Rethinking materials simulation with machine-learning strategies

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Scientific Machine Learning *Operator Learning* *Computational Mechanics*

Abstract Materials simulations are omnipresent across diverse scientific domains from physical, chemical, and materials sciences to mechanics and biology. Existing state-of-the-art direct numerical solvers (DNS) used for these simulations are accurate but computationally expensive for predicting materials evolution across timescales, due to the complexity of the underlying evolution equations, the nature of multiscale spatio-temporal interactions, and the need to reach long-time integration.

In this talk, I will discuss how we can rethink and accelerate such materials simulations and go beyond these limitations by blending classical computational solvers with various machine-learning strategies. I will discuss two strategies. The first strategy is based on a hybrid approach that integrate a community (phase-field) direct numerical solver (DNS) with a machine-learned solver. I will discuss some of the trade-offs to account for in terms of solution reconstruction and stability with such strategy [1] and I will describe how to integrate DNS with recurrent neural networks or neural operators to enable accurate extrapolation and efficient time-to-solution predictions of the predicted dynamics [2,3,4,5]. The second strategy is based on a physics-informed, multi-layer neural network which uses physical governing equations as its building blocks. Here the neural network acts as a reduced-order model replacing DNS. I will illustrate this strategy on the thermo-mechanical and thermal responses of composite materials [6,7]. For both of these strategies, I will discuss how the type of speed one can gain and how we can harness these emerging techniques for materials design and process optimization.
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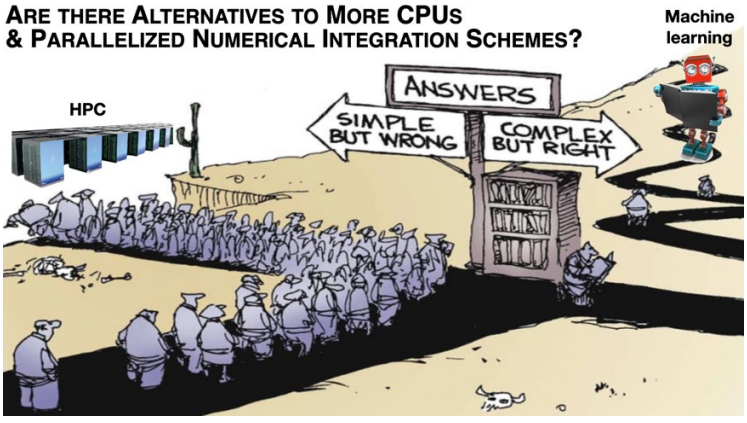

Figure 1 – Rethinking materials simulations with a machine-learning strategy. *Most of the current efforts to minimize computational costs have focused primarily on leveraging high-performance computing (HPC) and advanced numerical integration schemes. Emerging advances in machine learning offer an alternative (tortuous) route to achieve unprecedented speed up and comparable accuracy with direct numerical simulation results.*

References

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