Adaptive Control of Multi-Scale Models

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We present a general approach for mathematically and computationally modeling events that take place at multiple spatial and temporal scales. A basic premise of the approach is that, in any simulation, one has specific target outputs that are the quantities of interest: purpose of the calculation. These quantities of interest can often be represented as functionals on the solution of some mathematical system, such as partial differential equations, or systems of ordinary differential equations. The second fundamental hypothesis is that it is possible to compute relative error between events that take place at different scales. The base model, which is based on the finer scale of the event, is the so-called truth model. We replace the fine-scale model with a sequence of surrogates that have coarser scales and which are tractable using available computational resources. The surrogate models are systematically adapted until they deliver results for the quantities of interest within a specified level of accuracy, all being determined using a posteriori error estimates.

The general approach involves the computation of solutions of the adjoints, calculations of residuals, and determining sequences of a posteriori error estimates to guide the calculation. We describe examples of the application of these methodologies to problems in molecular statics that are encountered in nano manufacturing, as well as the general methodologies applicable to stochastic systems. In concluding remarks, we discuss extensions of the adaptive modeling methods to stochastic, discrete, and continuous systems.