Name: Graham Pash

Research Statements

This information is vital to the overall evaluation of your application.

Field of Interest

a. *In terms a general audience would understand, describe an important, outstanding problem in computer science, applied mathematics or statistics that you would like to pursue in your research. (1/3)*
b. *Discuss the potential impact of your research on your field. How would it advance high performance computing in general? (1/3)*
c. *Provide an example of how it would advance a science or engineering application area or areas. (1/3)*

Uncertainty in inputs, observed data, and models necessitates uncertainty quantification to make predictions with quantified and potentially reduced uncertainty. Scientists and engineers are increasingly solving large-scale inverse problems, where model complexity prohibits direct simulation and Bayesian inference. A prominent method of reducing the cost of model evaluations is to construct surrogate models, which emulate the behavior of the modeled process but are computationally efficient. These data-driven methods, especially deep learning, have had increasingly significant impact in recent years and have shown tremendous promise in a number of fields. However, current data-driven surrogate models are not constrained by governing equations and thus the physics of the problem are only loosely enforced to the degree that they are learned by the model.

We propose an extension to current frameworks used to encode non-linear dynamics in neural networks through the direct use of non-linear scalar observables as activation functions. Furthermore, we suggest learning conservation laws to be used to constrain model future state prediction. If this framework is successful, it will permit physically constrained surrogate models to be trained quickly to accurately emulate full-physics simulations at a fraction of the on-line computational cost. This is an improvement over current methods that rely on reduced-order models derived through projection-based systems with constraints, whose constrained minimization problems approach the cost of full simulations.

The methodology and computational techniques developed as a result of this research will provide an important computational tool, which will be directly applicable to various problems in fluid dynamic, structural mechanics, and thermohydraulics in nuclear engineering where conservation; e.g., of mass, energy, and momentum, is critical. Surrogate and reduced order models that conserve will ultimately improve the scalability of complex models and allow for more accurate and informed decisions in high-consequence applications by combining their attractive efficiency with the stability of full simulation.

High Performance Computing

a. *Discuss the role of high performance computing in your research. (1/2)*
b. *How will you demonstrate the success of your research? (1/2)*

The role of high performance computing in computational predictive science cannot be understated. State of the art methods for full-scale simulation of complex systems rely on large finite element or finite volume codes and distributed computing to adequately simulate systems even just a single time. Moreover, methods for quantifying uncertainty, such as Markov Chain Monte Carlo algorithms, converge slowly and require many thousands (or even millions) of solves. Despite increases in computational capabilities, the sole use of expensive high-fidelity models remains intractable and motivates the deployment of reduced-order and surrogate models.

I propose a three-stage methodology for constructing a physically constrained neural network surrogate model. First, a low-dimensional embedding of the system dynamics is computed using an auto-encoder with the caveat that the activation functions form a truncated eigenfunction basis obtained by Extended Dynamic Mode Decomposition. Second, auxiliary networks trained to minimize conservation-law violations of the discretized domain learn latent constraints on system dynamics. Third, the embedded dynamics of the system are evolved in time, constrained by the auxiliary networks, and decoded to recover the future state prediction. Training such models will bring its own set of challenges and motivate the use of new computational capabilities to take advantage of parallelism to efficiently solve corresponding optimization problems.

To demonstrate success, we will compare our technique to other approaches first by comparing surrogate model performance with high-fidelity simulation of canonical problems, such the inviscid Burgers' equation. We will also compare our technique with other existing data-driven surrogate models in the literature through the replication of known experiments. Moreover, we will leverage uncertainty quantification to determine more information about the robustness of the surrogate model itself. As we progress, we will work with collaborators to construct and demonstrate experimental success through the performance of surrogate models on deployed systems.

Program of Study

Describe how the courses listed in your planned program of study would help prepare you to address the challenges you have described in questions 1 and 2. Discuss your rationale for choosing these courses. How will the science or engineering application courses you have selected impact your research?

The interdisciplinary Computational Science, Engineering, and Mathematics program focuses on three core areas that underpin computational science research: applicable mathematics, numerical analysis and scientific computation, and mathematical modeling and applications. The applicable mathematics thrust of the program will provide me with a strong and broad theoretical foundation of the mathematical tools of the mathematical tools of the field. The numerical analysis and scientific computing portion of the program will provide me with grounded experience in applying these mathematical abstractions to solve “real” problems. Finally, the mathematical modeling and applications concentration will provide me with a robust understanding of the role that modeling and computation play with regards to engineering applications. Moreover, I plan on fleshing out my coursework with planned courses in Parallel Systems, Artificial Intelligence, and Machine Learning. These courses will establish a firmer grasp of optimization routines and their specific shortcomings, especially with respect to emerging computational platforms and high performance computing. The Finite Element Methods and Numerical methods for Flow and Transport Problems courses will aid my understanding of current state of the art capabilities for high fidelity simulation. Furthermore, the Statistical and Discrete Methods for Scientific Computing class will offer a unique perspective on the role of statistics and uncertainty quantification for computational science.