive sampling in active manifolds to overcome the curse of dimensionality associated with training parametric surrogate models; and designing numerically stable and highly accurate partitioned analysis procedures for solving coupled surrogate models. In particular, we are developing novel approaches for reducing the dimensionality of highly nonlinear, steady and unsteady, multi-physics, multi-scale, computational models that mitigate if not break the Kolmogorov-width barrier using nonlinear approximation manifolds; can operate on embedded boundary models; can handle mesh adaptation; and are efficient in the context of MDAO under uncertainty. We are also developing innovative "on-the-fly" adaptive multi-fidelity approaches for MDAO under uncertainty that are synthesized from high-fidelity multi-physics models. We are developing rigorous and yet practical trust-region methods to manage the inexact objective and gradient evaluations produced by the framework to guarantee convergence.

In this lecture, we will focus on the recent achievements – that is, those accomplished so far during FY 2024.

At the highest fidelity level of numerical modeling, the research team at the University of Minnesota led by Candler has performed a series of trajectory optimization studies. To this end, they have parameterized a generic boost-glide vehicle geometry and computed a sequence of trajectories to obtain a reference geometry that maximizes range subject to specified constraints. For this purpose, they have relied on the flow solver US3D coupled with a one-dimensional conjugate heat transfer analyzer to represent the response of the thermal protection system. They have optimized two different types of trajectories: one characterized by a specified angle-of-attack; and another characterized by

a guided trajectory with pull-up and constant dynamic pressure glide. Their followup work will include the incorporation of moving control surfaces in the parametric high-dimensional model (HDM); and a controller in the numerical prediction of the trajectory. For this effort, they will rely on grid morphing approaches that they have recently developed to represent the control surface deflections and their effects on the body-fitted CFD mesh; and on the two-body (main system-control surface) representation of the dynamical vehicle system and the exact formulation of its governing equations that the Stanford University research team led by Farhat has derived and numerically studied during this reporting period.

Additionally, the Stanford University research team led by Farhat has completed during FY 2024 the development of a novel nonlinear projection-based model order reduction (PMOR) method and its tailoring to hypersonic flow problems. Unlike all other PMOR methods available in the literature, this method incorporates a model, formulated in its latent space, of the closure error associated with the traditional affine approximation. Furthermore, this closure model is constructed using a deep artificial neural network (ANN), which effectively blends PMOR at the high-dimensional fidelity level and deep learning at the latent space level. Using a Mach-parameteric version of the benchmark double cone hypersonic flow problem, where the Mach number is varied between 8 and 13, the Stanford research team has shown that the resulting CFD-based and ANN-augmented projection-based reduced-order model (PROM-ANN): can have a dimension that is almost as small as the intrinsic dimension of the solution manifold; its ANN component requires less than 2.7 minutes to train on a simple latptop; can be hyperreduced in less than 0.6 second on the same laptop to achieve computational efficiency in additional to low dimensionality; and most importantly, can solve the steady-state benchmark double cone hypersonic flow problem in less than 3 seconds on the aforementioned laptop, while delivering an accuracy level in the neighborhood of 99%. The followup research of this Stanford team will include the training of the PROM-ANN in the higher-dimensional parameter domain of hypersonic dive-pull-up-glide trajectories and their initial conditions – rather than the lower-dimensional Mach number parameter domain – to enable its application along the trajectories computed by the University of Minnesota.

The research team at the University of Notre Dame led by Zahr has made progress on three frontiers. First, they have extended their trust-region approach, which utilizes PROMs to accelerate hypersonic design problems, to handle problems with constraints that depend on the CFD solution. Their new approach integrates their existing trust-region method for unconstrained optimization problems into an augmented Lagrangian framework with necessary modifications to ensure global convergence. Second, they have improved their implicit shock tracking method that simultaneously determines optimal node locations and the corresponding flow solution to minimize an error metric. In particular, they have extended their method from inviscid flow problems to laminar and turbulent viscous flow problems, and have demonstrated its ability to produce accurate solutions on coarse grids. They have also developed a method for mesh-based parameterization of complex surfaces to ensure that nodes slide along complex vehicle geometries while fitting shocks near or on the surface. Finally, they have made similar improvements to their implicit feature tracking method, an approach to PMOR that concurrently determines an optimal domain mapping and generalized coordinates that minimize the approximation error. In particular, they have extended their original inviscid formulation to viscous hypersonic flow problems.

Led by Hemati, the second research team at the University of Minnesota has developed during FY 2024 a numerical framework for computing, for a given vehicle geometry, steady-state operating points at given altitudes and speeds, using a nonlinear model of the longitudinal motion of the vehicle and Newtonian aerodynamics. In this framework, a linear time-invariant model is extracted by lin-

earization about one such operating point; and a controller is designed based on the linear model and the principles of model predictive control (MPC) to stabilize the vehicle at that operating point. They have implemented the MPC controller and shown for a given vehicle geometry that it can stabilize the system when the open-loop counterpart is unstable, without violating the hard constraints on the magnitude of the control input (elevator/elevon deflections). They have also shown that in contrast, a controller based on the linear quadratic regulator violates the constraints for the same task. Furthermore, they have extended their numerical framework such that the vehicle operates at or close to the maximum lift-to-drag ratio for a set of pre-specified altitudes. They are currently implementing the MPC framework to design local controllers at each altitude corresponding to the latest steady-state computations. Future work will include the development of a scheduling scheme for the local MPC controllers so that the vehicle can fly through a segment of the trajectory obtained via joining the discrete altitude points utilized for the local controllers; and the extension of the framework to CFD-based PROMs for modeling the aerodynamics of the vehicle.

Led by Alonso, the second research team at Stanford University has developed SHARPE, a novel low-fidelity modeling framework for rapid, integrated analysis and design optimization of parametric boost-glide hypersonic vehicles. They have integrated this framework in an aero-thermal-structural-trajectory optimization procedure and used it to study multiple variations of problem setup; and to understand the importance of higher-fidelity modeling at different points along the vehicle's trajectory. To overcome the curse of dimensionality associated with training parametric PROMs or multi-fidelity models, they have derived adjoint-based sensitivity equations to optimally guide adaptive sampling at low computational cost. They have also combined both achievements to implement a framework for multi-fidelity and multi-disciplinary optimization of hypersonic boost-glide vehicles, and arbitrary trajectory-based objectives. They have demonstrated this framework, which is based on recursive Gaussian process regression, for multi-fidelity aero-thermal analysis using combinations of the low-fidelity analyzer SHARPE and the high-fidelity flow solver SU2.

At Rice University, the research team led by Heinkenschloss has developed complementary approaches for optimization using PROMs or more general surrogate models. Specifically, they have developed line-search based optimization algorithms using function approximations with tunable accuracy, to address the issue raised by the inexactness of the objective and/or constraint functions when approximated by PROMs or other surrogate models. In every iteration of their algorithms, the model must satisfy function error and relative gradient error tolerances that are automatically determined. Moreover, a bound for the model error is used to explore regions where the model is sufficiently accurate and use a current model as much as possible. The algorithms only use the models and error bounds: they never access directly the original objective function. The research team has proved first-order global convergence to a (local) solution of the original problem. In a complementary line of work, they have developed new algorithms for the refinement of the use of surrogate models in optimal control problems, including trajectory optimization problems for hypersonic vehicles. They have developed a new sensitivity analysis of the solution of optimal control problems with respect to component functions that are computationally intensive at the HDM level and thus are approximated by PROMs or other surrogate models (for example, lift and drag coefficients). They have also devised an initial approach for combining this sensitivity analysis with point-wise error estimates for the surrogate models, to determine whether the current parametric surrogate model is sufficiently accurate, or if not, determine where to refine it. This reduces the overall training cost of a surrogate model. They have demonstrated their approach on ODE-based trajectory optimization problems. Future work will include developing this approach for the optimal control problem governed by the two-body dynamical system developed at Stanford University.

Most importantly, we are committed to a paradigm shift in MDAO that will enable the fast, accurate, and robust design and optimization of hypersonic systems; the assessment of their stability, structural integrity, and maneuverability throughout their flight phases; and the guidance of ground and flight tests. We are training a new cadre of computational scientists both in the classroom and by reaching out and collaborating with researchers at AFRL and NRL, among others.

Koopman Operator Theoretic Methods for Efficient Training and Analysis of Deep Neural Networks

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Abstract

Our work concentrated on continuing to develop Koopman operator theoretical methods to provided theoretical foundations for neural network architectures, as well as developing prediction algorithms using Koopman operator theory. Our prediction algorithms have shown capability to beat state-of-the-art time-series prediction methods in complex biomedical time series and enabled performance-enhancing robotic prosthetics.

On the neural network analysis side, we continued to build an approach for identifying when the dynamics associated with training multiple deep neural network (DNN) models are topologically conjugate, via Koopman operator theory. We developed a rigorously founded theoretical approach to identify equivalence of algorithms in a data-driven manner. To validate our approach, we demonstrated that it can correctly identify a known equivalence between online mirror descent and online gradient descent. We then utilized it to study a variety of DNN architectures. First, we identified non-conjugate training dynamics between shallow and wide fully connected neural networks. Second, we characterized the early phase of training dynamics in convolutional neural networks, finding that ResNet-20 and LeNet have distinct dynamical regimes, but similarly transitions between regimes. Finally, we uncovered non-conjugate training dynamics in Transformers that do and do not undergo grokking. Our results, across a range of DNN architectures, illustrate the flexibility of our framework and highlight its potential for shedding new light on DNN training dynamics. Our approach is presenting a promising theoretical foundation for the design of AI architectures that can perform with small amount of data, enabling edge AI.

Our theoretical work on Koopman operator-based prediction concentrated on the observed shifts in prediction curves in complex noisy data. The source of the error was associated with hidden variables and initial condition phase shift. To facilitate such analyses in the Koopman operator framework, we continued to develop PyKMD, a data-driven scientific tool with a graphical user interface based on Koopman Operator Theory. It includes modules for advanced data preprocessing, dynamic mode decomposition, mode reduction, and Koopman modeling and prediction. To address the challenge of selecting an appropriate subspace of functions in Koopman Operator Theory, we also enhanced the

toolkit to enable experimentation with various observables, including monomials, trigonometric functions, and user-defined functions. We began development of PyGoSumD, a Python-based data analysis tool. PyGoSumD currently includes the DSample sampling algorithm and a sensitivity analysis module with state-of-the-art methods. We tested the framework in complex time series that are the source of prediction challenge benchmarks, and are at the same time of importance to the Air Force mission. Biomedical time series obtained from sensors that measure body functions are of such type. In absence of pilot performance data, we utilized PyKMD to predict blood glucose levels in patients with type 1 and type 2 diabetes and contrasted our predictions against the state-of-the-art prediction methodologies that included neural network based time series prediction methods. Our algorithms accurately predicted blood glucose levels 30 minutes ahead, and beat state-of-the-art algorithms by a substantial margin. Additionally, we used the PyKMD framework in the context of data-driven methods for robotic neurorehabilitation for people with impaired hand-grasping abilities. The developed real-time surface electromyography (sEMG) signal processing framework, based on the most influential parameters obtained through PyGoSumD sensitivity analysis, accurately assesses and predicts grip strength using a limited number of sEMG sensors. The predictive models of this type can be used to prototype advanced robotic rehabilitation devices by using them in concert with the Robotic Operating System. These types of approaches can be used in future AI-enabled pilot support methodologies, where pilot performance is enhanced using (e.g. soft robotic) prosthetics.

We are utilizing these methods in a cross section of problems of interest to the Air Force, including transitions such as participation in the DARPA AIR program.

Developments for Design under Uncertainty of Transient Systems

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Abstract

Challenges associated with uncertainty quantification of transient, time-dependent systems share similar limitations to gradient-based design under uncertainty (GbDuU) due to the need for large samples spaces and higher-order / higher-fidelity models. The additional computational costs associated with uncertainty quantification (UQ) must demonstrate benefits in robust and reliable design, as well as inform decision-making by identifying critical interdisciplinary couplings due to uncertainty. These challenges are being addressed by in-house efforts to incorporate UQ within the MSTC digital engineering enterprise, as well as leveraging several external foundational efforts, including: embedded emulator neural networks for design exploration; gradient-enhanced robust design optimization; stability and control of uncertainty aeroelastic systems; and, uncertainty quantification of transient thermal management. An update is provided for progress on the stochastic characterization of a dynamic system where the coefficients of the state variables are considered to be uncertain, and the resultant non-deterministic behavior of the time-dependent state variables must be calculated through simulation. For even the simple case of a linear time-invariant system in state-space form, the propagation of mean and variance over time becomes a linear time-varying system. This system is unstable for normal/gaussian coefficients, but may be characterized over specified time intervals, and may be stable for bounded distributions. Future directions in thermal management and aeroelasticity under uncertainty are considered.

Towards large-scale quantum accuracy materials simulations

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Abstract

Electronic structure calculations, especially those using density functional theory (DFT), have been very useful in understanding and predicting a wide range of materials properties. The importance of DFT calculations to engineering and physical sciences is evident from the fact that 20% of computational resources on some of the world's largest public supercomputers are devoted to DFT calculations. Despite the wide adoption of DFT, and the tremendous progress in theory and numerical methods over the decades, the following challenges remain. Firstly, the state-of-the-art implementations of DFT suffer from system-size and geometry limitations, with the widely used codes in solid state physics being limited to periodic geometries and typical simulation domains containing a few hundred atoms. This limits the complexity of materials systems that can be treated using DFT calculations. Secondly, there are many materials systems (such as strongly-correlated systems) for which the widely used model exchange-correlation functionals in DFT, which account for the many-body quantum mechanical interactions between electrons, are not satisfactory. Addressing these challenges will enable large-scale quantum-accuracy DFT calculations, and can significantly advance our *ab initio* modeling capabilities to treat complex materials systems.

This talk will focus on our recent advances in tackling these challenges. I will present the the progress in developing systematically convergent real-space methods based on higher-order adaptive finite element discretization, development of algorithms for large-scale eigenvalue problems that are at the heart of enabling large-scale DFT calculations, and efficient scalable numerical implementation of the methods (including mixed precision algorithms) that can take advantage of exascale computing architectures. I will also present on the progress in improving the model accuracy of DFT.

Schrödinger's control and estimation paradigm with spatio-temporal distributions

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Abstract

In a 1931 visionary contribution, Erwin Schrödinger, the father of Quantum Mechanics, laid out the foundations of large deviations' theory and of likelihood estimation in his quest to understand how randomness creeps into the description of the quantum world. In recent years, almost a century later, Scrödinger's paradigm has served as the blue print of novel stochastic control methods to regulate uncertainty by enforcing soft-probabilistic constraints on stochastic dynamics, and furthermore, the serendipitous confluence of stochastic control with the theory of Monge-Kantorovich optimal mass transport has renewed interest and provided new impetus to Schrödinger's original program [1].

We herein report theoretical and computational advances on a novel type of control and estimation problems [2-4], in the same vein as that of Scrödinger bridges, where control design allows regulation of spatio-temporal marginals for stochastic dynamics. The new formalism addresses practical stochastic control problems where the duration of an experiment is itself random. Such problems are typified by the landing of a module about a specified target, following a spacial distribution that depends on the time of landing. Examples of practical interest also include inverse problems to identify underlying stochastic dynamics for diffusive particles from observed absorption or deposition rates.

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Rigorous Optimal Uncertainty Quantification & Optimization

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Abstract

The success and survival of autonomous systems greatly depends on the systems' ability to quantify and reason about incomplete and uncertain information in actionable ways. Optimal Uncertainty Quantification (OUQ) provides a rigorous theoretical framework to this end by tractably bounding statistical measures of quantities of interest. Although OUQ is rigorous in theory, the rigor is lost in practice due to numerical solution approaches. This issue is further amplified when the quantities of interest are induced by dynamical systems. This works seeks to account for these issues and develop an *end-to-end rigorous OUQ* framework to support system, control, and mission design and optimization under uncertain and incomplete information by leveraging advancements in global optimization and validated numerics. In this talk we outline end-to-end rigorous OUQ, its core technology gaps, preliminary results, and potential applications.

Multiscale Stochastic Modeling, Conditioning, and Simulation of Rare Events

Roger Ghanem

In the first two years of this effort we constructed switching diffusion models that encode the interaction between fine scale damage accumulation and coarse scale behavior of composite and polycrystalline material systems. We also constructed estimators of the joint model that can be informed from only coarse-scale observations.

In the last year of this project, we leverage this multiscale stochastic construction to efficiently characterize the extremes of the behavior of associated material systems. Specifically, we characterize the first passage of coarse-scale stress, coarse-scale strain, and fine scale damage indicator beyond their respective critical values. We develop both computational tools for exploring these extremes as well as analytical connections to extreme-value theory.

Real Time Bayesian Inference and Prediction for High Fidelity Digital Twins Governed by Linear Time Invariant Dynamical Systems

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Abstract

Digital twins often demand real-time inference and prediction under uncertainty. We consider a class of such problems that are governed by linear time-invariant PDE systems, with inferred parameter fields representing boundary or volumetric forcing. This class includes transport or wave propagation source inversion problems from sensor data. We show that the discrete parameter-to-observable map has block Toeplitz structure, and that this structure can be exploited to design real-time FFT-based algorithms for computing the Bayesian posterior and posterior predictive, using the full high fidelity forward model. This is accomplished via offline precomputations that involve a modest number of full PDEs solutions (equal to the number of sensors), and an online real-time inference component that maps well onto GPU clusters. We demonstrate the algorithms on a problem of megathrust tsunami inference from near-field seafloor pressure sensors, governed by coupled acoustic–gravity waves. Despite the fact that a single forward wave propagation requires over 30 minutes on 1,792 CPU cores, and that there are $O(10^8)$ inversion parameters representing the seafloor motion, the Bayesian inverse problem can be solved exactly (up to discretization error) given real-time data in a fraction of a second of online time on a modest GPU cluster (24 Nvidia A100s). This represents a 100,000$\times$ speedup over a classical inverse solver.

From Many-Body Quantum Systems to Classical Turbulence: Novel Horizons of Tensor Networks

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Abstract

The objective of this research is to move towards quantum computing for modeling & simulation of turbulence and combustion systems. The essential idea is based on the use of a novel quantum-inspired tensor network (TN) algorithm, to be utilized for deterministic and stochastic description of such systems. Belonging to the class of TN algorithms, the matrix product state (MPS) was originally developed for approximating the state of quantum many-body systems, exploiting their correlation structure to accurately capture the underlying physics in a low-rank form (i.e., in a massively reduced state space). Here, the TN/MPS is invoked to simulate several reactive flow systems in scenarios where DNS, LES and RANS are the reference methods. Related to DNS, the governing equations of turbulent reacting flows are recast in the context of MPS, and their time evolution is simulated for various degrees of truncations. For LES and RANS, the TN/MPS is utilized for solving the PDF-FDF transport equations of chemically reactive turbulent flows. Due to their inherent capabilities, these equations are high dimensional. This curse of dimensionality can be managed via TN and is employed to tackle the Fokker-Planck form of the PDF/FDF under several conditions, instead of the modelled Langevin form as is typically done via Monte Carlo methodologies. Work is also in progress in using trotterization and variational (real or imaginary) time evolution for solving the linear convection-diffusion equation. The ansatz is implemented on the IBM Torino quantum computer, showing that the circuit depth is suitable for adequate hardware.

Versatile Mathematical Tools for Directed Energy Simulations

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Abstract

Achieving targeted specifications for fieldable fiber high-power laser systems remains challenging, despite progress in recent years. Roadblocks have persisted partly due to the complex trade-space of fiber parameters and nonlinearities in laser systems operating at high-power. This project aims to mitigate such difficulties by developing versatile mathematical tools, based on rigorous and foundational mathematics, to improve reliability, accuracy, and efficiency of state-of-the-art methodologies for analysis of optical fibers and amplifiers.

This year's report from Portland focuses on a new adaptive algorithm for computing eigenmodes and propagation constants of optical fibers with complex microstructure. It is motivated by last years' findings on the high sensitivity of the computed mode losses to modeling choices for certain fibers and their relation to fine-scale modal features we unearthed. To address the challenge of creating a general purpose mode computation tool for any fiber, we construct an adaptive eigenvalue algorithm, based on a dual-weighted residual error estimator. We show that the algorithm captures fine scale features arising in varied locations in various microstructures without any expert input and provides converged confinement loss values.

This year's report from Austin focuses on three subjects: 1) Quantitative comparison of two distinct fiber amplifier models (a high-fidelity Maxwell model developed in Austin, and a lower-fidelity coupled-mode-theory model developed in Portland); 2) Stability result for a model acoustic waveguide problem with impedance BC, leading to the theory of non-self-adjoint operators, which is the first step towards analyzing the bent fiber problem (an open problem thus far); and 3) Analysis of pulsed lasers using a novel formulation generalizing the classical nonlinear Schrödinger equation. We shall present a complete analysis and numerical results for the linearized problem in the space-time domain. Depending upon material constants, the problem is either hyperbolic or elliptic in space-time.

Abstract: Tensor networks: structure learning, uncertainty quantification, and PDE solutions
Alex Gorodetsky

In this talk we introduce a project seeking to develop automated computational techniques with quantified uncertainty for using tensor networks to exploit low-dimensional structure in solutions for high dimensional forward and inverse problems. We investigate tensor-network approaches to discover this structure and seek to answer some fundamental computational questions. For example, we seek to understand how do we choose an optimal tensor network structure? How do we adapt structures to specific data and problem settings? How do we leverage the unique multi-linear nature of tensor networks to perform rapid inference? How do we embed these methods to enable fast forward and inverse uncertainty quantification?

To address these questions, we develop probabilistic computational mathematical tools. Specifically, we will develop fast computation routines for tensor networks with arbitrary structure through randomized numerical linear algebra; investigate the performance of probabilistic ensembles of tensor network structures – as opposed to deterministic or probabilistic representations of fixed structures; discover and investigate randomized graph construction strategies to progressively build a network that balances edge growth and rank growth; and develop probabilistic tensor network approaches to the solution of high-dimensional PDEs and high-dimensional data problems (tensors with more than billions of elements) with quantified uncertainty for both forward and inverse problems.

Our approach is based on the following algorithmic development activities. We will develop core algorithms that leverage randomization for tensor network computing. These include new sampling techniques for inference of tensor networks, the application of graph learning approaches to tensor network learning, and embedding randomized linear algebra into the multi-linear setting.

The outcomes of this project will include new algorithms for computing with tensor networks and demonstrations of their effectiveness on challenging high-dimensional PDE problems. We aim to show that this technology enables general and adaptable scalability that is applicable to wide ranging systems of interest.

GPT-PINN and TGPT-PINN: Linear and nonlinear model order reduction toward efficient non-intrusive Meta-learning of parametric PDEs

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Abstract

Efficient multi-precision training of machine learning algorithms for parameter to solution maps promise significant gains, in both accuracy and efficiency, over the corresponding single-level machine learning algorithms, while providing a reduced carbon footprint.

In this talk, we present the recently proposed Generative Pre-Trained PINN (GPT-PINN). It mitigates both challenges in the setting of parametric PDEs. GPT-PINN represents a brand-new meta-learning paradigm for parametric systems. As a network of networks, its outer-/meta-network is hyper-reduced with only one hidden layer having significantly reduced number of neurons. Moreover, its activation function at each hidden neuron is a (full) PINN pre-trained at a judiciously selected system configuration. The meta-network adaptively "learns" the parametric dependence of the system and "grows" this hidden layer one neuron at a time. In the end, by encompassing a very small number of networks trained at this set of adaptively-selected parameter values, the meta-network is capable of generating surrogate solutions for the parametric system across the entire parameter domain accurately and efficiently. Time permitting, we will discuss the Transformed GPT-PINN, TGPT-PINN, which achieves nonlinear model reduction via the addition of a transformation layer before the pre-trained PINN layer.

Spectral correctness of the approximation of the first-order form of Maxwell's equations

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July 9, 2024

Abstract

I will discuss the role of involutions in the approximation of Maxwell's equations written in first-order form and with non-homogeneous magnetic permeability and electric permittivity. Although the Sobolev smoothness index of the solution may be smaller than $\frac{1}{2}$, it is shown that the approximation is spectrally correct. The convergence proof is based on a duality argument. One essential idea is that the smoothness index of the dual solution is always larger than $\frac{1}{2}$ irrespective of the regularity of the material properties, whereas the smoothness of the solution may be smaller than $\frac{1}{2}$.

Discrete involutions play a key role in the analysis. The take home result from this work is that the discontinuous Galerkin approximation of Maxwell's equation naturally enforces Gauss's law. No extra stabilization has to be added. This result holds true for the discontinuous Galerkin approximation of the ideal MHD equations.

Multi-Scale Approaches for Physics Understanding and Model Development of Turbulent Combustion

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Abstract

Data Assimilation (DA) is needed to systematically bridge the gap between available experimental data and high-fidelity numerical simulations. The DA problem in combustion faces challenges from nonlinearity, extremely sparse, indirect, and incomplete data, multi-scale nature of the flow, and the presence of shocks and other features with sharp gradients. Recently, we have investigated the performance of three filtering-based sequential data assimilation (DA) methods applied to compressible flows. The three methods that are considered are the Ensemble Kalman Filter (EnKF), the Extended Kalman Filter (EKF), and the Particle Filter (PF). Their suitability at handling a combination of strongly nonlinear discontinuities and non-Gaussian statistics is of interest. Initial implementation of the DA is focused on the one-dimensional Euler equations of gas dynamics. The ability of the methods to handle sparse data as well as large deviations between prior data and truth solutions is evaluated.

Initial results show that the realizability of the solutions during the DA process is a challenge. To address this, we have implemented and evaluated several positivity-enforcing variable transformations. For the non-reacting flow, these transformations show that such a procedure is capable of maintaining thermodynamic realizability, yielding higher quality state estimates than before. For the one-dimensional detonation tube, the variable transformation approach is able to avoid the non-physical thermodynamic states. The current implementation however did not prevent the generation of new local extrema in the solution which is an area of future work.

Data-Driven Reduced-Order Modeling for Turbulent Combustion Model Development

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Abstract

Even with the rapid advancement in high performance computing, direct numerical simulations (DNS) remain restricted to small-scale turbulent combustion physics. While large-eddy simulations (LES) are well suited to model large-scale physics, the effects of small-scale physics must be incorporated through closure models, most of which are assumption-based and cannot represent the true physics, especially at practical conditions in aerospace systems. Against this landscape, the present work focuses on developing a data-driven reduced-order modeling framework to: 1) formulate appropriate model reduction techniques to inform effective reduced-order models (ROMs) from representative turbulent reacting flow DNS to represent subgrid-scale (SGS) or subfilter-scale (SFS) physics (referred to as DNS-ROM); and 2) enhance LES by incorporating DNS-ROM for SGS/SFS physics to enable efficient and accurate turbulent combustion simulations in aerospace systems (referred to as hybrid LES/DNS-ROM framework). In this talk, we examine the framework in two aspects. First, we investigate the use of POD basis to representative SFS physics (e.g., stresses, scalar fluxes, and reaction rates) based on the DNS data of premixed turbulent flames at high Karlovitz number conditions. We show that with reasonable number of POD modes, the SFS physics can be well represented. Second, we study the LES/DNS-ROM coupling using a 1D burgers' equation with prescribed initial spectrum to mimic the isotropic homogeneous turbulence decays. We show that the hybrid LES/DNS-ROM framework can accurately match the filtered DNS solutions.

Structure-preserving particle method for the Landau equation modeling plasma collisions – some extensions

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Abstract

In the past two years, we have developed a collisional particle-in-cell (CPIC) method for plasma dynamics which can account for the collisional effects modeled by the Landau operator. The method is derived from the gradient-flow formulation of the Landau equation, thereby preserving the collision invariants and entropy structure at the semi-discrete level. In this talk, we will discuss extensions of this method we explored last year in two directions: 1) We introduce a particle method for the multi-species Landau equation which is the more realistic setting for plasma applications. 2) We introduce a fully discrete entropy-dissipative and energy-conservative particle method by employing the discrete gradient integrator.

Inference of Forcing Kernels in Generalized, Multi-Physics, Dynamic Systems

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Abstract

The multi-physics dynamics of high-speed, shocked, droplet-laden flows are intricate. The accurate theoretical and experimental prediction of these dynamics in technologies relevant to the Air Force, such as rotating detonation engines and the erosion of missile cones by condensed droplets, has proven tremendously challenging. Central to modeling and observation challenges are (1) the extreme dynamical and thermodynamical scales, and (2) a marginal general understanding of the non-linear, stochastic and intermolecular, inter-phase forcing. Fast processes limit the observable data to snapshots of shadowgraphs of the droplet shape, while a reduced fidelity of process-scale models for droplet deformation and shock dynamics prevents a reliable engineering analysis. We discuss efforts towards the development of a method that infers forcing kernels of systems of computational, multi-physics, and particle clouds from limited, high-fidelity data with confidence intervals. Firstly, we present a method derived to replace a Wiener process in general Langevin models with a set of random forcing variables, whose distributions are tuned to match the observed statistics. We show that this gives rise to an exact deterministic, first-order, hyperbolic Liouville equation. Analytical PDF solutions for canonical models of particle-laden flows serve to establish a relationship between the Langevin and Liouville approaches. Secondly, we discuss a generalized variational formulation for a cloud moment dynamics system of ODEs, which minimizes the cost function based on sparse, limited data of the cloud moments to obtain information about the cloud's forcing function through adjoint operators. This adjoint-based inverse formulation is tested for a one-dimensional, two-way coupled shock-cloud interaction.

New shock mathematics: Humans, machinery and AI

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Abstract

What large-scale cohesive behaviors – desirable or dangerous – could suddenly emerge from systems with interacting humans, machinery and software including AI? When will they emerge? How will they evolve and be controlled? Here we offer some initial thoughts on these urgent questions by introducing new empirically-grounded shock formation mathematics that accounts for entity diversity – akin to encoding tokens in high-dimensional vector spaces in machine learning/AI. We discuss some preliminary solutions for the time-to-cohesion and growth-of-cohesion for two species, and some generalizations for an arbitrary number of species. These solutions reproduce – and offer a microscopic explanation for – an anomalous nonlinear growth feature observed in related real-world systems, including AI itself (e.g. so-called AI grokking in a a modular addition test case). Our theory suggests good and bad 'surprises' (extreme events) will appear sooner and more strongly as humans-machinery-AI etc. interact more – but it also offers a rigorous approach for understanding and controlling this.

Learning and Meta-Learning of Partial Differential Equations via Physics-Informed Neural Networks: Theory, Algorithms, and Applications

George Em Karniadakis and Jerome Darbon (Brown University)
Houman Owhadi and Andrew Stuart (Caltech)
Robet M. Kirby and Shandian Zhe (University of Utah)
Charbel Farhat (Stanford University)

July 11, 2024

At **Brown University**, we have developed a novel neural network architecture to address high–dimensional optimal control problems with linear and nonlinear dynamics. It allows us to solve path planning problems involving many agents in real time. Our approach relies on introducing a time-dependent symplectic network into the architecture that allows us to send the original optimal control problem into the solution of a Hamilton-Jacobi partial differential equation. In addition, we propose a general latent representation of the symplectic map, which greatly improves model expressivity based on the universal approximation theorem. We have successfully demonstrated the efficacy of our novel architecture for path planning problems with obstacle and collision avoidance, including systems with Newtonian dynamics and non-convex environments, up to dimension 512. Our method shows significant promise in handling efficiently both complex dynamics and constraints.

In addition, we have developed a new version of physics-informed networks based on the Kolmogorov-Arnold Metworks (KANs), the so-called PIKANs. We have performed a fair comparison with PINNs and published a paper https://arxiv.org/abs/2406.02917. Moreover, we have tackled many linear and nonlinear PDEs in high dimensions using PINNs (over 100,000 dimensions) and demonstrated that PINNs can beat the curse-of-dimensionality (https://arxiv.org/pdf/2402.07465, https://arxiv.org/pdf/2404.05615).

At **Caltech**, the initial focus of the group was on GP-based solutions of forward and inverse problems. Among several advantages, our formulation leads to a perspective on PINNs-like methodologies which, in addition to allowing practical computations, is also amenable to analysis and deeper theoretical understanding than afforded by neural network-based approaches. This approach leads to new methods and a deeper understanding of existing methods. In a follow-up work, we are currently generalizing the proposed approach to rough nonlinear PDEs (SPDEs) while maintaining theoretical and computational guarantees. This generalization has the potential to be extended to singular PDEs (e.g., KPZ) and lead to a natural framework for analyzing such PDEs that might be simpler than regularity structures/rough paths.

Under this broad umbrella, the work of co-PI Stuart has focused on two questions: (i) the development of uncertainty quantification through a Bayesian interpretation of the GP-based methodology; (ii) a study of inverse problems and the implied novel priors that follow from adopting a GP-based approach. A paper in area (i) has been submitted for publication and may be found on the arXiv (https://arxiv.org/abs/2405.13149), and work in area (ii) is ongoing.

The proposed GP-based approach also fits into a broader GP-based framework (Computational Graph Completion) enabling the completion of computational graphs (in which nodes and edges represent possibly unknown variables and functions) with known connectivity. Under this umbrella, the work of CoPI Owhadi in collaboration with Bamdad Hosseini has focused on applications towards learning generative models with rigorous a priori error estimates (https://arxiv.org/abs/2402.08077) and towards the learning of arbitrary nonlinear differential equations (with rigorous a priori error estimates) in the presence of scarce data. The work of CoPI Owhadi has also been focused on a generalization of the Computational Graph Completion framework towards the setting where the connectivity of the graph may be unknown. This generalization enables the co-discovery of graphical structures and functional dependencies within data. While causal inference methods suffer from their super-exponential complexity with respect to the number of underlying variables, the proposed approach has polynomial complexity, and it, therefore, opens potential applications to the discovery of very large graphs/hypergraphs. A paper has been accepted for publication in PNAS (https://arxiv.org/abs/2311.17007).

At the **University of Utah**, we have completed two projects covering our collaborative MURI work on PINNs and Operator Learning. In the first project, we analyze, benchmark, and generally compare one PINN approach to another. Using Kolmogorov n-widths as a measure of effectiveness of approximating functions, we judiciously apply this metric in the comparison of various multitask PIML architectures. We compute lower accuracy bounds and analyze the model's learned basis functions on various PDE problems. This is the first objective metric for comparing multitask PIML architectures and helps remove uncertainty in model validation from selective sampling and overfitting. We also identify avenues of improvement for model architectures, such as the choice of activation function, which can drastically affect model generalization to "worst-case' scenarios, which is not observed when reporting task-specific errors. We also incorporate this metric into the optimization process through regularization, which improves the models' generalizability over the multitask PDE problem. In our second project, we examine the Fourier Neural Operators (FNOs), a popular operator learning framework. In our experience, collecting training data for the FNO can be a costly bottleneck in practice because it often demands expensive physical simulations. To alleviate this challenge, we have developed Multi-Resolution Active learning of FNO (MRA-FNO), which can dynamically select the input functions and resolutions to lower the data cost as much as possible while optimizing the learning efficiency. We first propose a probabilistic multi-resolution FNO and develop an effective Bayesian training algorithm with Monte-Carlo ensembles. To conduct active learning, we maximize a utility-cost ratio as the acquisition function to acquire new examples and resolutions at each step. We use moment matching and the matrix determinant lemma to enable tractable, efficient utility computation. Furthermore, we develop a cost annealing framework to avoid over-penalizing high-resolution queries at the early stage. We have shown the advantage of our method in

several benchmark operator learning tasks.

At **Stanford University**, the research team has made significant advances on three different fronts: the acceleration of projection-based model order reduction (PMOR) by modeling the closure error in the latent space using deep learning; the design of a multi-modal loss function for regularizing the nonparametric probabilistic method (NPM) for modeling and quantifying model-form uncertainty and performing digital twinning; and the expansion of the scope of their physics-based machine learning (PBML) framework for multiscale material modeling. In the first arena, the team has demonstrated the ability of their PMOR-deep learning framework to solve in real-time challenging, parametric, hypersonic flow problems using projection-based reduced-order models of dimensions as low as the intrinsic dimension of the solution manifold. In the second front, they have developed a parameter-free regularization approach for NPMs loss function and demonstrated the potential of the regularized NPM for constructing a digital twin of the instance type for the structural health monitoring of a fighter aircraft. In the third area, the team has expanded the scope of their PBML framework for data-driven constitutive modeling to guarantee not only dynamic stability, material stability, internal variable stability, objectivity, and consistency, but also fading memory, the recovery of elasticity, material non-inversion, and the second law of thermodynamics. Most importantly, they demonstrated the ability of this PBML framework to genuinely discover the constitutive law of the multiscale soft good used in Perseverances parachute canopy, rather than simply regress its stress-strain data.

SDDC Solutions of Kinematic Dynamo Problems

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Abstract

The Spectral Difference with Divergence Cleaning (SDDC) method has been used to successfully model a number of nonlinear MHD problems [1, 2]. The spectral difference method is a versatile high order method that can be used for unstructured grids and can be massively parallelized. In this study, the SDDC method is applied for solving two kinematic dynamo problems. The first kinematic dynamo problem was solved in a cubic box with all periodic boundary conditions. The SDDC method is verified to capture the 'Cigar' structures published in the literature [3]. The second kinematic dynamo problem adopts a spherical shell geometry and non-penetrative and stress-free boundary conditions [4]. The SDDC method will be employed to predict Sunspot cycles [5].

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Transport information geometric computations

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Abstract

We provide a numerical analysis and computation of neural network projected schemes for approximating one-dimensional Wasserstein gradient flows. We approximate the Lagrangian mapping functions of gradient flows by the class of two-layer neural network functions with ReLU (rectified linear unit) activation functions. The numerical scheme is based on a projected gradient method, namely the Wasserstein natural gradient, where the projection is constructed from the L^2 mapping spaces onto the neural network parameterized mapping space. We establish theoretical guarantees for the performance of the neural projected dynamics. We derive a closed-form update for the scheme with well-posedness and explicit consistency guarantee for a particular choice of network structure. General truncation error analysis is also established on the basis of the projective nature of the dynamics. Numerical examples, including gradient drift Fokker-Planck equations, porous medium equations, and Keller-Segel models, verify the accuracy and effectiveness of the proposed neural projected algorithm.

If time allows, I will also discuss some updates on other developments in 2023-2024, such as deep JKO methods, high-order computations of mean field control problems, regularized Wasserstein proximal sampling methods, and convergence analysis in stochastic differential equations.

New frontiers in greedy approaches for linear and nonlinear model reduction

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Abstract

We report on new linear and nonlinear model reduction methods applied to differential equations. For linear reduction of linear (time-invariant) dynamical systems, we present a greedy-type algorithm that builds a reduced order model through progressive enrichment of a linear low-dimensional subspace approximation in the frequency domain. A significant feature of our procedure is that it is directly applicable to parametric differential equations and comes with *a posteriori* error bounds, and in particular that through sectorial properties of the differential equation operator yields *a priori* error estimates and rates of convergence. We demonstrate that in practice our procedure produces reduced order models whose accuracy on particular parameter values is comparable to gold-standard non-parametric methods such as balanced truncation. We also discuss recent work on nonlinear model reduction leveraging deep learning-based snapshot transformations that can effectively learn low-dimensional latent approximations to solutions of transport-type and -dominated differential equations.

MURI: Innovations in Mean-Field Game

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Abstract

In the year 2023-2024, the MURI team continue developing fundamental breakthroughs on mean field games (MFG) theory, fast and scalable numerical schemes based on AI and high order computational methods, and modeling in social science and engineering applications. Selected results are presented below.

AI and Sampling algorithm:

- Wasserstein proximal operators describe score-based generative models and resolve memorization.
- Numerical analysis of a first-order computational algorithm for reaction-diffusion equations via the primal-dual hybrid gradient method.
- Tensor train based sampling algorithms for approximating regularized Wasserstein proximal operators.
- A deep learning algorithm for computing mean field control problems via forward-backward score dynamics.

Theoretical result:

- We propose a way to discretize the common noise operator, in random optimal control problems. This allows us to study new types of quantum games, which rely on a time discrete family of semi-circle possesses.

In-context learning:

- PDE generalization of in-context operator networks: A study on 1d scalar nonlinear conservation laws.
- In-context operator learning with data prompts for differential equation problems.
- Prompting in-context operator learning with sensor data, equations, and natural language.

Primal-dual damping algorithms:

- Numerical analysis of a first-order computational algorithm for reaction-diffusion equations via the primal-dual hybrid gradient method.
- Primal-dual hybrid gradient algorithms for computing time-implicit Hamilton-Jacobi equations.

- A Primal-dual hybrid gradient method for solving optimal control problems and the corresponding Hamilton-Jacobi PDEs.

Engineering applications:

- Research on game theory meets data augmentation, federated learning, edge computing, LEO satellite networks.

Mean field modeling for spatial evolutionary games:

- Agent-based EGT Model of the Emergence of Symbolic Norms.
- An Approximation Framework for Large-scale Spatial Systems.

Parametric model reduction of stochastic systems via population dynamics

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Abstract

The aim of this work is to learn models of population dynamics of physical systems featuring stochastic effects and a dependence on physics parameters. The learned models can act as surrogates of classical numerical models to efficiently predict the system behavior. By population dynamics we refer to the evolution of the ensemble of samples (particles) 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.

Inference-oriented model reduction for linear Bayesian smoothing problems

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Abstract

We consider the Bayesian smoothing problem of inferring the unknown initial condition of a linear dynamical system from noisy linear measurements taken after the initial time. When endowed with a Gaussian prior and Gaussian noise model, this defines a linear-Gaussian Bayesian inverse problem whose posterior statistics can be optimally approximated in a low-rank subspace defined by the dominant generalized eigenvalues of the matrix pencil consisting of the Hessian of the log-likelihood and the prior precision. We use this subspace to define an *inference-oriented* projection-based reduced model via Petrov-Galerkin projection of the full system operators onto this inference-oriented subspace. We exploit connections between this new procedure and balanced truncation, a system theoretic control method, to prove that the new reduced model recovers the optimal posterior approximation in certain limits. Numerical experiments demonstrate that the reduced model can be used to accelerate an ensemble-based inference algorithm by orders of magnitude while high accuracy in the posterior approximation.

Title. A Semi-Lagrangian Adaptive-Rank Method (SLAR) for Linear Transport and Nonlinear Vlasov-Poisson Systems.

PI. Jingmei Qiu, University of Delaware, FA9550-22-1-0390.

Abstract. High order semi-Lagrangian methods for kinetic equations has been well-developed in the past few decades. In this work, we propose a semi-Lagrangian finite difference method that explore the adaptive-rank structure of the Vlasov-Poisson solution to further improve computational efficiency. Besides using extra large time stepping sizes via the semi-Lagrangian setting, the proposed method explores the low rank structure of the Vlasov solution by the cross approximation of matrices, which is also known as the CUR decomposition or pseudo-skeleton approximation. Such approximation could be obtained by selecting the columns and rows that best represent the solution matrix via a randomized pivoting strategy. Following the semi-Lagrangian update of the Vlasov solution via cross approximation, we apply a singular value truncation, as well as a mass conservative projection, of the Vlasov solution, for numerical stability and local mass conservation. The computational complexity scales linearly with respect to the mesh size N per dimension, in contrast to a N^2 for traditional full rank schemes, in each time step. A wide range of benchmark tests are performed, to demonstrate the efficiency and effectiveness of the proposed scheme.

Kernel Methods with Machine Learning and Adaptivity

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Abstract

Kernel methods, which include the more well known Radial Basis Function (RBF) based methods, have grown in popularity over the last three decades for the purposes of interpolation, numerical differentiation, quadrature/cubature and the solution of partial differential equations (PDE). These methods are straightforward to implement–analogous to polynomial based methods–and can be highly accurate even in the presence of scattered data and on complex domains. Due to these recent successes we investigate new computational tools that

- combine the benefits of kernel methods with advances in machine learning to overcome issues of stability in the numerical integration of semi-discrete PDEs.
- automatically adapt local kernel methods to achieve a prescribed tolerance on the accuracy of the approximation.

These computational tools will inform improved numerical simulations of the interaction between lasers operating at high power and the medium that the laser is propagating through.

A Machine Learning Framework for High-Dimensional Mean Field Games and Optimal Control

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Abstract

This project develops a machine learning framework for the numerical solution of high-dimensional mean field games and optimal control problems, e.g., problems in which the state space dimension is in the tens or hundreds. The framework targets applications where optimal controls can be obtained from the value function, and the latter satisfies high-dimensional Hamilton-Jacobi-Bellman (HJB) equations. We combine the approximation power of neural networks with the scalability of Lagrangian PDE solvers to mitigate the curse of dimensionality (CoD) that limits the use of traditional numerical solvers. Specifically, we parameterize the value function with a neural network and train its weights using a tailored objective function that includes penalty terms enforcing the HJB equations. A key benefit of our framework is that no training data is needed, e.g., no numerical solutions to the problem must be computed before training.

In this talk, I will summarize the outcomes of the project, highlight opportunities for practical applications, and present open challenges.

Deep Learning applied to Graph Problems

Amin Saberi

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Abstract: Geometric deep learning aims to generalize neural models to non-Euclidean domains such as graphs and manifolds. The field has made promising advances and remarkable performance improvements over the last few years. The goal of this project is to develop a foundational understanding of this new and exciting area.

The focus of today's talk is on MAGNOLIA, a Graph Neural Network (GNN) based algorithm for solving graph matching problems. We are studying Online Bayesian bipartite matching and introduce a graph neural network (GNN) approach that emulates the problem's combinatorially-complex optimal online algorithm, which selects actions (e.g., which nodes to match) by computing each action's value-to-go (VTG) -- the expected weight of the final matching if the algorithm takes that action, then acts optimally in the future. We train a GNN to estimate VTG and show empirically that this GNN returns high-weight matchings across a variety of tasks. Moreover, we identify a common family of graph distributions under which VTG can be efficiently approximated by aggregating information within local neighborhoods in the graphs. This structure matches the local behavior of GNNs, providing theoretical justification for our approach.

Information Geometric Regularization of the Barotropic Euler Equation

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Abstract

A key numerical difficulty in compressible fluid dynamics is the formation of shock waves. Shock waves feature jump discontinuities in the velocity and density of the fluid and thus preclude the existence of classical solutions to the compressible Euler equations. Weak "entropy" solutions are commonly defined by viscous regularization, but even small amounts of viscosity can substantially change the long-term behavior of the solution. In this work, we propose the first inviscid regularization of the multidimensional Euler equation based on ideas from semidefinite programming, information geometry, geometric hydrodynamics, and nonlinear elasticity. From a Lagrangian perspective, shock formation in entropy solutions amounts to inelastic collisions of fluid particles. Their trajectories are akin to that of projected gradient descent on a feasible set of non-intersecting paths. We regularize these trajectories by replacing them with solution paths of interior point methods based on logarithmic barrier functions. These paths are geodesic curves according to the information geometry induced by the barrier function. Thus, our regularization amounts to replacing the Euclidean geometry of configuration space with a suitable information geometry. We extend this idea to infinite families of paths by viewing Euler's equations as a dynamical system on a diffeomorphism manifold. Our regularization embeds this manifold into an information geometric ambient space, equipping it with a geodesically complete geometry. Expressing the resulting Lagrangian equations in Eulerian form, we derive a regularized Euler equation in conservation form. Numerical experiments on one and two-dimensional problems show its promise as a numerical tool. While we focus on the barotropic Euler equations for concreteness and simplicity of exposition, our regularization easily extends to more general Euler and Navier-Stokes-type equations.

A Scientific Foundation Model for PDEs: Multi-Operator Learning and Extrapolation

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Abstract

Foundation models have been successful in addressing various language and image processing tasks. In this talk, we introduce a multi-modal scientific foundation model for predicting and discovering partial differential equations, named PROSE-PDE. Our model, designed for bi-modality to bi-modality learning, is a multi-operator learning approach which can predict future states of spatiotemporal systems while simultaneously learning the underlying governing equations of the physical system. We will discuss extrapolation tests, generalization of physical features, and other computational studies.

ABSTRACT

Title: Machine Learned Turbulence Modeling (MLTM)

Investigators: Christopher Schrock (PI)
Organization: Air Force Research Laboratory, Aerospace Systems Directorate (WPAFB, OH)
Presenter: Christopher Schrock

This effort seeks to improve Reynolds Averaged Navier Stokes (RANS) models and predictive capabilities for aerospace systems design and analysis. The task is exploring machine learning (ML) approaches to increase accuracy of RANS solvers. Over the past several years, this effort has examined acceleration of RANS solvers using ML initialization, the development of an elliptic input feature (EIF) input space and output basis, and development of turbulence modeling approaches employing Graph Neural Networks. Results will be presented to highlight developments which have occurred during the first year of this renewal lab task. Over the past year, work has focused on the incremental implementation of MLTMs within a CFD solver, model feature importance studies, turbulence realizability encoding within network architecture.

Data-Driven Discovery of Optimized Multifunctional Material Systems Center of Excellence (RX, AFOSR, CMU)

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Abstract

This center of excellence has been focused on engineering and scientific questions at the intersection of materials science and machine learning/artificial intelligence and developing the workforce in these areas.

For this review, two students from the center will be presenting some of their work.

Zach Varley (zvarley@andrew.cmu.edu) will present on: In the context of multimodal image registration, we derive generalized non-standard 3rd and 4th order Edgeworth series expansions of mutual information. We then join this formulation with fast Fourier transforms for dense computation of mutual information over discrete image shifts, conventionally called the cross mutual information function. Traditional binning based approaches to its calculation, although straightforward to implement and faster than brute force methods, require a number of cross correlations that grows quadratically with the number of bins. Edgeworth series expansions effectively reduce this computational burden to 10 cross correlations for a 3rd order expansion, and 15 for a 4th order expansion. We benchmark the accuracy and run-time performance of several variants of our method and compare the results with those of the binned cross mutual information function.

Alex Gourley (agourley@andrew.cmu.edu) will present on: Binder jetting technology is capable of producing ceramic and metallic parts, but low green densities and spreading anomalies reduce the predictability and processability of resulting geometries. In-situ feedback presents a method for robust evaluation of spreading anomalies. Developing models to process images trained on small quantities of data reduces the number of required builds to refine processing parameters in a multivariate space. In this study, we generated and compared U-Net semantic segmentation models for visually different powders using single builds for training data, identifying the challenges of extending existing segmentation methods to visually lighter oxide powders. Leveraging preexisting analysis tools allowed for rapid analysis of oxide powder by providing an accessible framework for implementing neural networks. Robust analysis techniques and the demonstration of correcting anomalies with processing parameters show promise for the development of automation with in-situ feedback.

Navigating the mapping between process and microstructure

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Abstract

Microstructure sensitive design rests on two assumptions: (1) that the mapping between process and microstructure are continuous and (2) that this mapping is continuously invertible. These assumptions are made for convenience, since they allow for an incremental approach to materials design, but designers are not cognizant of the larger mathematical implications of these assumptions. A *homeomorphism* is a very specific functional mapping in topology defined precisely as above, and for which a considerable number of behaviors have been shown to be true. Typically, designers and materials engineers work together in *very* narrow regions of design space where they intuit these might be satisfied. This has the disadvantage that it makes the design strategy needlessly restricted and that, if the intuition is wrong, a considerable uncertainty as to 'what went wrong' is generated.

We propose to investigate the mapping between process and microstructure with phase field modeling as a random process to generate microstructure samples under controlled processing conditions. These will be used to develop neural networks that will map these microstructures into a *latent space*, i.e. the low dimensional manifold on which, by hypothesis, the microstructure samples would lie. The topological properties of this mapping between the process variables and the microstructure manifold could then be investigated independently. As an example, dimensionality, a topological property, can estimated from these samples alone to characterize the microstructure latent space.

From here, other hypotheses may be tested in order to validate (or reject) the claim that process is homeomorphic to microstructure. Examples may be homology, the number of connected regions, the number of 'holes,' the number of 'tunnels,' etc. which must be the same between the domains if the mapping were homeomorphic. With some exploration, this could give some estimate of the bounds of the region of homeomorphism.

The potential implications of studying the microstructure manifold in the latent space, are (1) being able to understand the result of process limitations on microstructure, (2) finding rare events, (3) navigating along independent dimensions in microstructure space, which are directly related to necessary changes in processing space, and (4) developing a methodology for identifying the extent

Mesh Generation and AI-enhanced Algorithms for Modeling Complex Materials Systems

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Abstract

This presentation will focus on the latest updates in developing the Deep Learning-Driven Domain Decomposition (DLD^3) algorithm and its application for modeling linear elastic problems. DLD^3 is a novel, generalizable AI-driven modeling framework capable of approximating the field in problems with arbitrary geometries, boundary conditions (BCs), and material properties. This method combines a set of pre-trained Fourier Neural Operator (FNO) models with the Schwarz Domain Decomposition (DDM) technique to approximate the field. A partitioning algorithm is employed to break down a given domain into several subdomains with 50% overlap, where the FNO model can predict the response during DDM iterations. The FNO model needs to be trained using a dataset with millions of entries consisting of subdomains with various shapes, BCs, and material properties. This training dataset is constructed using an automated finite element (FE) modeling framework involving virtual geometry reconstruction and meshing algorithms, which are developed through prior support from the Comp Math program. Despite the high cost of constructing the training dataset and subsequently training the FNO models, the generalizability of DLD^3 sets it apart from other scientific AI/ML algorithms. In this work, we show the excellent accuracy of DLD^3 for modeling plane strain linear elasticity problems with various geometries and BCs. Compared to an FE simulation, this technique can significantly reduce the operation cost (no mesh generation is required) and computational cost (does not involve solving a linear system of equations) of the simulation. We also discuss plans for further expanding DLD^3 and its future applications for modeling nonlinear problems.

of homeomorphic regions in latent space where incremental changes may be safely made. Additionally, since homeomorphism is transitive, if a sub-region of a processing-microstructure region were homeomorphic to a region in property space, this would give a direct homeomorphic mapping between process and property, a longstanding dream of materials design. If this were true, materials characterization could be separated from materials design, at least over that region, and processes could be directly modified to produce desired properties. All of these would enable true autonomous materials development with microstructure design. We will present on plans for work beginning in the fall, some seedling work on dimensionality estimation and some work on developing criterion for microstructure descriptors.

Feature-Informed Data Assimilation: Making Sense of Binary-Sensor Observations

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Abstract

Abstract: Many sensors report feature data, e.g., shock locations and level curves, in a binary form. In doing so, a sensor converts a continuous state variable into a positive or negative reading. Estimation of the state and parameters of the system from binary observations is challenging due to at least two reasons. First, information content of binary observations is lower than that of their continuous counterparts, which hinders the system's observability and identifiability. Second, the discrete nature of binary observations poses a challenge to variational data assimilation methods. We show that a dynamical system with continuous forward model and observation operators is almost surely non-identifiable under binary observations and establish a metric to quantify the degree of non-identifiability of the system. We supplement this theoretical result with numerical experiments, which demonstrate that binary observations contain valuable information for parameter estimation. We propose two variational approaches to parameter estimation from binary observations: a constrained optimization and a constraint-free optimization. We apply our algorithms to analyze in-host virus dynamics and immune response to COVID-19.

Title. MURI: Tensor Approaches for Simulating Kinetic Systems

PIs
Andrew Christlieb, Michigan State University
Jingwei Hu, University of Washington
Jingmei Qiu, University of Delaware
Edgar Solomonik, University of Illinois Urbana-Champaign
Daniele Venturi, University of California, Santa Cruz
Lexing Ying, Stanford University

Dates: 2024-2029

Abstract. Our team proposes to systematically develop an interlocking research framework to advance tensor network methods for simulating high-dimensional kinetic models. Our research efforts are organized as three core thrusts. These include a direct multi-scale time integration of tensor network solutions on a low-rank manifold with preservation of solution structures and modeling hierarchy (Thrust 1 and part of Thrust 2), and a data-driven learning approach in discovering tensor network decomposition and model reduction for extremely high-dimensional probability density functions for quantification of uncertainties and optimal control (Thrust 2). The core technical challenges in tensor network computations arise from previous two thrust, lead to a focused discussion on robust tensor decomposition and optimization tools in Thrust 3, covering the topic of tensor network topology optimization, low-rank tensor network representation of high-dimensional functions and operators, and data-driven learning of tensor network representations. While the proposal is inspired by nonequilibrium plasmas simulations and control of plasma instabilities, the underlying methodology promises wide-ranging applications, extending to multiple areas critical to the DoD's interests.

Heterogeneous Data Fusion by Graph-based Stochastic Models to Achieve Combinatorial Generalization of New Insights into Powder-based Fabrication

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Abstract

During the development of new manufacturing processes, it is essential to discover defect mechanisms and thereby establish process control. However, many relationships between the defects and potential process variables are unknown yet due to limited or even absent historical measurements. As such, traditional methods, including state-of-the-art multi-physics simulations and machine learning, struggle to effectively obtain the relationships without directly observed data. This project will establish a theoretical framework to achieve the capability of combinatorial generalization (CG) that can empower AI to make inferences on new scenarios given piecewise knowledge learned by fusing multiple data sources, such as multi-physics simulation and experimental data. The research will develop theories and algorithms based on physics-informed Graphnets and generative AI to solve CG problems, helping discover unmeasurable defect mechanisms in powder-based fabrication. The research includes three thrust areas including the (1) development of physics-informed machine learning algorithms to integrate multi-modal data from low-cost measurements and multi-scale simulations to generalize insights into anomalies that are difficult to measure, (2) generation of piecewise information from low-cost measurements by experiments and machine learning, and (3) extraction of informative data from computational fluid dynamics simulation and computer experiment. Through close collaboration with HP Inc., use cases will be developed to explore the concept of CG and its applications in accelerating discoveries of defect mechanisms in powder-based fabrication. The proposed research can benefit a wide range of manufacturing processes, leading to new discoveries in defect formation for manufacturing engineering and material sciences. This project also features a strong educational aspect involving the interaction of all teams with graduate students from FAMU, a historically black college/university (HBCU). Their graduate students will have opportunities to conduct experiments and simulations for their research during their internships at HP.

HBCU-led Center for scientific machine learning for the materials sciences

PI: Yunjiao Wang (Texas Southern University)
co-PIs: Daniel Vrinceanu (Texas Southern University),
Noushin Ghaffari (Prairie View A&M University)
Lin Li (Prairie View A&M University)
Mohsen Taheri Andani (Texas A&M University)
Veera Sundararahgavan (University of Michigan)

Abstract

The proposed Center for Scientific Machine Learning for Material Sciences brings together a multidisciplinary team of experts in applied mathematics, physics, statistics, optimization, and machine learning, in collaboration with materials scientists. The primary objective of the center is to develop a foundational SciML framework that will drive advancements in materials design and discovery. This comprehensive framework will encompass uncertainty quantification, predictive simulation, and optimization tools. By focusing on the Electron beam powder bed fusion (EBPBF) platform, the center will leverage the inherent equivalence between electron beam processing and scanning electron microscopy, utilizing sensor data to facilitate data-driven and principle-guided scientific exploration. The center places a strong emphasis on knowledge development and building diversity in the scientific community, fostering the growth of SciML and Data Science programs in Historically Black Colleges and Universities (HBCUs). A background on Electron beam powder bed fusion (EBPBF) platform, sensor data collection and control of microstructure will be provided, as well as the current work on topographical analysis using multisensor data integration.

Enhanced Entropy Filtering and Online Bayesian Optimisation of Polynomial-Multigrid Cycles for High-Order Methods

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Abstract

In the first part of this talk we will present an enhanced variant of our positivity-preserving entropy filtering approach. Through the incorporation of a range of algorithmic enhancements this new approach is around $\sim$2.4 times more efficient with third order solution polynomials and $\sim$6.4 times faster with fourth order solution polynomials. With these enhancements we will show how entropy can serve as a cost-effective alternative to quadrature based anti-aliasing. Results will be presented for a NACA 0021 aerofoil in deep stall at $Re = 270\,000$ demonstrating how this approach results in a twofold decrease in run-time compared with over-integration.

In the second part of the talk we will outline how Bayesian optimisation can be used to learn polynomial multigrid cycles at run-time. This is accomplished through a combination of cycle parameterisation along with a novel application of *stochastic rounding*. It will be shown how this technique can identify cycles for a turbulent cylinder flow problem at $Re = 3900$ which outperform hand-tuned cycles in time-to-solution by a factor of two.

Modeling Unknown Stochastic Systems via Generative Models

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Abstract

We present a numerical framework for modeling unknown stochastic systems by using observation data. The framework is based on flow map learning (FML), which utilizes the data to approximate the flow map operator of the unknown system. Once the flow map is approximated, FML creates an iterative time marching scheme that can produce long-term system predictions. For unknown stochastic systems, since the noises can not be directly observed, we utilize generative models in FML to approximate the unknown stochastic flow map in distribution. Various generative models such as GANs, normalizing flow, diffusion map, autoencoder-decoder can be incorporated in the framework. Extensive numerical examples demonstrate the effectiveness of the proposed approach, particularly for producing very long-term system predicions using only short bursts of data.

Nonlocal Attention Operator: Towards an Interpretable Foundation Model

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Abstract

Despite recent popularity of attention-based neural architectures in core AI fields like natural language processing (NLP) and computer vision (CV), their potential in modeling complex physical systems remains under-explored. Learning problems in physical systems are often characterized as discovering operators that map between function spaces based on a few instances of function pairs. This task frequently presents a severely ill-posed PDE inverse problem.

In this work, we propose a novel neural operator architecture based on the attention mechanism, which we coin Nonlocal Attention Operator (NAO), and explore its capability towards developing a foundation physical model. In particular, we show that the attention mechanism is equivalent to a double integral operator that enables nonlocal interactions among spatial tokens, with a data-dependent kernel characterizing the inverse mapping from data to the hidden parameter field of the underlying operator. As such, the attention mechanism extracts global prior information from training data generated by multiple systems, and suggests the exploratory space in the form of a nonlinear kernel map. Consequently, NAO can address ill-posedness and rank deficiency in inverse PDE problems by encoding regularization and achieving generalizability. Lastly, we empirically demonstrate the advantages of NAO over baseline neural models in terms of the generalizability to unseen data resolutions and system states. Our work not only suggests a novel neural operator architecture for learning an interpretable foundation model of physical systems, but also offers a new perspective towards understanding the attention mechanism.

Adaptive, data-driven model reduction for shock-dominated flows to enable many-query computational physics

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Abstract

We introduce a series of model reduction methods to reduce the cost of shock-dominated flow simulations that aim to circumvent the well-known Kolmogorov n-width reducibility limitation. The first approach seeks to align flow features in the solution with corresponding features in the reduced basis by deforming the underlying domain, which effectively removes the convection-dominated nature of the solution. We also introduce two forms of online adaption to improve the robustness and prediction potential of reduced-order models, one of which injects high-fidelity information from previous time steps into the reduced basis, and the other enriches the global basis functions with piecewise polynomials. We use the proposed methods to solve a number of relevant two- and three-dimensional compressible flows with complex discontinuity surfaces and demonstrate the potential of the method to provide accurate approximations with very few degrees of freedom.

DeepONet for fast data assimilation in transitional high-speed flows

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Abstract

Deep operator networks (DeepONet) are an efficient model for learning functionals. However, a key challenge is the availability and computational cost of training data in high dimensions. The specific problem of interest in his work is transition to turbulence in hypersonic boundary layers, and in particular the estimation of the oncoming instability waves from wall-pressure data. This inverse problem is nonlinear, ill-conditioned, and may have non-unique solutions. While use of DeepONet has the potential to significantly accelerate the data-assimilation loop by replacing the high-fidelity Navier-Stokes solution, model errors can appreciably compromise the accuracy of the estimated state. The sampling of the training data must therefore minimize the epistemic uncertainty of the trained DeepONet model, while also minimizing the number of training data in order to reduce the computational cost. These objectives are achieved by optimally sampling the space of possible solutions, preferentially along the most uncertain directions and with aid of a physics-based model. Our DeeONet-based algorithm successfully assimilates wind-tunnel measurements of a Mach 6, transitional, boundary layer over a 7-degree half-angle cone. The estimated state compares favorably to the only known solution form an ensemble-variational approach.

Universal Approximation of Dynamical Systems by Semi-Autonomous Neural ODEs and Applications

Enrique Zuazua

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This presentation reports on the recent collaborative efforts of our team at the intersection of control theory and machine learning.

We will primarily address the challenge of modeling dynamical systems using neural network architectures. Our focus lies in the introduction of semi-autonomous neural ordinary differential equations (SA-NODEs), a refined version of the conventional vanilla NODEs, designed with a reduced parameter footprint. We explore the universal approximation capabilities of SA-NODEs for dynamical systems, supported by both theoretical analysis and computational experiments that showcase the proficiency of SA-NODEs in capturing the behaviors of diverse ODE systems and transport equations. Furthermore, we conduct a comparative analysis between SA-NODEs and vanilla NODEs, showing the superior performance of our approach.

This presentation is inspired on our ongoing collaboration with Ziqian Li, Kang Liu, and Lorenzo Liverani.