

Mathematical Opportunities in Digital Twins (MATH-DT)

Dates

December 11-13, 2023

Location

Van Metre Hall
George Mason University (Arlington Campus)
3351 Fairfax Dr, Arlington, VA 22201

Organizing Committee

Harbir Antil (George Mason University)
Benjamin Seibold (Temple University)
Kathrin Smetana (Stevens Institute of Technology)

Local support team: Ratna Khatri (US Naval Research Lab), Juan Cebal (GMU), Rainald Löhner (GMU), and Mahamadi Warma (GMU)

Sponsors

National Science Foundation
Center for Mathematics and Artificial Intelligence, George Mason University
College of Science, George Mason University
SIAM DC-Baltimore Section

In Cooperation With

Association for Women in Mathematics

Schedule of Mathematical Opportunities in Digital Twins (MATH-DT)

December 11–13, 2023

Monday, December 11, 2023

8:00AM - 9:00AM	Breakfast / Registration
8:45AM - 9:30AM	Welcome address by the Organizers, Andre Marshall (VP Research, GMU), and David Manderscheid (NSF DMS Division Director)
9:30AM - 11:00AM	Session 1 (Plenary Talks)
11:00AM - 11:30AM	Coffee
11:30AM - 12:30PM	Session 2 (Applications Panel)
12:30PM - 1:30PM	Boxed Lunch
1:30PM - 3:00PM	Session 3 (Plenary Talks)
3:00PM - 4:00PM	Dream Big & Report - Discussion
4:00PM - 5:30PM	Poster / Demo Session (Jointly with SIAM DC-Baltimore Section)
5:30PM - 6:00PM	SIEMENS (Demo)

Tuesday, December 12, 2023

8:00AM - 9:00AM	Breakfast / Registration
9:00AM - 10:30AM	Session 4 (Plenary Talks)
10:30AM - 11:00AM	Coffee
11:00AM - 12:00PM	Session 5 (Applications Panel)
12:00PM - 1:00PM	Boxed Lunch
1:00PM - 2:30PM	Session 6 (Funding Agency Panel) (Jointly with SIAM DC-Baltimore Section)
2:30PM - 4:30PM	Dream Big & Report II
4:30PM - 5:00PM	NVIDIA (Demo)
5:30PM - 7:00PM	Conference Dinner

Wednesday, December 13, 2023

8:00AM - 9:00AM	Breakfast / Registration
9:00AM - 10:30AM	Session 7 (Plenary Talks)
10:30AM - 11:00AM	Coffee
11:00AM - 12:15PM	Dream Big & Report III - Final Presentations
12:30PM - 1:30PM	Boxed Lunch

Notes

1. MATH-DT has “in Cooperation with Association for Women in Mathematics (AWM)” status. This conference supports the Welcoming Environment Statement of the AWM.
2. Each **Plenary talk** will be 20-minutes followed by a moderated panel discussion of 30 minutes.
3. Each **Applications Panelist** will give 10-minute talk followed by a moderated panel discussion of 30-minutes.
4. Each **Funding Agency** will give 7-8-minute introduction followed by a moderated panel discussion of 30-minute.
5. Session assignments are on the next page.

Session 1: Plenary Talks

Omar Ghattas (The University of Texas Austin, USA)

Julianne Chung (Emory University, USA)

Reinhard Laubenbacher (University of Florida, USA)

Session 2: Applications Panel I

Stefan Boschert (SIEMENS)

Sharon Di (Columbia University)

Mustafa Megahed (ESI Group)

Session 3: Plenary Talks

Roland Wüchner (Technical University Braunschweig, Germany)

Rainald Löhner (George Mason University)

Bart Van Bloemen Waanders (Sandia National Laboratories)

Session 4: Plenary Talks

Enrique Zuazua (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

Carol Woodward (Lawrence Livermore National Laboratory, USA)

Karen Veroy-Grepl (Eindhoven University of Technology, Netherlands)

Session 5: Applications Panel II

Brent Bartlett (NVIDIA)

Aldo G Badano (FDA)

Juan Cebal (George Mason University)

Session 6: Funding Agencies Panel

National Science Foundation

Air Force Office of Scientific Research

Office of Naval Research

Army Research Office

DARPA

Department of Energy

National Institute of Health

Session 7: Plenary Talks

Arvind K. Saibaba (North Carolina State University, USA)

Akil Narayan (University of Utah, USA)

Lise Marie Imbert-Gérard (University of Arizona)

Plenary Speakers

1. [Julianne Chung](#) (Emory University)

Title. Feedback Flow from Physical to Virtual: Mathematical Opportunities in Inverse Problems, Uncertainty Quantification, and Data Assimilation

Abstract. Digital twins have gained widespread interest recently as a tool for accelerating scientific discovery and revolutionizing industries. Central to any successful digital twin is the bidirectional interaction between the virtual representation and the physical counterpart. In this talk, we focus on the feedback flow from physical to virtual, that is, the process of combining physical observations to update the virtual models in a rigorous, systematic, and scalable way. We describe challenges and opportunities for digital twins in the field of inverse problem methodologies, uncertainty quantification, and data assimilation.

2. [Omar Ghattas](#) (The University of Texas)

Title. Geometric Neural Operators for Digital Twins

Abstract. A digital twin is a computational model of a physical system that continually updates its knowledge of the system by assimilating observational data, and in turn informs decisions and controls the system to achieve a desired goal, over a continually evolving time horizon. When the model takes the form of a system of PDEs, and when the data assimilation and optimal control problems must be solved under uncertainty, the computations underlying digital twins quickly become prohibitive. Efficient surrogates of the maps from parameters or decision variables to objective functions, which involve solution of the forward PDEs, is key to making digital twins tractable. Unfortunately, constructing such surrogates presents significant challenges when the parameter/decision dimension is high and the forward model is expensive, which limits the amount of available data.

Deep neural networks have emerged as leading contenders for overcoming the challenges of constructing infinite dimensional surrogates, which are known as neural operators. We demonstrate that black box application of DNNs for problems with infinite dimensional parameter fields leads to poor results when training data are limited due to the expense of the model. Instead, by constructing a network architecture that captures the geometry of the map – in particular its smoothness, anisotropy, and intrinsic low-dimensionality – one can construct a dimension-independent reduced basis neural operator with superior generalization properties using just limited training data. We employ this reduced basis neural operator to make tractable the solution of PDE-constrained Bayesian inverse problems and optimal control under uncertainty, with applications to inverse wave scattering, inverse hyperelasticity, inverse earthquake subduction, and optimal flow control.

This work is joint with Thorsten Becker, Lianghao Cao, Peng Chen, Dingcheng Luo, J. Tinsley Oden, Thomas O’Leary-Roseberry, Simone Puel, Umberto Villa, and Keyi Wu.

3. [Lise Marie Imbert-Gérard](#) (University of Arizona)

Title.

Abstract.

4. [George Karniadakis](#) (Brown University)

Title. Modular Building of Digital Twins using Neural Operators

Abstract. We will present a new data assimilation framework, the DeepM&Mnet, for simulating multiphysics and multiscale problems at speeds much faster than standard numerical methods using pre-trained neural networks (NNs). We first pre-train DeepONets that can predict independently each field, given general inputs from the rest of the fields of the coupled system. DeepONets can approximate nonlinear operators and are composed of two sub-networks, a branch net for the input fields and a trunk net for the locations of the output field. DeepONets, which are extremely fast, are used as building blocks in the DeepM&Mnet and form constraints for the multiphysics solution along with some sparse available measurements of any of the fields. We demonstrate the new methodology and document the accuracy of each individual DeepONet, and subsequently we present two different DeepM&Mnet architectures that infer accurately and efficiently fields in electroconvection, hypersonics and oil & gas applications. The DeepM&Mnet framework is general and can be applied for building any complex multiphysics and multiscale models based on very few measurements using pre-trained DeepONets in a plug-and-play mode.

5. [Reinhard Laubenbacher](#) (University of Florida)

Title. The Mathematics of Medical Digital Twins

Abstract. The digital twin concept has its origins in industry. One industrial equipment manufacturer advertised its digital twin capabilities to its customers as "No unplanned downtime" for its products. There is a compelling aspirational analog in healthcare: "No unplanned doctor visits." Of course, the challenges of building digital twins for human patients are incomparably greater than for machinery. Nonetheless, there are now several instances of what might be called digital twins in medicine, and many more ongoing development projects. Aside from our incomplete understanding of human biology, relative sparseness of data characterizing human patients, and logistical difficulties in implementing computational models in healthcare, there are many mathematical and computational problems that need to be solved. Examples include calibration and validation of multi-scale, hybrid, stochastic computational models, forecasting algorithms, and optimal control methods. This talk will describe some of these problems and outline a mathematical research program for the field.

6. [Roland Wüchner](#) (Technical University Braunschweig, Germany)

Title. Digital Twins in the Built Environment – Challenges and Potentials

Abstract. The built environment includes structures and systems with immense social, economic and environmental impacts, such as bridges, water networks, traffic and crowd management, all kinds of buildings, and conventional and renewable energy plants. Given the large amount of building material these structures require, it is of utmost importance to enable efficient material use through optimal design, long-term smart operation, and possibly retrofitting or an adapted utilization strategy. Modern numerical methods and simulations in combination with robust sensor systems can be combined to form digital twins in order to achieve this. The following special challenges of these structures must be considered and solved:

Most structures such as bridges and tall buildings are unique, i.e. built only once, which places very high demands on the predictive capabilities of numerical simulations in the design phase, but also for the evaluation of “what-if” scenarios during operation. Hence, verification and validation of the numerical approaches are extremely important, and purely data-driven approaches for predictions are not feasible due to the lack of training data for the structures under consideration with their emerging changes during operation. Since physics-based models and simulations are indispensable and additional sensor data is available, the combination of both in hybrid FEM-ROM or FEM-ML approaches appears promising.

The actual simulation requirements – which are very immense - arise from the special characteristics of civil engineering structures. These are large, flexible structures with complex geometry and heterogeneous materials such as reinforced concrete which are immersed in their environment. Thus, the simulation techniques within the specific digital twin may require multi-scale (e.g. local concrete damage in large structures) and multi-physics (e.g. fluid-structure interaction with wind or water flows) approaches. Moreover, significant variations in material properties and boundary conditions (e.g. foundation conditions) may occur during installation and operation, which can necessitate the quantification of uncertainties.

Another aspect is the comparatively long service life. Therefore, the digital twin must be effectively adaptable even in the event of component replacement or rebuilding scenarios. This could be summarized as the need for a “maintainable digital twin”, which has direct consequences on data management, software planning, interfaces between components, and a modular model setup and suitable update algorithms. Another aspect are the very different time scales (e.g. vibrations of structures versus aging of materials). While this may require suitable coupling approaches for (possibly barely) coupled phenomena with inherently very diverse time scales, the requirement for real-time calculations is much more relaxed for long-term phenomena.

The assessment of the structural condition and the detection of emerging, possibly local damage may require a digital twin model with many (preferably spatially distributed) parameters. This leads to inverse problems with very high dimensionality, which require efficient numerical methods for twinning (e.g. adjoint approaches). In cases where structures are also affected by complex multiphysics phenomena, the operation, identification

and updating of the specific digital twin requires efficient approaches for the solution of coupled forward and inverse problems, which encourages the further development of coupled adjoint sensitivity analysis. A large number of scenarios in which digital twins could be advantageously deployed and used in civil engineering can be envisioned. A non-exhaustive list includes:

- Detection of aging in steel and reinforced concrete structures (bridges, high-rises, stadiums, power plants, etc.);
- Detection of soil/foundation softening for structures;
- Maintenance of structures and buildings;
- Condition assessment of used components for reuse scenarios to support circularity;
- Adaptation of structures to climate change and/or varying load conditions.

7. Rainald Löhner (George Mason University)

Title. Digital Twins in the Built Environment – Methods and Requirements

Abstract. The term ‘digital twin’ can mean different things in different realms - even in a specialized field like civil engineering. The data stored in the digital twin can encompass vastly different information. In some instances a BIM enumeration of parts (e.g. number of buildings in a neighbourhood) is already considered by some a digital twin. This data can be enriched by accounting for the parts (number, type, dimensions, manufacturer, . . . of: walls, doors, flooring, piping, HVAC systems, lighting, kitchen, etc.). And enriched further by the CAD data for visualization or product life cycle management. And enriched further by the detailed or approximate (ROM, POD, ML) computational models and sensors that monitor aspects of the built environment throughout its life. These ‘information rich’ digital twins have emerged as a result of three megatrends: a) the pervasive use of CAD systems, b) the widespread availability and use of computational tools to ‘pre-compute, only then build’ and ‘pre-compute, then operate’; and c) the emergence of precise, rugged, connected and cheap cameras and sensors that may be used to monitor structures.

The simple ‘data storage’ digital twins which are often used for product life management pose interesting mathematical requirements in the field of massive data storage and retrieval/comparison, pattern recognition, labeled data update, and data maintenance.

The ‘information rich’ of ‘high fidelity’ digital twins pose mathematical and software requirements along the complete simulation/digital twin chain:

Pre-processing: For large, unique engineering structures, extensive predictive numerical models are created in the design phase before the actual realization of the specific product. In order to simplify the workflow to deploy a digital twin, the CAD or BIM models used for computational mechanics should be built with ‘digital twin readiness’ in mind. The goal is to achieve a level of automation such that if a part of the structure is changed, all metier-specific inputs (grids, material parameters, boundary conditions, ROMs, ...) are automatically updated.

Workflow and Training: As could be seen from above, new methods and software developments are required for the creation of integrated workflows in relation to the definition, setup, operation, updating and maintenance of digital twins for engineering structures. This also places particular demands on the work of standardization committees. In addition, (university) education and professional training must reflect the overall increase in complexity due to the growing number of models involved (possibly of various fidelity) and their dependencies and interactions in digital twins.

Solvers: The combination of computational tools and sensors has opened the possibility to detect aging, weakening or operational hazards in real time, simplifying maintenance and improving operational efficiencies and security. In order to make this possibility a reality, a number of mathematical challenges need to be addressed. Solvers need to be improved further (and, yes, this includes linear algebra running efficiently on advanced hardware, better preconditioners, robust nonlinear convergence and adaptive refinement). As many of the sensor/model adaptation/update tasks can be cast as optimization problems, optimization methods that operate robustly and reliably with a very high number of parameters and non-convex optimality criteria and input-based parameter adaptation need to be developed. The same applies to UQ and stochastic analysis.

Post-processing: Given that ‘high fidelity’ digital twins may yield too much (or confusing) information to operators, the data must be condensed and visualized in an intuitive, metier-specific way. This will require adaptations on a case-by-case basis, but general principles based on sound mathematical foundations may help.

The talks will focus on these aspects and highlight them on two applications: detection of weakening in structures and digital twin enhanced command and control centers for crowds (DTEC4).

8. [Akil Narayan](#) (The University of Utah)

Title. Model selection, combination, and management: Sowing with exploration and reaping with exploitation

Abstract. Modern simulation-based scientific models are complex and multi-faceted, involving computationally demanding physics-based modeling and discretization, reliable and robust data assimilation, and an accurate accounting for uncertainty in the face of unknown model parameter values and/or genuine stochasticity. To meet such demands, many simulations of real-world systems often involve combinations of homogenized, microscale, or reduced order model components that target accuracy of specific system subcomponents. To complicate matters, individual subcomponents may have several competing models whose query cost and accuracy payoff for system-wide prediction is opaque. For example, there may be numerous ways to identify macroscopic closure terms that are informed through analysis of a suite of microscale models.

We discuss how computational exploration-exploitation meta-algorithms can accomplish model selection and combination for digital-twin scale applications: An exploration phase is devoted to learning about model relationships and interactions, followed by an exploitation phase that uses information learned in exploration to make decisions about optimal

model selection. This framework leads to flexible procedures, capable of managing disparate models and multi-modal data in adaptive and real-time scenarios. We will identify existing theoretical guarantees for such procedures along with promising and impactful directions for new analysis and algorithm development.

9. [Arvind Saibaba](#) (NC State)

Title. Randomized Low-rank Approximations in Scientific Computing

Abstract. Randomized numerical linear algebra (RandNLA) is emerging as a powerful tool to tackle large-scale linear algebra problems—such as low-rank approximations, least squares, linear systems, and matrix functions—in scientific computing and data science. RandNLA can overcome computational bottlenecks associated with classical NLA algorithms by exploiting problem structure, making judicious use of access to the underlying matrices, and enabling high-performance computing. In this talk, we will show how randomization for low-rank approximations can be used to obtain orders-of-magnitude reductions in applications of relevance to scientific computing such as sensitivity analysis, tensor decompositions, Bayesian inverse problems, and reduced order modeling.

10. [Karen Veroy-Grepl](#) (Eindhoven University of Technology, Netherlands)

Title. Parametric Model Order Reduction in the Multi-scale Materials Setting

Abstract. Digital twins for multi-scale materials are extremely challenging due to the huge computational cost required for multi-scale simulations. Such simulations are crucial in understanding structure-property relations (i.e., the effect of the microstructure on a component’s macroscopic properties), and are thus essential in the optimal design of materials for specific applications, in production process control, or to enable (for example) estimation of microstructural parameters through macroscale measurements. However, even just two-scale simulations are very computationally expensive particularly in multi-query contexts such as optimization, material design, and inverse problems. To make such analyses amenable, the microscopic simulations can be replaced by inexpensive parametric surrogate models.

In this talk, we present some recent work on parametric model order reduction methods to construct efficient surrogates for parametrized microstructural problems. The proposed methodology can account for parameters involving loading, material property, and geometry. The methods are tested on several (composite) microstructures, where large deformations, rotations, and finite-strain plasticity in combination with relatively large variations in the shape of inclusions are considered. The method is applied to two-scale examples, where the surrogate model achieves a high accuracy and significant speed up, thus demonstrating its potential in realistic two-scale engineering applications and material design.

11. [Bart van Bloemen Waanders](#) (Sandia National Labs)

Title. Post-optimality sensitivities with respect to model-discrepancy for optimization of complex systems

Abstract. Digital twins require a fusion of numerical modeling and outer-loop analysis to support decision-making for complex systems. In this talk, PDE-constrained optimization serves as the outer-loop analysis and the goal is to achieve an optimization solution at the highest possible model fidelity. However, implementing large scale optimization (objective functions, adjoints, Hessians) is often intractable for high-fidelity models. To that end, we present a novel use of post-optimality sensitivities with respect to model discrepancy using lower-fidelity PDEs to achieve a higher-fidelity optimization solution. We demonstrate our approach on various numerical exemplars, including control of Stokes to emulate control of Navier Stokes.

12. [Carol Woodward](#) (Lawrence Livermore National Lab)

Title. Developing and Deploying Software for Use in Multi-Temporal-Scale Applications on High Performance Computing Systems

Abstract. In collaboration with Cody J. Balos, David J. Gardner, Steven B. Roberts, and Daniel R. Reynolds

Effective digital twins rely on robust numerical software that can be utilized in multiple computing environments. This software must provide implementations of numerous methods including algorithms for optimization, algebraic solvers, time evolution, and data assimilation, among others. The SUNDIALS software library provides efficient, adaptive time integration algorithms for use in application codes with time dynamics. Through the Exascale Computing Project, the team has rearchitected the software platform to provide new flexibilities for accommodating use on hybrid computer architectures, use in varied application contexts, and use of several algebraic solver and data structure classes. Through the DOE SciDAC program the team has researched new methods for multiscale applications as well as deployed the software to several applications. In this talk I will discuss considerations for development of software for public distribution and use on high performance computing systems using examples from SUNDIALS' experience. The importance of the three areas of method research, capability development, and applications deployment will be discussed along with recent results and application examples. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC. LLNL-ABS-854222.

13. [Enrique Zuazua](#) (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

Title. Control and Machine Learning

Abstract. Control theory and Machine Learning share common objectives, as evident in Norbert Wiener's definition of "Cybernetics" as "The science of control and communication in animals and machines."

The synergy between these fields is reciprocal. Control theory tools enhance our comprehension of the efficacy of certain Machine Learning algorithms and offer insights for their enhancement. However, this often bounces intricate queries back.

Consider the control of a linear finite-dimensional system—as example. A sharp mathematical solution exists: it suffices to ensure the Kalman matrix’s rank is full. Yet, computing these matrices in high dimensions presents a new challenge. DeepMind has made remarkable contributions, introducing artificial intelligence solutions to the old problem of matrix multiplication.

The interplay between Control and Machine Learning opens up a new captivating scientific landscape to be explored but this can become a labyrinthine task. And this is surely part of the overall ambitious program of developing Digital Twins technologies. In this talk, we will present some of the contributions from our team at the interface between Control and Machine Learning, which can modestly contribute to this noble and complex task.

Applications Panel

1. [Aldo Badano](#) (FDA)

Title: Digital Twins and Other Synthetic Humans in the Regulatory Evaluation of Medical Devices

Abstract: Applications of digital twin technology in regulatory science differ from applications in other industries because of data complexity, data sparsity, data privacy, and data ownership issues. To realize the potential of digital twins in biomedicine, several scientific challenges need to be addressed including commutability, bias mitigation, wide-sense generalizability, and platforms, standards, and protocols for in silico databanks.

2. [Stefan Boschert](#) (SIEMENS)

Title: Challenges for Digital Twins in Industrial Applications

Abstract: Digital Twins have become very popular in the last decade. Its development strongly benefited from advances in simulation technology and the rising availability of data so many products are already equipped with Digital Twin technology. However, there are several challenges from an industry point of view, that need to be tackled before Digital Twins can leverage their full potential. In the talk I will give some examples of potential industrial applications, where existing technologies come to its limits in actual realization.

3. [Brent Bartlett](#) (NVIDIA)

Title: Creating Geospatial Workflows with Digital Twin

Abstract: Edge sensors are quickly becoming indispensable to many different use cases and can provide rich information streams to enrich virtual representations of the real world. The amount of data these sensors create is growing at an incredible rate and new system architectures are needed to effectively update Digital Twins. This talk will present how NVIDIA Holoscan can be utilized to create geospatial processing workflows that link sensor data to a digital twin with examples of FMV and SAR data streaming into and NVIDIA Omniverse digital twin.

4. [Juan R. Cebral](#) (George Mason University)

Title: Biomedical Digital Twins from Virtual Patient Populations

Abstract: Personalization of surgical procedures and medical therapies requires understanding the most likely responses of each individual patient to the different treatment

options. However, assessing treatment outcomes and potential complications depends on the patient’s individual anatomical and physiologic characteristics, which are difficult to determine with certainty. Building a digital twin of a given patient that reproduces the salient features associated with therapeutic outcomes provides the opportunity to make more informed, objective, and personalized clinical decisions. To achieve this goal, we envision building a virtual patient population (i.e. computational models) with varying anatomical and physiologic characteristics and pre-compute synthetic images and/or physiologic curves that could be directly compared to actual patient data and measurements. Next, the virtual patient with the closest (i.e. most similar) imaging and physiologic data can be identified using statistical and/or machine learning approaches. Once so identified, this (approximate) digital twin can be used to assess different therapeutic options and inform the clinical decision-making process.

As an example, we investigate different interventional procedures used for occlusive stroke treatment. The outcomes of these procedures largely depend on the patient’s individual brain vascular collateralization, which provide alternative avenues of flow to the area of the brain affected by an arterial occlusion. The human brain contains collateral vessels (i.e. communicating arteries) that join the main feeding arteries at the level of the circle of Willis at the base of the brain, as well as a network of smaller collaterals at the surface of the brain called pial collaterals or leptomeningeal arteries. However, there is a large variability of these collateral vessels among the population. Even tough medical images such as computed tomography angiography (CTA) can depict the larger collaterals, their resolution is limited, and smaller vessels are not clearly visualized. Nevertheless, temporal imaging such as multi-phase CTA provide valuable information about the delayed filling of smaller arteries feeding the affected area of the brain (through collaterals). This information can be directly used to identify a digital twin within a virtual patient population with varying levels of brain collateralization that best matches (i.e. explains) the patient’s temporal curves. Finally, the patient data can be augmented with data from the digital twin and/or different treatment options could be investigated using the digital twin. Thus, improved understanding of the underlying anatomy and effects of interventions on a patient-specific basis using the corresponding digital twin has the potential to further improve patient management.

The proposed strategy poses a number of mathematical and computational challenges, including: 1) creating virtual patient populations with the correct anatomical variability (e.g. using constrained constructive optimization methods to extend vascular models), 2) creating synthetic data that can be compared to patient data (e.g. performing transport simulations to create virtual angiograms and quantifying specific features from medical images and virtual images), 3) identifying digital twins that best match patients’ data (e.g. using statistical correlations, machine learning models, etc.), 4) using the digital twins to assess best options for a patient (e.g. performing numerical simulations of medical procedures, identifying statistical associations between anatomical and physiological characteristics and intervention outcomes, creating machine learning models to predict outcomes, etc.)

5. [Sharon Di](#) (Columbia University)

Title: AI for Urban Transportation Digital Twin

Abstract: Transportation digital twins have become increasingly popular tools to improve traffic efficiency and safety. However, the majority of effort nowadays is focused on the “eyes” of the digital twin, which is object detection using computer vision. I believe the key to empowering the intelligence of a transportation digital twin lies in its “brain,” namely, how to utilize the information extracted from various sensors to infer traffic dynamics evolution and devise optimal control and management strategies with real-time feedback to guide the transportation ecosystem toward a social optimum.

My research aims to employ tools including machine learning and game theory to develop an urban transportation digital twin, leveraging data collected from the NSF PAWR COSMOS city-scale wireless testbed being deployed in West Harlem next to the Columbia campus. In this talk, I will primarily focus on two solutions: (1) scientific machine learning that leverages both domain knowledge and available data, and (2) mean field game that bridges the gap between micro- and macroscopic behaviors of multi-agent dynamical systems. In the first topic, physics-informed deep learning will be introduced and applied to traffic state estimation and uncertainty quantification. In the second topic, I will introduce how to model behaviors of new actors (e.g., a large number of autonomous vehicles) in a transportation system and their interaction with existing actors (e.g., human-driven vehicles).

6. [Mustafa Megahed](#) (ESI Group)

Title: Hybrid Twins for diverse Data Sets in Industrial Applications

Abstract: Given the very large differences in data sources, acquisition frequency, accuracy and formats, the large variety in reasons behind using digital twins and the large assortment of data analysis and machine learning tools available the question arises “How straight forward is it to apply digital twins in industrial applications?”. This talk will explore these aspects and how they impact industrial implementation. The hybrid twin concept is introduced as applied to material behavior, manufacturing outcome and vehicle safety predictions.

Contributed Posters

1. [Facundo Airaudó](#) (George Mason University)
On the use of risk measures in digital twins to identify weaknesses in structures
2. [Reza Akbarian Bafghi](#) (University of Colorado Boulder)
Accelerating PINNs implementations in PyTorch and TensorFlow
3. [Antonio Álvarez López](#) (Universidad Autónoma De Madrid)
Optimized classification with neural ODEs
4. [Mohammad Atif](#) (Brookhaven National Laboratory)
Towards enabling digital twins capabilities for a cloud chamber
5. [Charles Beall](#) (Stevens Institute of Technology)
Randomized reduced basis methods for advection-diffusion problems
6. [Prajakta Bedekar](#) (Johns Hopkins University and National Institute of Standards and Technology)
Time-dependent antibody kinetics for previously infected and vaccinated individuals via graph-theoretic modeling
7. [Filip Belik](#) (University of Utah)
Dynamic arterial bulk conductivity from blood pressure
8. [Md Rezwan Bin Mizan](#) (University of Houston)
Reduced order modeling of the Kuramoto-Sivashinsky equation using proper orthogonal decomposition
9. [Mingchao Cai](#) (Morgan State University)
A combination of physics-informed neural networks with the fixed-stress splitting iteration for solving Biot's model
10. [Sean Carney](#) (George Mason University)
PDE constrained optimization with distributional uncertainty
11. [Rujeko Chinomona](#) (Temple University)
Real-time interactive simulation of reality with neuroscience applications
12. [Kamala Dadashova](#) (North Carolina State University)
Parameter subset selection for identifiability analysis in mPBPK model
13. [Alejandro Diaz](#) (Rice University)
Nonlinear manifold reduced order models with domain decomposition

14. [Emmanuel Fleurantin](#) (George Mason University and University of North Carolina at Chapel Hill)
A data driven study of the drivers of stratospheric circulation via reduced order modeling and data assimilation
15. [Jithin George](#) (Northwestern University)
Walking into the complex plane to “order” better time integrators
16. [Sebastian Gutierrez Hernandez](#) (Georgia Institute of Technology)
Parametric geodesics and control problems in Wasserstein space
17. [Sebastian Kaltenbach](#) (Harvard University)
Korali - part 2: Bayesian inference
18. [Kai Fung \(Kelvin\) Kan](#) (Emory University)
LSEMINK: a modified Newton-Krylov method
19. [Prashant Kambali](#) (Villanova University)
Hybrid Modeling Approaches for Dynamic Systems: Bridging Nonlinear Physics, Machine Learning, and Expert Insights in Engineering and Medicine
20. [Rohit Khandelwal](#) (George Mason University)
A discontinuous Galerkin method for optimal control of the obstacle problem
21. [Hyunah Lim](#) (University of Maryland College Park)
Mathematical modelling of the impacts of screening and vaccination in HPV
22. [Anton Malandii](#) (Stony Brook University)
Adaptive importance sampling for topology optimization in uncertain environment
23. [Zhaobin Mo](#) (Columbia University)
Physics-Informed Deep Learning for Traffic State Estimation: A Survey and the Outlook
24. [Soyoung Park](#) (University of Maryland)
Mathematical modelling of the impacts of screening and vaccination in HPV
25. [Aseem Milind Pradhan](#) (George Mason University)
A digital cerebral vasculature database for stroke management
26. [Rhea Shroff](#) (University of Florida)
Accelerating the computation of tensor z -eigenvalues
27. [Priscila Silva](#) (University of Massachusetts Dartmouth)
Predictive system resilience modeling
28. [Moyi Tian](#) (Brown University)
Community robustness under edge addition in synthetic and empirical temporal networks

29. [Shanyin Tong](#) (Columbia University)
Large deviation theory-based adaptive importance sampling for rare events in high dimensions
30. [Deepanshu Verma](#) (Emory University)
Neural Network Approaches for Parameterized Optimal Control

Abstracts

On the use of risk measures in digital twins to identify weaknesses in structures

Facundo Airaud¹

¹George Mason University

Given measurements from sensors and a set of standard forces, an optimization based approach to identify weakness in structures is introduced. The key novelty lies in letting the load and measurements to be random variables. Subsequently the conditional-value-at-risk (CVaR) is minimized subject to the elasticity equations as constraints. CVaR is a risk measure leads to minimization of rare and low probability events which the standard expectation cannot. The optimization variable is the (deterministic) strength factor which appears as a coefficient in the elasticity equation, thus making the problem nonconvex. Due to uncertainty, the problem is high dimensional and, due to CVaR, the problem is nonsmooth. An adjoint based approach is developed with quadrature in the random variables. Numerical results are presented in the context of a weakened region in a plate and a large structure with trusses similar to those used in solar arrays or cranes.

Accelerating PINNs implementations in PyTorch and TensorFlow

Reza Akbarian Bafghi¹

¹University of Colorado Boulder

We want to introduce two Python packages that accelerate the implementation of Physics-Informed Neural Networks (PINNs) using the PyTorch and TensorFlow frameworks. These packages streamline user interaction by abstracting PDE issues.

Optimized classification with neural ODEs

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¹Universidad Autónoma De Madrid

Classification of $O(N)$ points becomes a simultaneous control problem when viewed through the lens of neural ordinary differential equations (neural ODEs), the time-continuous limit of residual networks. We estimate the likelihood that each number of neurons below $O(N)$ may be required for that task in the worst-case scenario, when the points are independently and uniformly distributed in $[0, 1]^d$. Notably, we quantify how this probability evolves with respect to N when the dimension d grows. Furthermore, assuming a generic condition on the point distribution, we propose a new constructive algorithm for classification that steers entire clusters of d points at once, leading to a reduced maximal complexity of $O(N/d)$ neurons.

Towards enabling digital twins capabilities for a cloud chamber

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Particle-resolved direct numerical simulations (PR-DNS), which resolve not only the smallest turbulent eddies but also track the development and motion of individual particles, are arguably an essential tool for exploring aerosol-cloud-turbulence interactions at the fundamental level. For instance, PR-DNS may complement experimental facilities designed to study key physical processes in a controlled environment and therefore serve as digital twins for such cloud chambers. In this poster we present our ongoing work aimed at enabling the use of a PR-DNS model for this purpose. We consider two approaches: traditional HPC techniques and emerging machine learning methods. Future research directions are outlined as well.

Randomized reduced basis methods for advection-diffusion problems

Charles Beall¹

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In this project, we develop randomized model reduction methods for advection-diffusion problems with sharply discontinuous source terms. To study such problems, we must solve the advection-diffusion equation, a partial differential equation (PDE) used to model systems such as a liquid dye being dissolved in a flowing fluid, or the combination of heat conduction and convection through a medium. This PDE arises often in the sciences, from fluid dynamics [1] to semiconductor physics [2], although in such contexts, the equation is almost always unsolvable by hand, so we rely on computer algorithms to efficiently obtain accurate approximations to the solutions. Our goal is to obtain a faster result than with direct numerical simulations like finite difference or finite element schemes. We employ randomized methods from data science to allow for parallel-in-time computation [3] and generation of a reduced order model. Compared to direct simulations, the reduced model produces a solution space of much lower dimension, meaning the computational complexity is greatly reduced. Thus, simulations with the reduced model allow for a further speedup in computational runtime, with the added benefit of maintaining accuracy. As a novel contribution, we consider the case of sharp discontinuities in source functions, partition the time domain into overlapping subintervals with overlap around the discontinuities, and construct a reduced basis on each subinterval. This allows for the construction of a reduced solution that combines information from the reduced bases, rather than relying on a single reduced basis to capture information throughout the time domain. We present a test case to show that this approach can provide significant improvements in accuracy compared to the construction of only one reduced basis over the whole time domain.

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Time-dependent antibody kinetics for previously infected and vaccinated individuals via graph-theoretic modeling

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Modeling the deterioration of antibody levels is paramount to understanding the time-dependent viral response to infections, vaccinations, or a combination of the two. These events have been studied experimentally, but also benefit from a rigorous mathematical underpinning. Disease/vaccination prevalence in the population and time-dependence on a personal scale simultaneously affect antibody levels, interact non-trivially, and pose considerable modeling challenges. We propose a time-inhomogeneous Markov chain model for event-to-event transitions coupled with a probabilistic framework for post-infection or post-vaccination antibody kinetics. This approach is ideal to model sequences of infections and vaccinations, or personal trajectories in a population. We use synthetic data to demonstrate the modeling process as well as estimation of transition probabilities. This work is an important step towards a comprehensive understanding of antibody kinetics that will allow us to simulate and predict real-world disease response scenarios. Modeling the deterioration of antibody levels is paramount to understanding the time-dependent viral response to infections, vaccinations, or a combination of the two. These events have been studied experimentally, but also benefit from a rigorous mathematical underpinning. Disease/vaccination prevalence in the population and time-dependence on a personal scale simultaneously affect antibody levels, interact non-trivially, and pose considerable modeling challenges. We propose a time-inhomogeneous Markov chain model for event-to-event transitions coupled with a probabilistic framework for post-infection or post-vaccination antibody kinetics. This approach is ideal to model sequences of infections and vaccinations, or personal trajectories in a population. We use synthetic data to demonstrate the modeling process as well as estimation of transition probabilities. This work is an important step towards a comprehensive understanding of antibody kinetics that will allow us to simulate and predict real-world disease response scenarios.

Dynamic arterial bulk conductivity from blood pressure

Filip Belik¹

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Impedance cardiography is a non-invasive procedure in which an alternating electrical current is passed into the human body to measure total conductivity. Currents are primarily

conducted through the arteries and blood as they generally exhibit lower resistivity compared to the muscle, skin, and fat. This conductivity can then be used to study important physiological parameters such as stroke volume, heart rate, and cardiac output. We propose an analytical forward model to understand the complicated relationship between blood pressure measured at the upper arm and the electrical conductivity of the radial artery at the wrist. This model involves several steps. First, the transport of a pressure wave down the brachial artery, through the bifurcation of the brachial artery into the ulnar and radial arteries, and then the transport down the radial artery to the wrist. Next, reduced Navier Stokes equations are matched with a moving boundary to model the pulsatile nature of blood flow alongside the elasticity of the tube wall. Finally, Maxwell-Fricke equations are used alongside the shear stress-induced orientation and deformation of red blood cells to calculate the bulk conductivity of the blood.

Reduced order modeling of the Kuramoto-Sivashinsky equation using proper orthogonal decomposition

Md Rezwan Bin Mizan¹, Ilya Timofeyev¹, Maxim Olshansky¹, and Alexander Mamonov¹

¹University of Houston

Proper Orthogonal Decomposition (POD) techniques are widely utilized in various scientific fields to streamline complex, data-driven spatio-temporal dynamics. In this study, we present a POD-Reduced Order Model (POD-ROM) for the one-dimensional Kuramoto-Sivashinsky (KS) equation, known for its chaotic attractor. Our FOM simulation was conducted over an extended time period to capture snapshots within this attractor. We constructed our basis using truncated Singular Value Decomposition (SVD), effectively representing the attractor. This single basis was then employed to construct our ROM using Galerkin projection. We demonstrate that the POD-ROM can accurately reproduce the statistical features of the KS equation's attractor, independent of initial conditions. Additionally, we show that this basis allows short-term predictions of the KS dynamics. Our findings suggest that a POD-ROM, based on a single basis, is effective for both long-term and short-term predictions of the chaotic KS dynamics. Furthermore, we have developed a criteria for the automatic selection of the reduced model's dimension, based on the cumulative variance of the singular values.

Keywords: Kuramoto-Sivashinsky Equation, Proper Orthogonal Decomposition (POD), spatio-temporal dynamics, Reduced Order Model (ROM)

A combination of physics-informed neural networks with the fixed-stress splitting iteration for solving Biot's model

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TBA

PDE constrained optimization with distributional uncertainty

Sean Carney¹

¹George Mason University

A critical task when seeking to quantify and minimize the risk of rare, outlier events, such as structural failures or climate catastrophes, is to account for uncertainty in the underlying physical models. Uncertainty in physical systems is modeled with random variables, however, in practice there may be some nontrivial ambiguity in the underlying probability distribution from which they are sampled. This work describes an analytic framework and computational methods that guarantee minimizers are robust to such ambiguities.

Real-time interactive simulation of reality with neuroscience applications

Rujeko Chinomona¹

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In this project, we delve into some crucial aspects of digital twins, focusing on real-time interaction and the simulation of real-time data. Unlike traditional high performance computing, which typically involves running simulations and creating visualizations afterward, our Virtual Simulation Of Reality (VISOR) project enables real-time interaction and immediate visualization, fostering an intuitive understanding of the physical system and allowing

on-the-fly adjustments. As part of the VISOR project, we have developed a computational neuroscience tool called Neuroscientific Virtual Simulation Of Reality (Neuro-VISOR). This tool simulates the Hodgkin-Huxley equations, which describe the active electrical signal processing in neurons. Our primary goal is to create real-time, interactive simulations tailored to assist researchers in their neuroscientific experiments, ultimately working towards the development of digital twins for neuroscience research. We also address some of the numerical challenges related to computing accurate solutions to the Hodgkin-Huxley equations in real-time, ensuring a seamless and fluid visualization experience. During our demonstration, participants will have the opportunity to explore Neuro-VISOR. Equipped with a virtual reality (VR) headset, they can visualize the current system state in real-time and make instant adjustments. Some noteworthy features of the current simulation model include the capability to directly modify voltage at specific neuron points, insert a clamp on a designated neuron point, and create synaptic connections between different neurons.

Parameter subset selection for identifiability analysis in mPBPK model

Kamala Dadashova¹

¹North Carolina State University

We consider a minimal PBPK (mPBPK) model of the brain for antibody therapeutics. This model is the reduced form of an previous multi-species platform brain PBPK model. The original PBPK model consists of 100 differential equations, whereas the mPBPK model contains 16 differential equations, improving the speed of simulations. The reduced model includes 31 parameters, and their values are taken from the original brain PBPK model. We implement a local sensitivity-based parameter subset selection (PSS) algorithm to determine identifiable parameters based on verified threshold values. We also compare results to a more standard PSS algorithm. One objective is to determine which parameters have the greatest influence on model predictions and how changes in these parameters affect model responses. This information can be utilized to improve the model's performance and facilitate subsequent uncertainty analysis. We systematically verify obtained results using qualitative methods and quantitative techniques based on energy statistics.

Nonlinear manifold reduced order models with domain decomposition

Alejandro Diaz¹

¹Rice University

This poster discusses the integration of nonlinear-manifold reduced order models (NM-ROMs) with domain decomposition (DD). NM-ROMs approximate the full order model (FOM) state in a nonlinear-manifold by training a shallow, sparse autoencoder using FOM snapshot data. These NM-ROMs can be advantageous over linear-subspace ROMs (LS-ROMs) for problems with slowly decaying Kolmogorov n-width. However, the number of NM-ROM parameters that need to be trained scales with the size of the FOM. Moreover, for "extreme-scale" problems, the storage of high-dimensional FOM snapshots alone can make ROM training expensive. To alleviate the training cost, DD is applied to the FOM, NM-ROMs are computed on each subdomain, and are coupled to obtain a global NM-ROM. This approach has several advantages: Subdomain NM-ROMs can be trained in parallel, each involve fewer parameters to be trained than global NM-ROMs, require smaller subdomain FOM dimensional training data, and subdomain NM-ROMs can be tailored to subdomain-specific features of the FOM. The shallow, sparse architecture of the autoencoder used in each subdomain NM-ROM allows application of hyper-reduction (HR), reducing the complexity caused by nonlinearity and yielding computational speedup of the NM-ROM. The proposed DD NM-ROM with HR approach is numerically compared to a DD LS-ROM with HR on 2D steady-state Burgers' equation, showing an order of magnitude improvement in accuracy of the proposed DD NM-ROM over the DD LS-ROM.

A data driven study of the drivers of stratospheric circulation via reduced order modeling and data assimilation

Emmanuel Fleurantin¹

¹George Mason University and University of North Carolina at Chapel Hill

Stratospheric dynamics are strongly affected by the absorption/emission of radiation in the Earth's atmosphere and waves which propagate upward from the troposphere perturbing stratospheric zonal flow. Reduced order models of stratospheric wave-zonal interactions, which parameterize radiative drivers and tropospheric perturbation, have been used in the past to study interannual variability in stratospheric zonal winds and sudden stratospheric warming (SSW) events. These models are most sensitive to two main parameters Λ , which forces the mean radiative zonal wind, and h which acts as a perturbation parameter representing the effect of waves propagating upward from the troposphere. These parameters have been taken to be constant or have been given various time dependent parameterizations

to account for seasonal, solar, and other possible forcings. In this work, we take one such reduced order model (Ruzmaikin 2002) in conjunction with 20 years of atmospheric reanalysis data provided by the European Center for Medium Weather Forecasting (ECMWF) to estimate Λ and h using various methods in data assimilation. We employ a particle filter to estimate constants in previous parameterizations of Λ and h as well as ensemble smoothing with multiple data assimilation (ESMDA) to estimate time series for $\Lambda(t)$ and $h(t)$ such that model output closely matches the reanalysis data. We provide some analysis of the resulting time series, compare them to previous parameterizations, and examine them around known historical SSW events. This allows a data driven examination of these important parameters through the lens and tractability of a reduced order model.

Walking into the complex plane to “order” better time integrators

Jithin George¹

¹Northwestern University

Most numerical methods for time integration use real time steps. Complex time steps provide an additional degree of freedom, as we can select the magnitude of the step in both the real and imaginary directions. By time stepping along specific paths in the complex plane, integrators can gain higher orders of accuracy or achieve expanded stability regions. We show how to derive these paths for explicit and implicit methods, discuss computational costs and storage benefits, and demonstrate clear advantages for complex-valued systems like the Schrodinger equation. We also explore how complex time stepping also allows us to break the Runge-Kutta order barrier, enabling 5th order accuracy using only five function evaluations for real-valued differential equations.

Parametric geodesics and control problems in Wasserstein space

Sebastian Gutierrez Hernandez¹

¹Georgia Institute of Technology

In the work “Parameterized Wasserstein Hamiltonian flow”, the authors propose a parametric formulation to solve Wasserstein Hamiltonian Flows numerically. In this poster, we

offer a short introduction to this topic and some recent developments. In particular, we show that when the considered distributions are Gaussians, this formulation can convert the Wasserstein geodesic and barycenter problems into equivalent problems in Euclidean space, which allows us to design efficient algorithms to compute the Wasserstein barycenter even in higher dimensions. Additionally, we apply the parametric formulation to control problems in the Wasserstein space.

Korali: Stochastic Optimization and Bayesian Inference **Sebastian Kaltenbach¹**

¹Harvard University

During this demo session, we are presenting Korali (<https://www.cse-lab.ethz.ch/korali/>), a high-performance framework for uncertainty quantification, optimization, and deep reinforcement learning. Korali's engine provides support for large-scale HPC systems and a multi-language interface compatible with distributed computational models. This presentation will focus on addressing (stochastic) optimization challenges as well as Bayesian inverse problems with Korali and showcase algorithms such as CMA-ES and Transitional Markov Chain Monte Carlo. In case evaluating the original model is expensive, we demonstrate how a surrogate model can be used instead. Moreover, we show how Korali is used within DCoMEX, a European High Performance Computing Joint Undertaking project.

LSEMINK: a modified Newton-Krylov method **Kai Fung (Kelvin) Kan¹**

¹Emory University

This paper introduces LSEMINK, an effective modified Newton-Krylov algorithm geared toward minimizing the log-sum-exp function for a linear model. Problems of this kind arise commonly, for example, in geometric programming and multinomial logistic regression. Although the log-sum-exp function is smooth and convex, standard line search Newton-type

methods can become inefficient because the quadratic approximation of the objective function can be unbounded from below. To circumvent this, LSEMINK modifies the Hessian by adding a shift in the row space of the linear model. We show that the shift renders the quadratic approximation to be bounded from below and that the overall scheme converges to a global minimizer under mild assumptions. Our convergence proof also shows that all iterates are in the row space of the linear model, which can be attractive when the model parameters do not have an intuitive meaning, as is common in machine learning. Since LSEMINK uses a Krylov subspace method to compute the search direction, it only requires matrix-vector products with the linear model, which is critical for large-scale problems. Our numerical experiments on image classification and geometric programming illustrate that LSEMINK considerably reduces the time-to-solution and increases the scalability compared to geometric programming and natural gradient descent approaches. It has significantly faster initial convergence than standard Newton-Krylov methods, which is particularly attractive in applications like machine learning. In addition, LSEMINK is more robust to ill-conditioning arising from the nonsmoothness of the problem. We share our MATLAB implementation at <https://github.com/KelvinKan/LSEMINK>.

Hybrid Modeling Approaches for Dynamic Systems: Bridging Nonlinear Physics, Machine Learning, and Expert Insights in Engineering and Medicine

Prashant Kambali¹

¹ Villanova University

This research endeavors to pioneer advanced techniques for modeling dynamic systems by synergistically incorporating nonlinear physics, machine learning methodologies, and expert insights. The interdisciplinary approach aims to enhance the accuracy and predictive capabilities of models in diverse fields such as engineering and medicine. By amalgamating the precision of nonlinear physics with the adaptability of machine learning algorithms and the nuanced understanding provided by expert insights, this study seeks to unlock new frontiers in system modeling. The outcomes hold significant promise for optimizing design processes, improving decision-making in complex systems, and advancing personalized medical diagnostics and treatments.

A discontinuous Galerkin method for optimal control of the obstacle problem

Rohit Khandelwal¹

¹George Mason University

This article provides a priori error estimates for an optimal control problem constrained by an elliptic obstacle problem where the finite element discretization is carried out using the symmetric interior penalty discontinuous Galerkin method. The main proofs are based on the improved L_2 -error estimates for the obstacle problem, the discrete maximum principle, and a well known quadratic growth property. All the existing results require restrictive assumptions on mesh which is not assumed here. Quasi-optimal rate of convergence is derived for both state and control variables, in a realistic, locally distributed optimal control setting.

Mathematical modelling of the impacts of screening and vaccination in HPV

Hyunah Lim¹

¹University of Maryland, College Park

Cervical cancer is one of the most frequent cancers women may suffer, which caused about 342,000 death cases in 2020 worldwide. It is known that cervical cancer is highly attributable to HPV, while HPV has no medical treatment leading to cure of infection but realistic prevention only available from vaccine. However, HPV vaccines are overly expensive for individuals, and many countries including South Korea has been vaccinating young female population only for cost-effectiveness. We wish to study the impacts of different vaccine strategies such as vaccinating males and females altogether in South Korea, and also experiment on the impact of detection in early cancer stages for females through screening, to find the ideal strategy for our society to take. Although we experiment on South Korean data, our model is not regional, and we expect it to contribute to researches similar in different countries also.

Adaptive importance sampling for topology optimization in uncertain environment

Anton Malandii¹

¹Stony Brook University

The paper addresses the problem of topology optimization in the presence of uncertainty. The risk of failure of a structure is measured by conditional value-at-risk (CVaR). For the considered structures, estimation of CVaR requires a very large number of scenarios of failures. It is not possible to evaluate the performance of the model for every scenario because of the high computational costs associated with solving partial differential equations (PDEs). To tackle this computational complexity, we use an adaptive importance sampling approach. We efficiently estimate and minimize the CVaR by sampling failure scenarios depending on their impact. By carefully selecting critical failure scenarios, we significantly reduce the computational burden associated with solving PDE for each scenario. We validated the suggested approach with two numerical case studies.

Physics-Informed Deep Learning for Traffic State Estimation: A Survey and the Outlook

Zhaobin Mo¹

¹Columbia University

For its robust predictive power (compared to pure physics-based models) and sample-efficient training (compared to pure deep learning models), physics-informed deep learning (PIDL), a paradigm hybridizing physics-based models and deep neural networks (DNNs), has been booming in science and engineering fields. One key challenge of applying PIDL to various domains and problems lies in the design of a computational graph that integrates physics and DNNs. In other words, how the physics is encoded into DNNs and how the physics and data components are represented. We offer an overview of a variety of architecture designs of PIDL computational graphs and how these structures are customized to traffic state estimation (TSE), a central problem in building a transportation digital twin. When observation data, problem type, and goal vary, we demonstrate potential architectures of PIDL computational graphs and compare these variants using the same real-world dataset.

Mathematical modelling of the impacts of screening and vaccination in HPV

Soyoung Park¹

¹University of Maryland

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A digital cerebral vasculature database for stroke management

Aseem Milind Pradhan¹

¹George Mason University

Human cerebral collateral circulation acts as a vital safeguard against interruptions in blood flow, especially during strokes. The quality of collateral circulation significantly affects stroke treatment outcomes. However, assessing this circulation is subjective due to limitations in current metrics, and advanced imaging techniques cannot capture detailed collateral structures, leaving us with an incomplete understanding of the cerebral vasculature.

In this study, we use a constructive constrained optimization algorithm to extend arterial trees reconstructed from MR images, generating realistic vascular models spanning from the aortic arch to cerebral arteries as small as 50 micrometers. These models can incorporate various Circle of Willis configurations and collateral vessel distributions to accommodate individual subject differences. Consequently, we aim to establish a comprehensive database of cerebral vasculatures (i.e., a virtual population) by combining multiple segmented geometries with varied extended arterial trees. We have developed a distributed lumped parameter model coupled with a mass transport solver to enable *in silico* angiographies for such large vascular networks. These virtual angiograms can be compared to patient-specific angiograms,

identifying a model within the population (digital twin) that best approximates the patient’s cerebral vasculature.

It is essential to note that this model differs from a traditional digital twin, as information transfer between the virtual model and the patient occurs infrequently, typically only during their imaging sessions. Nevertheless, these virtual geometries facilitate blood flow simulations providing data inaccessible through conventional imaging. They can predict the impact of interventions like blockages, hemorrhages, or catheter insertion on a patient’s hemodynamics. This innovative approach offers promising prospects to enhance stroke management by providing a deeper understanding of cerebral vasculature and the consequences of various interventions.” Human cerebral collateral circulation acts as a vital safeguard against interruptions in blood flow, especially during strokes. The quality of collateral circulation significantly affects stroke treatment outcomes. However, assessing this circulation is subjective due to limitations in current metrics, and advanced imaging techniques cannot capture detailed collateral structures, leaving us with an incomplete understanding of the cerebral vasculature.

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Accelerating the computation of tensor Z -eigenvalues

Rhea Shroff¹

¹University of Florida

Efficient solvers for tensor eigenvalue problems are important tools for the analysis of higher-order data sets. Here we introduce, analyze and demonstrate an extrapolation method to accelerate the widely used shifted symmetric higher order power method for tensor Z -eigenvalue problems. We analyze the asymptotic convergence of the method, determining the range of extrapolation parameters that induce acceleration, as well as the parameter that gives the optimal convergence rate. We then introduce an automated method to dynamically approximate the optimal parameter, and demonstrate its efficiency when the base iteration is run with either static or adaptively set shifts. Our numerical results on both even and odd order tensors demonstrate the theory and show we achieve our theoretically predicted acceleration.

Predictive system resilience modeling

Priscila Silva¹

¹University of Massachusetts Dartmouth

Resilience is the ability of a system to respond, absorb, adapt, and recover from a disruptive event. Dozens of metrics to quantify resilience have been proposed in the literature. However, fewer studies have proposed models to predict these metrics or the time at which a system will be restored to its nominal performance level after experiencing degradation. This talk presents three alternative approaches to model and predict performance and resilience metrics with techniques from reliability engineering, including (i) bathtub-shaped hazard functions, (ii) mixture distributions, and (iii) a model incorporating covariates related to the intensity of events that degrade performance as well as efforts to restore performance. These models are general, and therefore, are highly applicable to digital twins in several ways, as they can enhance the understanding, performance, and management of physical systems or processes represented by digital twins, as well as critical infrastructure, cybersecurity, and machine learning systems. However, data in these areas is not shared widely. For this reason, historical data sets on job losses during seven different recessions in the United States are used to assess the predictive accuracy of these approaches, including the recession that began in 2020 due to COVID-19. Goodness of fit measures and confidence intervals as well as interval-based resilience metrics are computed to assess how well the models perform on the data sets considered. The results suggest that both bathtub-shaped functions and mixture distributions can produce accurate predictions for data sets exhibiting V, U, L, and J shaped curves, but that W and K shaped curves that respectively experience multiple shocks, deviate from the assumption of a single decrease and subsequent increase, or suffers a sudden drop in performance cannot be characterized well by either of those classes proposed. In contrast, the model incorporating covariates is capable of tracking all of types of curve noted above very well, including W and K shaped curves such as the two successive

shocks the U.S. economy experienced in 1980 and the sharp degradation in 2020. Moreover, covariate models outperform the simpler models on all of the goodness of fit measures and interval-based resilience metrics computed for all seven data sets considered. These results suggest that classical reliability modeling techniques such as bathtub-shaped hazard functions and mixture distributions are suitable for modeling and prediction of some resilience curves possessing a single decrease and subsequent recovery, but that covariate models to explicitly incorporate explanatory factors and domain specific information are much more flexible and achieve higher goodness of fit and greater predictive accuracy. Thus, the covariate modeling approach provides a general framework for data collection and predictive modeling for a variety of resilience curves.

Community robustness under edge addition in synthetic and empirical temporal networks

Moyi Tian¹

¹Brown University

Communities often represent key structural and functional clusters in complex networks. Many real-world networks exhibit the property of edge densification over time and observed networks may erroneously present false edges. Therefore, it is important to understand how communities change as the network changes and examine the limits of the robustness of communities under expanding the network by edge addition. We study the effect of edge addition on both real-world temporal networks and its digital twins, the simulated dynamic networks using synthetic data with controlled edge-addition strategy. We present experimental methodologies designed for synthetic and empirical cases and demonstrate results from applying four state-of-the-art community detection algorithms, i.e., Infomap, Label propagation, Leiden, and Louvain, on various network datasets. Our findings suggest that the robustness of communities depends strongly on the choice of detection method.

Large deviation theory-based adaptive importance sampling for rare events in high dimensions

Shanyin Tong¹

¹Columbia University

Rare and extreme events like hurricanes, energy grid blackouts, dam breaks, earthquakes, and pandemics are infrequent but have severe consequences. Because estimating the probability of such events can inform strategies that mitigate their effects, scientists must develop methods to study the distribution tail of these occurrences. However, calculating small probabilities is hard, particularly when involving complex dynamics and high-dimensional random variables. In this poster, I will discuss our proposed method for the accurate estimation of rare event or failure probabilities for expensive-to-evaluate numerical models in high dimensions. The proposed approach combines ideas from large deviation theory and adaptive importance sampling. The importance sampler uses a cross-entropy method to find an optimal Gaussian biasing distribution, and reuses all samples made throughout the process for both, the target probability estimation and for updating the biasing distributions. Large deviation theory is used to find a good initial biasing distribution through the solution of an optimization problem. Additionally, it is used to identify a low-dimensional subspace that is most informative of the rare event probability. This subspace is used for the cross-entropy method, which is known to lose efficiency in higher dimensions. The proposed method does not require smoothing of indicator functions nor does it involve numerical tuning parameters. We compare the method with a state-of-the-art cross-entropy-based importance sampling scheme using three examples: a high-dimensional failure probability estimation benchmark, a problem governed by a diffusion partial differential equation, and a tsunami problem governed by the time-dependent shallow water system in one spatial dimension.

Neural Network Approaches for Parameterized Optimal Control

Deepanshu Verma¹

¹Emory University

We present numerical approaches for deterministic, finite-dimensional optimal control problems whose dynamics depend on an unknown or uncertain parameter. The objective is to amortize the solution over a set of relevant parameters in an offline stage to enable rapid decision-making and be able to react to changes in the parameter in the online stage. To tackle the curse of dimensionality arising when the state and or parameter dimension are high-dimensional, we represent the policy using neural networks. We compare two training paradigms: First, our model-driven approach leverages the dynamics and definition of the objective function to learn the value function of the parameterized optimal control problem and obtain the policy using a feedback form. Second, we use actor-critic reinforcement learning to approximate the policy in a data-driven way. Through a two-dimensional convection-diffusion equation, featuring high-dimensional state and parameter spaces, we investigate the accuracy, efficiency, and scalability of both training paradigms. While both paradigms

lead to a reasonable approximation of the policy, the model-driven approach is more accurate and reduces the number of PDE solves significantly.
