Bias-variance tradeoff in accelerating multiscale solid mechanics with Model Order Reduction and machine learning

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Recent advances in materials science and manufacturing techniques are enabling the advent of new high-performance material systems with highly-tailored microstructures. Together with a push for less reliance on costly and environmentally harmful experimental material characterization campaigns, these recent shifts underscore the importance of developing efficient high-fidelity multiscale analysis techniques. In particular, computational homogenization (FE^2) is seen as a powerful tool for unravelling small-scale phenomena in complex materials and linking them to macroscale performance with no loss of generality. Yet, FE^2 still does not see widespread application due to the extreme computational cost associated with embedding and solving microscopic boundary-value problems at each and every macroscopic material point. The development of effective ways to accelerate FE^2 simulations has therefore given rise to a new and highly-active research community.

A popular approach to accelerate computational homogenization is to substitute its costly micromodel computations by fast approximate solutions. Here, two main approaches can be distinguished: Model Order Reduction (MOR) techniques can be used to reduce the complexity of the original microscopic boundary-value problem based on snapshots of full-field microscopic solutions, or micromodels can be altogether bypassed in favor of machine learning-based surrogate models trained on homogenized stress-strain data. Although no consensus currently exists on a definitive approach with broad applicability, substantial progress in these two directions has been made over the last few years, in particular concerning accurate representations of highly-nonlinear and path-dependent microscopic material behavior.

In this work, we present an integrated overview of our recent developments in MOR- and machine learning-based tools for accelerating FE^2 simulations in solid mechanics. We frame and compare different methods not only in their ability to reproduce relevant material behavior but also in terms of their unique levels of balance between physics-based bias and data-driven variance. The discussion includes pre-trained and adaptive hyper-reduced projection MOR models for plasticity and fracture [1], active learning of constitutive models for composite materials with Gaussian Processes [2], hybrid data-driven surrogates with embedded physics-based constitutive models [3] and graph-based learning for full-field predictions of path-dependent microscopic behavior. We summarize our main findings along these fronts and provide a sketch of future research directions.

References

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