Adaptive Multiscale Modeling of Polymeric Materials

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Outline

• Principles of goal-oriented error estimation and model adaptivity
• Application: Semiconductor manufacturing
• Base model definition
• Continuum surrogate models
• Coupled problem: Arlequin method
  - 1-D model problem (mathematics)
  - 3-D uniform problem
• Error estimates
• Concluding remarks and future work
Goals Methodology

1. Define **Base Model** (fine scale):

   \[ \text{Find } u \in U \text{ s.t. } B(u; v) = F(v) \forall v \in V \]

2. Define **Quantity of Interest**:

   \[ \text{Given } u, \text{ find } Q(u) \]

   \[ Q : U \rightarrow \mathbb{R} \]

- **Base model** captures events of interest, but intractable
- Never “solved”, used as comparison for other models
- May be challenging to define, but is considered necessary
3. Replace base model by (a sequence of) **Surrogate Models:**

Find \( u_0 \in U \) s.t.

\[
B_0(u_0; v) = F_0(v) \quad \forall v \in V
\]

- Must be tractable
- Ideally captures coarse scale features of base model
- May involve fine and coarse scale models (and the interface between the two)

2. **Error** in Quantity of Interest:

\[
\mathcal{E} = Q(u) - Q(u_0)
\]

- Must estimate error
- Reduce error by model adaptivity

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Adjoint Problem

Optimal Control problem for $Q$:

$$Q(u) = \inf_{v \in M} Q(v)$$

$$M = \{ v \in U : B(v; w) = F(w), \ \forall w \in V \}$$

$B(u; v) = F(v), \ \forall v \in V$ (Primal)

$B'(u; v, p) = Q'(u; v), \ \forall v \in U$ (Adjoint)

Surrogate Primal and Adjoint Problems:

$$B_0(u_0; v) = F_0(v), \ \forall v \in V$$

$$B'_0(u_0; v, p_0) = Q'_0(u_0; v), \ \forall v \in U$$
Error Estimation

Error Estimate*:

\[ Q(u) - Q(u_0) = R(u_0; p) + \Delta \]

where: \( R(u_0; p) = F(p) - B(u_0; p) \)

and \( p \) is the solution to

\[ B'(u; v, p) = Q'(u; v), \quad \forall v \in V \]

Remainder:

\[ \Delta = O(\|u - u_0\|^r), \quad r \geq 2 \]

* Oden, Prudhomme, JCP, 2002
Adaptive Modeling

Goals Algorithms:
\( \mathcal{R}(u_0; p) \approx \mathcal{E} = Q(u) - Q(u_0) \)

\( \tilde{u}_1 \)

\( Q(u) - Q(\tilde{u}_1) = \mathcal{E}_1 \)

\( |\mathcal{E}_1| \leq \gamma_{\text{tol}} ? \)

\( \tilde{u}_2 \)

\( Q(u) - Q(\tilde{u}_2) = \mathcal{E}_2 \)

\( |\mathcal{E}_2| \leq \gamma_{\text{tol}} ? \)

\( \tilde{u}_3 \)

\( Q(u) - Q(\tilde{u}_3) = \mathcal{E}_3 \)

\( |\mathcal{E}_3| \leq \gamma_{\text{tol}} ? \)
Nanoindentation of a thin Aluminum film to study the initial stages of plastic deformation under the action of an indenter.

Nanoindentation

Base Model: Molecular Statics

Surrogate Model: Quasicontinuum

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Nanoindentation

Force vs. displacement curve comparing the evolution of the base, QC, and Goals solutions.

Exact and estimated relative errors for the Goals solution.
Step and Flash Imprint Lithography

Template

Photocurable Acrylate

Wafer

Transfer Layer

UV

Polymerization

(Densification
(Equilibrium configuration at room temperature)
Need for Multiscale

Continuum models are unable to simulate roughness.

A molecular approach is suited for simulating roughness.
1. Base model
2. Quantity of interest
3. Interface conditions for the surrogate model
4. Error estimation
5. Adaptation
Polymerization Step

Initiation: \[ I + h\nu \rightarrow R_1^\bullet + R_2^\bullet \]

Propagation: \[ M + R^\bullet \rightarrow MR^\bullet \]
\[ M_nR^\bullet \rightarrow M_{n+1}R^\bullet \]

Termination: \[ M_nR^\bullet + M_mR^\bullet \rightarrow M_{n+m} \]

Arrhenius Law: \[ P = Ce^{-E_a/\kappa T} \propto k \]
One Realization of Polymerization
Molecular Potentials

Calibration by Inverse Analysis under way

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Given:
1. Lattice with $N$ molecules, each with position $x_i$
2. $N_i$ neighbors/molecule.
3. $E_{ik}(x_i, x_k) = \text{potential energy between particle } i \text{ and neighbor } k$.

Goal:
Find $x^* = \arg \min_x E(x)$

System of Equations:
$$\frac{\partial E(x^*)}{\partial x} = f(x^*) = 0$$
Densification Step

Base Primal and Adjoint Problems: For $u, v, p \in \mathbb{R}^{3N}$

$$B(u; v) = \sum_{i=1}^{N} \sum_{k=1}^{N} \frac{\partial E_{ik}}{\partial u_i} \cdot v_i$$

$$B'(u; v, p) = \sum_{i=1}^{N} \sum_{j=1}^{N} v_j \cdot \sum_{k=1}^{N} \frac{\partial^2 E_{ik}}{\partial u_i \partial u_j} p_i$$

$$Q(u) = \frac{1}{M} \sum_{m=1}^{M} u_m \cdot e_1$$

Solver:
- Inexact Newton Trust Region Method
- TAO/PETSc (http://www.mcs.anl.gov/petsc)

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Densification Step
Initial Parallel Calculations

- 100x100x100 particles
- ~3,000,000 D.O.F.
- 370 CPU hours on 64 processors
Construction of Continuum Model

Virtual Experiments on RVE's:
- Isotropy, homogeneity
- Must be validated against molecular model
- Objectivity: frame indifference

Statistical Mechanics of Polymer Networks:
- Flory, Treloar, Weiner, Fried

\[ W_{\text{CMR}} = \alpha(I_1 - 3) + \beta(I_2 - 3) + \gamma(J - 1)^2 - (2\alpha + 4\beta)\ln J \]

\[ W = \hat{W}(I_1, I_2, I_3) \]
Virtual Experiments

Strain Energy Density vs. $\lambda_1$, uniaxial tension

Strain Energy Density vs. $\lambda_2$, uniaxial tension

Strain Energy Density vs. $\lambda_3$, uniaxial tension

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Model Coupling: Arlequin Method

- Ben Dhia, "Problemes mecaniques multiechelles: la methode Arlequin" CRAS (1998)
Find \((u, w) \in X, \lambda \in M\) such that:

\[
a((u, w), (v, z)) + b(\lambda, (v, z)) = l((v, z)) \quad \forall (v, z) \in X
\]

\[
b(\mu, (u, w)) = 0 \quad \forall \mu \in M
\]

where:

\[
a((u, w), (v, z)) = \int_{\Omega_c} \alpha_c W'(u)v'\,dx + \sum_{i=1}^{m} \alpha_d E'_i(w_i, w_{i-1})(z_i - z_{i-1})
\]

\[
b(\mu, (v, z)) = \int_{\Omega_o} \beta_1 \mu(v - \Pi z) + \beta_2 \mu'(v - \Pi z)'\,dx
\]

\[
l((v, z)) = f z_m
\]

**Theorem:** Let \(\alpha_c = \alpha_d = 1/2\) and \(\beta_2 > 0\).

Then, the above problem is well-posed.
Model Coupling: Arlequin Method

a) General case

b) Nodes on overlap region are aligned with particles

c) Nodes on $\Omega_0$ coincide with those of $\Omega_C$

Particle Coupling

Continuum Coupling
I-D Example: Part. vs. Cont. Coup.

**L2 Coupling:**

![Graph showing Arlequin Solution for L2 Coupling with continuum and particle models, and a line graph depicting displacements vs. x with x values ranging from 0 to 3. The graph shows the coupling parameter $(\beta_1, \beta_2) = (1, 0)$.]

**H1 Coupling:**

![Graph showing Arlequin Solution for H1 Coupling with continuum and particle models, and a line graph depicting displacements vs. x with x values ranging from 0 to 3. The graph shows the coupling parameter $(\beta_1, \beta_2) = (1, 1)$.]

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1-D Example: L2 vs. H1 Coup.
3-D Example: Uniform Springs

- Base model: 20x20x20 lattice (8000 dofs)
- Surrogate: 9 trilinear elements, 20x20x4 particles (612 dofs)
- Stretched under uniform loading
- Quantity of Interest: Final Length
3-D Example: Poor Continuum Model

Base Solution
Colored by Adjoint Solution

Surrogate Solution
20% Longer
3-D Example: Error Estimation

\[ \mathcal{E} \approx \mathcal{R}(u_0; p) = \mathcal{R}(u_0; p_0) + \mathcal{R}(u_0; p - p_0) \]

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3-D Example: Error Control

\[ |R(u_0, p_0)| = 12.3 \]

\[ |R(u_1, p_1)| = 10.3 \]

\[ |R(u_2, p_2)| = 8.59 \]
Concluding Remarks

- Modeling of SFIL process using lattice polymer
- Base model consists of spring model
  - Primal, adjoint in 3-D
- Construction of surrogate continuum models using virtual experiments on RVE’s
  - Nonlinear elastic continuua
  - Solved using FEM in 3-D
- Coupling method introduced
  - Well-posedness in 1-D, linear
  - 3-D, nonlinear capability
- Error estimation and control with (manual) adaptivity
Future Work: Short Term

- Complete implementation of automatic 3-D adaptivity
- Continue investigation of approximations of adjoint/residual for coupled problem
- Investigate the effects of various coupling terms in 3-D
- Solve problem relevant to SFIL process (shrinkage) using coupled formulation (continuum determined with virtual experiments) with error estimation and automatic adaptivity.
Future Work: Long Term

• Investigate mathematical properties of 1-D problems:
  - New coupling terms
  - Nonlinear potentials
  - Error estimation (dual/residual approx., remainder)
• Base model solution on a petascale level
• Fully parallel coupled algorithm for Large scale calculations
• Investigate parallel implementation of Goals algorithm
• Investigate statistical variations
• Apply tools to bio-molecular problems