Editorial: Machine Learning and *Physical Review Fluids*: An Editorial Perspective

Machine learning (ML) has become an important tool for modeling, prediction, and control of fluid flows. Increases in computational power, novel algorithms, and open-source software have facilitated the incorporation of ML in numerous experimental and computational studies and have created a fertile ground for new ideas in fluid mechanics. In turn, an ever-increasing number of papers are submitted to *Physical Review Fluids* (PRFluids) with ML content. At PRFluids, we welcome research on advances in fluid mechanics achieved through ML, and the goal of this editorial is to assist authors in the preparation of their papers.

Papers submitted to PRFluids are expected to make contributions to fluid mechanics, either through the discovery of mechanisms or through the deployment of novel computational, theoretical, and experimental approaches. We suggest that when ML is integrated in such efforts, there are at least three important aspects to address: (i) the physical content and interpretation of the result; (ii) the reproducibility of methods and results; and (iii) the validation and verification of models.

Physical mechanisms and their interpretation are essential. While training a regression algorithm could lead to the development of a hypothesis for a flow mechanism, this in itself is not a sufficient argument for publication in a fluid mechanics journal. For example, training classifiers of different regimes is interesting when one learns something about the underlying mechanics from the classifier. While algorithms such as neural networks and reinforcement learning provide remarkable results in modeling and flow control, articles in PRFluids should make distinct efforts to provide a physical interpretation of the underlying algorithms and their results. Changing from one network to the next or recovering one Reynolds-averaged Navier–Stokes (RANS) model or a large eddy simulation (LES) closure is not sufficient. We argue that prediction does not imply causation. Providing an explanation for a prediction or a causal mechanism is important.

Reproducibility of models is paramount. Papers should include both the code and data that make it possible for others to reproduce their findings. These can be provided via the supplemental information. A paper with methods and results that

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are reproducible is an opportunity for ML to boost fluid mechanics research. At the same time, ML algorithms and software entail hyperparameters that are not often reported. Testing the proposed ML algorithms in previously unseen flow data sets (by changing geometry or Reynolds numbers) should be reported and should not be an art that requires expert tuning.

Validation, verification, and uncertainty quantification remain the hallmarks of computational discovery in fluid mechanics, and they are broadly accepted as necessary by our community. These standards are often bypassed in ML studies, as the lack of rigorous theory does not offer (yet!) guarantees of convergence, while there is an ongoing debate about whether changing one or other parameter of ML algorithms, such as network depth, will provide consistent results. Even more, it is broadly recognized that ML algorithms harbor biases, and their interpretation is hindered by their complexity and heuristics. Validating ML models, as well as quantifying their uncertainties using data, is as important as it has been for classical computational fluid dynamics. Data-driven Bayesian inference provides metrics for quantification of modeling uncertainties that also account for the experimental ones. Verification may be more difficult because of the lack of theory, but it is possible to quantify the sensitivity of predictions using statistical tools and ML techniques such as cross validation.

We understand in particular how ML brings new perspectives on the development of phenomenological models (for turbulence, rheology, bubbles, etc.) that have been published extensively in fluid mechanics journals over the decades. These models were devised to have a domain of validity that could be understood, and the authors have demonstrated the errors and quantified uncertainties. For example, LES and RANS for turbulent flows are often devised to work in the inertial range of the turbulent cascade. Understanding the regime of validity for important models is critical for fluid mechanics as a subject in order to know how results generalize across Reynolds numbers and different geometries. We expect that ML models will maintain these standards while they help us cross new scientific frontiers.

We live in exciting times, with new algorithms and unprecedented data that enable new discoveries in fluid mechanics. We believe that we are not in a position to predict the maturity curve for this field. The plethora of approaches that have been enabled by the ML revolution will no doubt have an impact on fluid mechanics as a subject in ways that we cannot presently imagine. The intent of any journal must be to let the flowers bloom, and we do not want to squelch the creativity of the community. We argue that the job of editors and referees is to balance this blooming with guardrails so that papers published in PRFluids have a chance of archival value and real impact in fluid mechanics in the long term.

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