"Estimating and Control of Modeling Error: a systematic approach to multiscale modeling of large molecular and continuum systems"

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Summary

We have developed a general and rigorous approach of a posteriori error estimation of both modeling and discretization errors for general nonlinear problems. The approach is based on the idea of the existence of a base model, which is used as the datum with respect to which all other models of a given class, such as those involving coarser scales, or coarser discretizations, can be measured. The method allows the estimation of errors with respect to local quantities of interest. Once a modeling error is estimated, it can be systematically reduced through the implementation of the GOALS algorithm. We have demonstrated that these methods provide a rigorous and systematic approach to multi-scale modeling and are currently extending the technique to the analysis of very large-scale models of polymer materials.

"If error is corrected whenever it is recognized as such, the path to error is the path of truth." So said the renowned philosopher of science, Hans Reichenbauch, in his 1951 treatise, *The Rise of Scientific Philosophy*. Thus was laid the philosophical foundation of *a posteriori* error estimation. In the half-century that has followed Reichenbauch's work, *a posteriori* error estimation and control of numerical approximation error has reached the level of development where it has had a significant impact on adaptive meshing and in solution verification of finite element codes [1]. Only in very recent times has the notion been extended to general mathematical models of complex physical systems [2][3]. Our approach rests on the idea that to model a specific physical event, one has in hand a so-called base model that is of sufficient sophistication and detail that, with appropriate data, one could extract predictions of specific quantities of interest of sufficient accuracy to comfortably make predictions. The base model is never "solved", but acts as a datum with respect to how other models are compared. We then proceed to generate systematically a sequence of surrogate models that are designed to be not only tractable, but also progressively closer to the base model in the sense that they produce approximations of the quantities of interest that converge to the quantity of interest predictable by the base model. The sequence of surrogates is generated by the so-called "GOALS" algorithm. The key to the method of error estimation and control is the calculation of a residual functional: $R(u_0; p)$ in which u_0 is the solution of the surrogate problem and p is the solution of an adjoint problem corresponding to the particular quantity of

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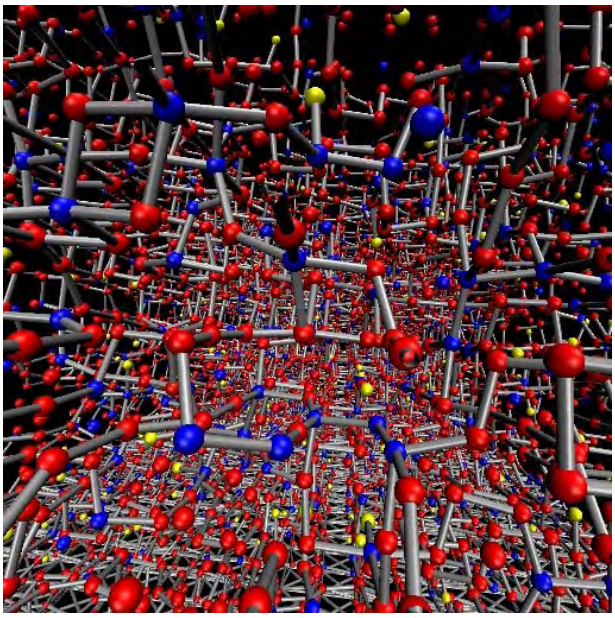
interest [3]. The GOALS algorithm employs a partition of the problem domain into sub-domains upon which the contribution of each sub-domain to the total residual can be calculated. Only sufficient information from the fine scale is used to produce predictions of quantities of interest within a preset level of accuracy. One thereby "recognizes error as such and then corrects it" and in this way attempts to "follow the path to truth."

Our particular application focuses on so-called "Step and Flash Imprint Lithography", a new method for manufacturing semiconductor devices. A key step in the process is the production of a polymer etch barrier that is used in the etching process of the nano-manufacturing of transistors. We hope to model nano-scale polymer systems and focus on specific features of the manufacturing process as our quantities of interest. We are developing a large-scale molecular statics program that implements the GOALS algorithm for these classes of applications

The accompanying figure demonstrates the polymer chains using our molecular model of the etch barrier in the SFIL process.



A lattice model of a polymer network generated in nano-manufacturing semi-conductor devices.

References

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