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Upscaling and Automation: New Opportunities for Multiscale Systems Modeling

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Defense and energy applications ubiquitously involve multiscale and multiphysics systems. The accurate modeling of these systems, critical to achieve superior performances and optimized designs, has challenged generations of computational physicists due to the mathematical and numerical complexities involved in the development of their computable representations. One of the fundamental challenges associated with modeling multiscale processes is the development of rigorous models at the scale of interest (system-scale), which is typically much larger than the scale at which the physics is best understood (fine-scale). Coarse-graining techniques are a suite of mathematical strategies that allow one to perform rigorous scale translation, while bounding a priori upscaling errors. Yet, they require substantial time and mathematical expertise to use. This is due to the number analytical manipulations and rigorous approximations (e.g., series expansions) involved during model development that quickly become analytically intractable for systems of realistic complexities (e.g., systems with large numbers of interacting physics, nested scales, and chemical species). While computational physics has primarily focused on the aggressive advancement of numerical strategies for the solution of discretized PDEs of complex multiscale multiphysics systems, the applied mathematical techniques necessary for model formulation have continued to heavily rely on the speed and mathematical skill of humans rather than machines. As a result, their application to systems of realistic complexities has been very limited. With this work, we suggest that combining upscaling and automation allows to go beyond human-centered limitations and to accelerate model development processes. In this talk we propose a method of automatic upscaling through symbolic computation. By streamlining the upscaling procedure and derivation of applicability conditions to just a few minutes, the potential for democratization and broad utilization of upscaling methods in real-world applications emerges. We demonstrate the ability of our software prototype, Symbolica, by applying it to thermal runaway in battery packs and reactive transport in large reactive systems.

Participation

In-Person

References

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