

## ESTIMATION OF MODELING ERRORS FOR A COUPLING METHOD

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**Key Words:** *Model Adaptivity, Multiscale Problems, Goal-oriented Error Estimation.*

### ABSTRACT

In this talk, we will review the main ideas of goal-oriented error estimation and adaptation for the control of modeling errors [1,2,3]. We will focus in particular on the extension of these ideas toward the development of a coupling method based on the Arlequin method (see [5]), for multi-scale modeling of nano-devices made of polymeric materials. We will present a new method in which a particle model is coupled to a continuum model via an overlap region as introduced in the Arlequin method. This coupling approach provides for a surrogate model that is an approximation of the true particle model. We will show here how to extend the goal-oriented adaptive modeling technique [3,6] so as to identify the regions in which the continuum and atomistic models should be used and thus to predict the position of the interface. We will show 1D and 3D examples in which the polymeric material is represented via a lattice-based molecular model. This work is part of an ongoing study of the application of these ideas to polymer materials used in semiconductor manufacturing.

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