"Bridging Scales in Cancer Modeling"

Regina Célia Cerqueira de Almeida
Laboratório Nacional de Computação Científica (LNCC)
http://lattes.cnpq.br/6688041530466410

Cancer arises from multiscale interactions that span tissues, cells, and molecular pathways. Computational modeling provides critical insights into disease mechanisms and treatment strategies. This talk explores hybrid multiscale frameworks and surrogate model reduction techniques for advancing cancer modeling and optimizing therapeutic approaches.

"Towards a Governable Hybrid AI Platform for Scientific Discovery"

Renato Cerqueira
Director, PUC-Behring Institute for Artificial Intelligence - PUC-Rio, Brazil
http://lattes.cnpq.br/0731606611183670

Over the past few years, the use of Artificial Intelligence has rapidly expanded across multiple stages of the scientific investigation process. From capturing and analyzing experimental observations, to exploring related literature, assisting in hypothesis formulation and verification, and even supporting the writing of research papers, AI technologies have already demonstrated a significant impact in accelerating discovery. Yet, as several authors have pointed out, this potential for efficiency gains comes with serious risks when AI is used inappropriately or without sufficient safeguards. In this talk, we will revisit emerging trends and risks in the use of AI for scientific investigation and argue for the need of a governable hybrid AI platform. By combining physics-based models, data-driven learning, and knowledge-centric approaches, such a platform would enable AI to be applied more effectively, safely, and transparently in research. Beyond efficiency, the focus should be on epistemic integration: how AI can contribute not only to prediction but also to explanation, justification, and validation of knowledge. A critical component of this vision is the systematic capture of the traces left by scientific processes, which provides a foundation for reproducibility and auditability, while also enabling meta-analysis and the acceleration of future discoveries. By advancing towards this vision, we aim to support a more agile, transparent, and trustworthy process of scientific discovery.

"Symbolic Regression for the Construction of Reduced Order Models for Acoustically Forced Combustion Instabilities"

Leonardo Santos de Brito Alves
Universidade Federal Fluminense (UFF)
http://lattes.cnpq.br/9363093814106081

The present work describes an ongoing collaboration between the DFCom Lab at UFF and EPRL at UCLA, funded by the US ARO. Its goal is the development of parametrized reduced order models (ROMs) for acoustically forced coaxial jet diffusion flames with flame lift-off and extinction predictive capabilities. Experiments performed at the EPRL provide the required datasets, whereas the ROMs are generated by the DFCom Lab. In order to do so, these datasets are first compressed using proper orthogonal decomposition (POD) and the ROMs for the POD coefficient dynamics are then developed using symbolic regression tools. Such an effort will lead to a better understanding of oscillatory combustion. This is relevant for the development of efficient fuel and oxidizer injection systems for liquid rocket engines and air-breathing propulsion systems.

"Universal Differential Equations for Hybrid Modeling in Process Systems Engineering: Concepts and Case Studies"

Maurício B. de Souza Jr.
Universidade Federal do Rio de Janeiro (UFRJ)
http://lattes.cnpq.br/4530858702685674

Process Systems Engineering (PSE) encompasses model-based strategies for the monitoring, control, and optimization of industrial processes. The selection between phenomenological (first-principles) and purely data-driven models depends on several factors, including the complexity of the process, the type and availability of data, and the computational resources required. In this context, hybrid modeling approaches, combining phenomenological and empirical models, offer a promising alternative by integrating first-principles knowledge with information extracted from data. These models improve interpretability while aiming to retain accuracy and flexibility in implementation. In our works, we investigated hybrid models based on Universal Differential Equations (UDEs), where universal approximators (e.g., neural networks) are embedded within differential equations to replace unknown or partially known terms. Specifically, we applied UDEs that combine Population Balance Equations (PBEs) with neural networks for the modeling of batch crystallization processes of potassium sulfate in water and paracetamol in ethano. Additionally, we employed neural networks integrated with mass balance equations to model gas-lifted oil production systems. Across all these cases, the UDE-based hybrid modeling approach demonstrated itself to be an efficient and flexible methodology, with strong potential for a wide range of PSE tasks.

"Recent Advances in Data Driven ROMs for Coupled Fluid Flow and Transport"

Gabriel Freguglia Barros
Universidade Federal do Rio de Janeiro (UFRJ)
http://lattes.cnpq.br/6712093008698539

In recent years, there has been significant interest in using data-driven methods to solve problems in science and engineering. Numerical simulations for these problems can be costly, making data-driven methods valuable for understanding and improving efficiency in quantifying and predicting states. This talk will review recent advancements in Scientific Machine Learning for Coupled Fluid Flow and Transport, such as dynamic mode decomposition, manifold learning, and variational autoencoders, as applied to relevant scientific and engineering problems. These problems are of interest in sustainable resource exploration, geophysics, and various industrial applications. We also assess strategies to improve model training efficiency such as the use of floating point compression in large datasets. In this talk, we will show how data-driven information can improve predictions, help explore parametric manifolds for unseen scenarios, and reconstruct high-dimensional simulations with lower-dimensional structures in a feasible time.

"Learning Physics from Videos"

J. Nathan Kutz
University of Washington
http://faculty.washington.edu/kutz

Sensing is a universal task in science and engineering. Downstream tasks from sensing include learning dynamical models, inferring full state estimates of a system (system identification), control decisions, and forecasting. These tasks are exceptionally challenging to achieve with limited sensors, noisy measurements, and corrupt or missing data. Existing techniques typically use current (static) sensor measurements to perform such tasks and require principled sensor placement or an abundance of randomly placed sensors. In contrast, we propose a SHallow REcurrent Decoder (SHRED) neural network structure which incorporates (i) a recurrent neural network (LSTM) to learn a latent representation of the temporal dynamics of the sensors, and (ii) a shallow decoder that learns a mapping between this latent representation and the high-dimensional state space. By explicitly accounting for the time-history, or trajectory, of the sensor measurements, SHRED enables accurate reconstructions with far fewer sensors, outperforms existing techniques when more measurements are available, and is agnostic towards sensor placement. In addition, a compressed representation of the high-dimensional state is directly obtained from sensor measurements, which provides an on-the-fly compression for modeling physical and engineering systems. Forecasting is also achieved from the sensor time-series data alone, producing an efficient paradigm for predicting temporal evolution with an exceptionally limited number of sensors. In the example cases explored, including turbulent flows, complex spatio-temporal dynamics can be characterized with exceedingly limited sensors that can be randomly placed with minimal loss of performance.