Statement of Research

I am a computational engineer and computational applied mathematician with expertise in Computational Engineering, Sciences, Engineering, and Mathematics (CSEM). My research has focused on **two thrusts** that motivate and drive each other. The first thrust is to develop *rigorous numerical analysis and scalable forward simulations, inversion, and Uncertainty Quantification (UQ) of engineering, science, and mathematical problems governed by complex multiscale multiphysics partial differential equations* with applications to geophysics, fluid dynamics, wave propagation, plasma physics, etc. The second thrust is to develop Scientific Machine Learning (SciML) approaches for reliable real-time forecast, calibration, and UQ of digital twins based on the developments of the first thrust.

Executive Summary on Research Interest. My research program unifies high-order, scalable PDE solvers with data-assimilative SciML and certified UQ to deliver real-time digital twins in wave propagation applications (seismic imaging, inversion, earthquake monitoring, subsurface) and large-scale fluid systems (high-Mach, and multiscale/multiphysics). I target faster-than-real-time prediction and control on GPU/CPU leadership systems with a runway to quantum-accelerated SciML. My goal is to translate these capabilities into deployable solutions. This will be accomplished by leveraging my *cross-disciplinary* expertise in large-scale uncertainty quantification, large-scale optimization constrained by partial differential equations, large-scale model and data/model reduction, scalable parallel algorithms for forward simulations and inverse problems, computational applied mathematics, HPC, and SciML.

I now present: a) some details of SciML goals and accomplishments in Section I and computational sciences & engineering contributions in Section II, b) ongoing and future work in Section III, and c) some flagship research experiences in Section IV.

I. `Learn2Solve` framework with model-constrained SciML methods

For a deep learning model to serve as a reliable basis for operational forecast, design, optimization, and decision-making, the following main challenges need to be addressed:

1. How to **automate** deep neural networks (DNNs) architecture (e.g. how many layers and how many neurons are on each layer for a particular application at hand)? *Addressing this question with mathematical rigor provides* **reliable** *architecture design approaches and helps avoid hours/days spent on currently demanding heuristic hyperparameter searches.*

2. Can we develop new optimization methods that are significantly more efficient than stochastic gradient descent—the main workhorse in machine learning training—especially for ill-conditioned loss landscapes (i.e. with flat or close to flat regions or regions with complicated saddle structures)? *Addressing this question could provide* **reliable** *training methods that reduce the number of epochs significantly, and thus cutting the training time substantially.*

3. How to incorporate not only the governing equations/physics but also their well-developed numerical treatments, that is, how to learn well-designed methods we use the problem? *Addressing this question allows us to incorporate our decades of successful experience in solving problems (as opposed to approaches that respect only the governing equations and that completely discard our*

solution methods). Such a method could not only solve challenging problems but also be **interpretable and reliable** *for* **out-of-distribution** *(***OOD***) dynamics/information/regimes. Such generalization capability is not possible with existing methods.*

4. How to quantify the error and/or uncertainty associated with a deep learning model? *Addressing this question provides us with* **predictive** *deep learning models. In particular, such a deep learning model informs us on regimes, such as spatial and temporal domains, in which it is* **reliable***, and when it faces* **OOD** *regimes (and thus needs to be updated/re-calibrated).*

5. How to update/calibrate a trained deep learning model online and/or in real-time when the baseline counterpart drifts away from it? *Addressing this question provides methods to* **adaptively** *maintain the* **reliability** *and accuracy of a deep learning model as a digital twin.*

6. Can we develop SciML approach capable of delivering similar accuracy to traditional methods? *Addressing this question would provide similar* **accuracy***, and thus* **reliability***—that is currently not possible with the contemporary SciML approaches—to traditional counterparts.*

7. Can we develop mathematical theoretical foundations for deep learning methods inspired by traditional computational applied mathematics? *Addressing this question provides* **confidence** *for not only developers but also practitioners of deep learning methods.*

Addressing the aforementioned questions requires interdisciplinary capabilities in applied mathematics, probability, scientific computing, and scientific deep learning. My group is one of a few groups with such capabilities. My research focus for the past six years on the `Learn2Solve` paradigm has been mainly revolving around the aforementioned questions (see, e.g., [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]). Let me now discuss some recent results for four questions out of the aforementioned seven questions. Addressing the other questions (in fact, all of them) is ongoing.

Addressing the first question. Our first attempt [11] introduces a two-stage framework for progressively developing neural architectures to adapt/generalize well on a given training data set. This is based on our interpretation of the depth of the network as time evolution, as in numerical methods for time-dependent problems. On a radically different path, we have developed a rigorous approach inspired by the topological optimization for adapting DNN architecture [10]. In this approach, adding/removing a neuron/layer is similar to adding/removing materials in topology optimization. Currently, capitalizing on our expertise in finite elements, our ongoing DNN architecture design is grounded in mesh adaptivity based on *a posterior* error estimation.

Addressing the third question. Our recent work [5, 9, 8] contributes a model-constrained tangent slope learning (`mcTangent`) approach for real-time simulations/forecasts. At the heart of `mcTangent` is the desire to encode the neural network tangent slope with the underlying governing equations **and their numerical methods**. As a result, our approaches, particularly `DGNet`, can achieve unprecedented ODD results for supersonic/hypersonic flows [9]. For inverse problems, our recent work [6, 8] develops a model-constrained deep learning approachs called `TNet` and `TAEN` that are capable of learning the Tikhonov method for inverse problems governed by partial differential equations in low data regimes, and thus providing real-time inverse/calibration solutions.

Addressing the fourth question for inverse problems. Principled Uncertainty quantification (UQ) in deep learning is extremely challenging and still an unsolved problem. Our recent work develops a model-constrained Bayesian DNN (`mcBNN`) for quantifying the uncertainty in DNN inverse solutions. At the heart of our approach is to learn our previously developed methods for quantifying associated uncertainty in inverse solutions. The preliminary work has been presented at various invited talks and published as a conference proceeding [12].

Addressing the seventh question. One of the reasons why many neural networks are capable of replicating complicated tasks or functions is their universal approximation property. Our recent work [7] provides a unified and constructive framework for the universality of a large class of activation functions, and hence neural networks, including most of the existing ones.

With the above foundational work, my group is one of the handful of research groups positioned to provide faster-than-real-time forecasts and calibrations of digital twins with quantifiable UQ. What remains is to detect when deep learning models are no longer accurate or reliable and to develop real-time approaches to recalibrate them. Tackling this and the other questions will be forthcoming.

II. Scalable and accurate computational sciences & engineering research

The foundation of my research group on reliable AI/ML methods for complex problem in sciences, engineering, and mathematics relies not only on available well-developed applied mathematics and scientific computation approaches but also new ones for new problems or problems without satisfactory approaches. Part of my research has been the continuation of new developments of applied mathematical methods and scientific algorithms for challenging problems (in plasma physics and earth system models, for example). This is reflected in several recent publications on advanced high-order discontinuous Galerkin methods for forward problems governed by complex multiphysics and multiscale PDEs [13, 14, 15, 16, 17, 18, 19, 20], deterministic and stochastic inverse problems [21, 22, 23, 24, 25, 26], and uncertainty quantification [27, 28]. I have also developed hybrid approaches that leverage the advantages of the reliability/accuracy of applied math methods and the speed of deep learning techniques [29, 30].

III. Ongoing and future work

Continuation of the `Learn2Solve` framework. Digital twins (DTs) are designed to be replicas of systems and processes. The key roles of DTs are to run hypothetical simulations to understand the implications at any point throughout the life cycle of the process, to monitor the process, to calibrate parameters to match the actual process, to quantify the uncertainties, etc. *The core of my research in the next 5-10 years* will continue the foundations that I have established on various faster-than-real-time SciML approaches for forward, inverse, and UQ problems. I will continue my unique interdisciplinary strength in both theoretical and algorithmic developments, and simultaneously transition to adapting them to building digital twins for physical processes/assets, including geophysics and fluid dynamics (such as numerical weather forecast, hurricanes, high-Mach flows), seismic imaging/inversion and subsurface characterization, renewable energy (fusion-energy systems such as Tokamak and stellarators), and rare mineral exploration/extraction processes. Raytheon Technologies, Lockheed Martin, and Trident & Zoetic realized the impacts of my work and have been investing in my `Learn2Solve` framework for digital twins that could support some of their missions. Federal agencies and companies have been and are expected to continue investing in my SciML research.

Quantum Algorithms for Scientific Computing. My research for the next 5-20 years will also be exploration/exploitation at the intersection of quantum computing and AI/ML/data-sciences. In particular, my interest lies in the mathematical foundations and quantum-accelerated SciML algorithms for Digital Twins applications.

IV. Flagship research experiences

i. Forward/inverse wave propagation + AI/ML

My experiences. I have been constructing end-to-end pipelines that integrate high-order forward solvers (elastic-acoustic & EM waves on GPUs/CPU leadership systems) with adjoint/Bayesian inverse methods, wrapped in data-assimilative SciML for real-time, UQ-aware digital twins. My `Learn2Solve` framework (e.g., `TNet/TAEN/mcBNN` for inverse problems and model-constrained UQ) directly advances reliable imaging/monitoring under streaming data.

ii. Large-scale fluid systems (HPC, advanced algorithms, ML, multiscale/multiphysics)

My experiences. I have two decades of parallel high-order DG/HDG/DPG methods and solvers for incompressible/compressible flows, MHD, shallow water equations, multilevel preconditioning, and operator-learning/SciML models with OOD-robustness (e.g., `mcTangent/DGNet`) to achieve faster-than-real-time prediction for high-Mach and complex flows. My work is built to translate: from rigorous numerics to real-time SciML digital twins to UQ-certified decisions.

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