Statement of Research

I am a computational engineer and computational applied mathematician with expertise in Computational Engineering, Sciences, Engineering, and Mathematics (CSEM). ourresearch has focused on **two thrusts** that motivate and drive each other. The first thrust is to develop *rigorous numerical analysis and scalable simulations of engineering, science, and mathematical problems governed by partial differential equations* with applications to plasma physics, geophysics, fluid dynamics, wave propagation, etc. The second thrust is to develop methods for data-driven predictive modeling based on the developments of the first thrust.

Goals. Since tenured, I have transitioned my research focus to (faster-than) real-time AI/ML approaches for both thrusts. The *long-term goal* of my research program is to bring SciDL (Scientific Deep Learning) to a mature stage where we have confidence in deploying SciDL tools—just like traditional tools but with unprecedented speed and possibly without a human in the loop. 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 reduction, scalable parallel algorithms for forward simulations and inverse problems, computational applied mathematics, and scientific deep learning. *My ultimate objective is to construct rigorous and reliable SciDL approaches for faster-than-real-time forecasts, calibrations, assimilation, optimizations, and optimal designs/controls of future digital twin models.*

I now present: a) some details of SciDL goals and accomplishments in Section I and computational math contributions in Section II, and e) ongoing and future work in Section III.

I. `Learn2Solve` framework with model-constrained deep learning 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 closed 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 that we have developed to solve a particular challenge? *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 skills). 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 by existing methods (see, e.g., our results for an ODD supersonic/hypersonic flows by clicking here).*

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 SciDL 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 SciDL approaches—to traditional counterparts.*

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, if not the only, with such capabilities. My research focus for the past five years on the `Learn2Solve` paradigm has been mainly revolving around the aforementioned questions (see, e.g., [1, 2, 3, 4, 5, 6, 7]). Let me now discuss three instances of our `Learn2Solve` paradigm.

Addressing the first question. Our first attempt 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. The preliminary results were reported in [8], and we are wrapping up the final version with rigorous mathematical proofs. On a complementary approach, we have developed a rigorous approach inspired by the topological optimization literature for adapting DNN architecture. This work has yielded significant results, both theoretically and numerically. We are in the process of completing a paper in this direction. In parallel, we have devised an adaptation strategy making use of our expertise on mesh adaptation in finite element methods. This approach is awaiting implementation and testing.

Addressing the second question. ourrecent work [5, 9] contributes a model-constrained tangent slope learning (`mcTangent`) approach. At the heart of `mcTangent` is the desire to encode the neural network tangent slope with the underlying governing equations and their numerical methods. For inverse problems, ourrecent work [6] develops a model-constrained deep learning approach called `TNet` that is capable of learning the Tikhonov method for inverse problems governed by partial differential equations in low data regimes.

Addressing the third question for inverse problems. Principled Uncertainty quantification (UQ) in deep learning is extremely challenging and still an unsolved problem. ourrecent work develops a model-constrained Bayesian DNN 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 [10]. It will be soon submitted.

Addressing the fourth and fifth questions. One of the reasons why many neural networks are capable of replicating complicated tasks or functions is their universal approximation property. ourrecent 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 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 re-calibrate them. This will be forthcoming from my research group.

II. Scalable and accurate computational math research

The foundation of my research group on reliable AI/ML methods for complex problem 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 high-order discontinuous Galerkin methods for forward problems governed by PDEs [11, 12, 13, 14, 15, 16, 17], deterministic and stochastic inverse problems [18, 19, 20, 21, 22, 23], and uncertainty quantification [24, 25]. 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 [26, 27].

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 is 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, and to quantify the uncertainties. *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 SciDL 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 earth systems (such as weather and hurricanes: ongoing), fusion systems (such as Tokamak: ongoing), and rare mineral exploration/extraction process (ongoing). 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 SciDL research.

Augmented reality and Quantum Algorithms for Scientific Computing. Augmented Reality (AR) is an interactive environment combining the physical processes/assets and their digital models. It has vast applications in healthcare, gaming, architecture, education, industrial manufacturing, etc. The work that I have carried out and will continue for `Learn2Solve` uniquely positions my group to develop key technologies/algorithms for future Augmented Reality (AR) systems. Half of my group, 3 graduate students and me, are working on quantum-accelerated algorithms for DTs. My research for the next 10-20 years will be on the mathematical foundations and quantum-accelerated SciDL algorithms for DTs and ARs with applications to earth system models, fusion processes/devices, and mineral exploration/extraction.

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