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Equation-Free Computation for Complex/Multiscale Systems Modeling

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In current modeling , the best available descriptions of a system often come at a fine level (atomistic, stochastic, microscopic, individual-based) while the questions asked and the tasks required by the modeler (prediction, parametric analysis, optimization and control) are at a much coarser, averaged, macroscopic level. Traditional modeling approaches start by first deriving macroscopic evolution equations from the microscopic models, and then bringing our arsenal of mathematical and algorithmic tools to bear on these macroscopic descriptions.

Over the last few years, and with several collaborators, we have developed and validated a mathematically inspired, computational enabling technology that allows the modeler to perform macroscopic tasks acting on the microscopic models directly. We call this the “equation-free approach, since it circumvents the step of obtaining accurate macroscopic descriptions and links with matrix-free iterative linear algebra.

I will argue that the backbone of this approach is the design of (computational) experiments. In traditional numerical analysis, the main code pings a subroutine containing the model, and uses the returned information (time derivatives, function evaluations, functional derivatives) to perform computer-assisted analysis. In our approach the same main code pings a subroutine that sets up a short ensemble of appropriately initialized computational experiments from which the same quantities are estimated (rather than evaluated). Traditional continuum numerical algorithms can thus be viewed as protocols for experimental design (where experiment means a computational experiment set up and performed with a model at a different level of description).

Ultimately, what makes it all possible is the ability to initialize computational experiments at will. Short bursts of appropriately initialized computational experimentation through matrix-free numerical analysis and systems theory tools like variance reduction and estimation- bridges microscopic simulation with macroscopic modeling. Remarkably, if enough control authority exists to initialize laboratory experiments "at will", this computational enabling technology can become a set of experimental protocols for the equation-free exploration of complex system dynamics.