ABSTRACT

Most attempts at the interface of physical modeling and machine learning (ML) employ computationally-generated data in order to drive the various statistical discovery objectives. This enables a direct transfer and application of ML tools and techniques, but removes valuable structure, symmetries and invariances that were present in the model. In order to rediscover this structure, if at all possible, ML tools would need copious amounts of data. Even when big data is available, it is important to ensure that predictions produced by ML models trained on this data satisfy these constraints. Purely data-based, modern ML tools as those based on deep neural networks (NNs) provide rich representations for learning complex nonlinear functions, but lack robustness and fail when higher-level abstractions implied by the physical structure are needed to make predictions. We will discuss some aspects in the development of multiscale deep learning approaches incorporating known physical constraints as prior knowledge. Examples will be provided in the development of surrogate and uncertainty quantification models for multiscale PDEs, and the development of multi-fidelity generative deep learning algorithms for fluid flows. Application of these techniques to molecular systems, inverse modeling and other will be highlighted.