# Coupling Methods for Multiscale Simulations and Adaptive Modeling


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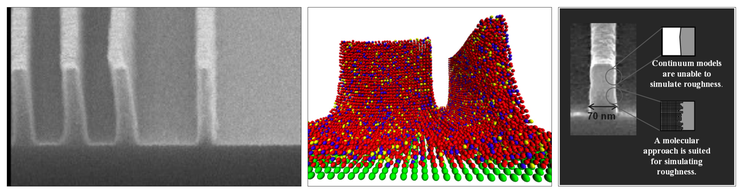
## Summary


We present here our recent progress on the development of multiscale approaches for coupling concurrent models used to describe phenomena spanning different spatial scales. The main approach is based on the Arlequin framework in which a reference particle model, supposedly intractable, is replaced by a coupled model that blends solutions from small and large scale models [1,2]: more explicitly, a continuum (large scale) model is used far from the regions of interest and a particle (small scale) model is kept in the local critical regions. We, in particular, describe

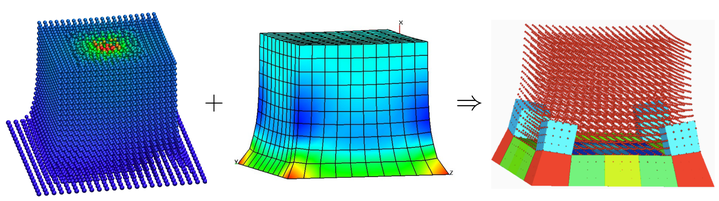
- a new coupling operator [3] that explicitly involves the size of the representative volume element (RVE) used to derive the continuum model from the particle model and show that it yields a well-posed formulation of the problem;
- an alternative approach to a classical adaptive method [4] to automatically adapt the position of the coupling zone in order to reduce modeling errors with respect to quantities of interest; the new approach is based on optimal control [5]; and
- an approach for the statistical calibration and validation of coarse-grained/continuum models and the stochastic coupling of models for uncertainty propagation.

Theoretical results are illustrated with recent numerical examples dealing with one- and two-dimensional problems.

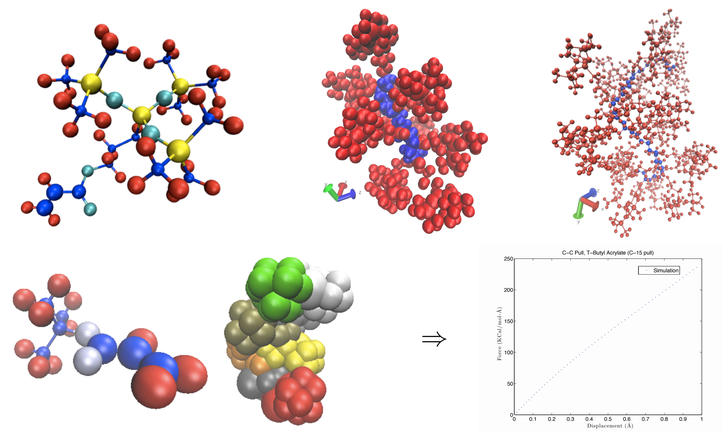

## Motivation




**Modeling of Nano-manufacturing Process:** Simulation of polymeric masks for the imprint of nanoscale features in micro-chips. Full particle model is intractable. The goal is to develop a concurrent approach that couples continuum and particle models.

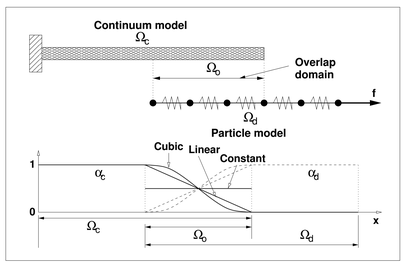


## Coarse-Graining Modeling

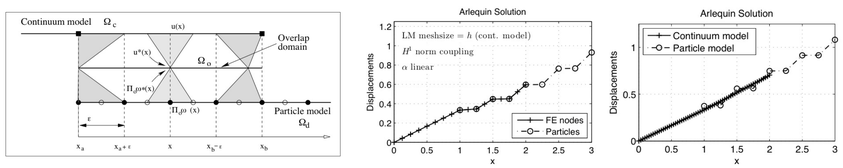


**Calibration of coarse-grained model:** Molecular simulations of Silicon mono-acrylate chains (shown with 1, 10, and 20 monomers, top) and of t-Butyl acrylate chains (shown with 1 and 8 monomers, bottom) using LAMMPS. These virtual experiments provide data to calibrate the parameters of the coarse-grained model in which the monomers are described as two particles bonded together. Calibration and validation of the coarse-grained models will be based on Bayesian inference.

## Coupling Method based on Arlequin Framework




1) Partition of energies.
2) Weight coefficients may be chosen constant, linear, cubic in overlap region.
3) Coupling through Lagrange multipliers: "averaging operator" is used to match the displacement and stress over the overlap region on .
4) Resulting mixed problem is well-posed.




Averaging Coupling Operator: $b(\mu,(u,w)) = \beta_0 \overline{\mu}\overline{(v-\Pi z)} + \beta_1 \int_{\Omega_o} \mu^*(v-\Pi z)^* dx$

## Adaptive Modeling

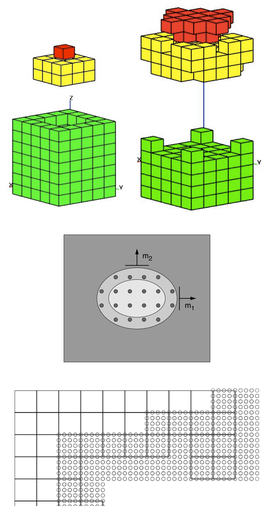
1. **Based on A posteriori Error Estimation:** Given a quantity of interest $Q$, estimate error in $Q$ as:

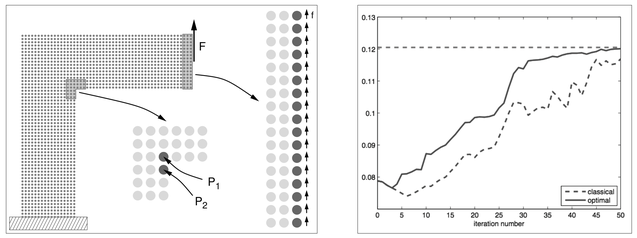
$$Q(u) - Q(u_0) = \mathcal{R}(u_0; p) + \Delta$$

where $u$ is the solution of fine-scale model, $u_0$ is the solution of the surrogate model (coupled model), $\mathcal{R}$ is the residual w.r.t. to fine-scale model, $p$ is the adjoint solution, $\Delta$ is a remainder involving higher-order terms w.r.t. the error.

2. **Based on Optimal Control:** Optimal control problem: Find the set of parameters $\mathbf{m}^*$ that minimizes the error $\mathcal{E}$ in the quantity of interest $Q$

$$\mathbf{m}^* = \underset{\mathbf{m}}{\operatorname{argmin}} \left[ \frac{1}{2} \big( Q(\mathbf{y}) - Q(\mathbf{y}_0(\mathbf{m})) \big)^2 \right]$$






## References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