

Upscaling and Automation: Pushing the Boundaries of Multiscale Modeling through Symbolic Computing

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In complex multi-scale system analysis, macroscopic differential equations are used to significantly increase computational efficiency and accurately model physical processes across multiple scales. Such equations can be systematically generated through rigorous *upscaling* techniques, which provide *a priori* error estimates and conditions under which the equations are valid (i.e., *applicability conditions*). However, the analytical derivations required in these techniques are time consuming, error-prone, and become quickly intractable for complex, multi-physical systems. To ease these complications, we propose a method of automatic upscaling through symbolic computation. By automating the analytical derivations, we democratize the utilization of upscaling techniques in practical applications and enable multi-scale model development in a feasible amount of time (i.e., seconds to minutes) with no requirements in analytical tractability, nor specialized expertise in mathematical model formulation. In this presentation, we demonstrate the ability of our software prototype, *Symbolica*, by reproducing homogenized advective-diffusive-reactive (ADR) systems from earlier studies and homogenizing a large ADR system deemed impractical for manual homogenization. We then discuss an application of *Symbolica* in Lithium ion battery packs to study heat transfer and thermal runaway.