Adaptive Control of Multiscale Modeling Error, with Applications to Large-Scale Molecular Systems

J. Tinsley Oden

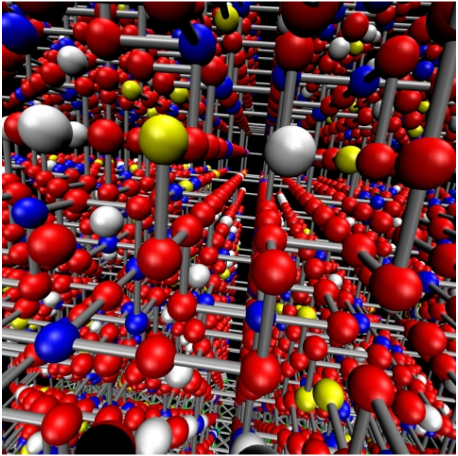
Institute for Computational Engineering and Sciences
The University of Texas at Austin

Office of Advanced Scientific Computing Research
2007 Applied Mathematics PI Meeting
Lawrence Livermore National Laboratory
Tuesday, May 22, 2007

RESEARCH TEAM

Collaborators:

Serge Prudhomme
Paul T. Bauman
Leszek Demkowicz
Chetan Jhurani
Jon Bass
Grant Willson
Elizabeth Collister



U.S. Department of Energy:

Office of Science's "Multiscale Mathematics" Program

INTRODUCTION

"If error is corrected whenever it is recognized, the path of error is the path of truth."

Hans Reichenbach, 1891–1953
The Rise of Scientific Philosophy, 1951

OUTLINE

- Introduction
- Anatomy of a Multi-scale Modeling Algorithm
- An Example: the Nano-indentation Problem
- Modeling of a Nano-manufacturing Process:
    1. The Polymerization Step
    2. The Densification Step
- Construction of Surrogates
- Coupling of Lattice/Continuum Models by the Arlequin Method
- Error Estimates and Adaptivity
- Conclusions

The Anatomy of Multi-scale Modeling

1. Define the Base Model for the finest scale:

   Find $u \in U$ s.t.
   $$B(u; v) = F(v) \; \forall v \in V$$

2. Target outputs
   Define the Quantities of Interest:

   Given u, find $Q(u)$
   $$Q : U \longrightarrow \mathbb{R}$$

- Is believed to capture the events of interest but is intractable.
- Is never "solved"*; is only a datum for assessing other models.
- May often be a sizable and complex undertaking – but in theory, is necessary.

* $Au = F$ in V'
$\Leftrightarrow B(u; v) = \langle Au, v \rangle \; \forall v \in V$

The Anatomy of Multi-scale Modeling

3. Replace the base model by a (sequence of) surrogates:

Find $u_0 \in U$ s.t.

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

- Must be tractable.
- Ideally captures coarser scale features of the phenomena.
- May involve fine scale and coarse scale components and interface.

4. Modeling Error:

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

- Must estimate $\mathcal{E}$.
- Reduce $\mathcal{E}$ by model adaptivity.

"Coarse graining", "homogenization", "model reduction", "up-scaling", "ensemble average",...

The Adjoint Problem

Optimal Control Problem for Q:

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

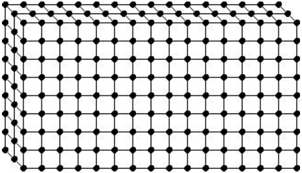
$$M = \{v \in U : \ B(v;w) = F(w), \ \forall w \in V\}$$

$$\begin{aligned} B(u;v) &= F(v), & \forall\, v \in V \quad & \text{(Primal)} \\ B'(u;v,p) &= Q'(u;v), & \forall\, v \in U \quad & \text{(Adjoint)} \end{aligned}$$

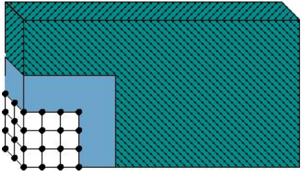
Surrogate Primal and Adjoint problems:

$$\begin{aligned} B_0(u_0;v) &= F_0(v), & \forall\, v \in V \\ B_0'(u_0;v,p_0) &= Q_0'(u_0;v), & \forall\, v \in U \end{aligned}$$

The Anatomy of Multi-scale Modeling



Base model ("u")



Surrogate model ("u_0")

Theorem* If u is a solution of the base model and u_0 an arbitrary member of U, then:

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

where $\mathcal{R}(u_0; p) = F(p) - B(u_0; p)$ and p is a solution of the adjoint problem,

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

and Δ is a remainder involving terms of $\mathcal{O}(\|u - u_0\|^r), \ r \geq 2$.

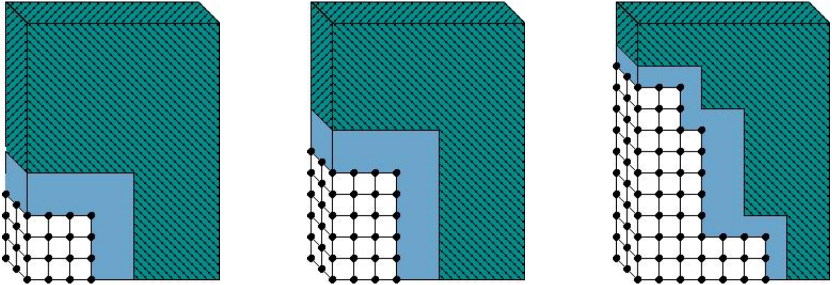
*Oden & Prudhomme, *J. Comp. Phys.* (2002).

*Oden, Prudhomme, Romkes, & Bauman, SIAM J. Sci. Comput. (2006).

Adaptive Modeling Algorithms

"GOALS ALGORITHMS"

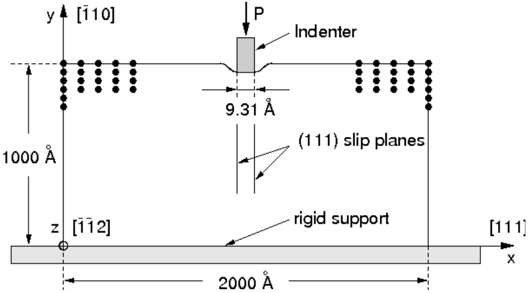
$$\mathcal{R}(u_0; p) \approx \mathcal{E} = Q(u) - Q(u_0)$$

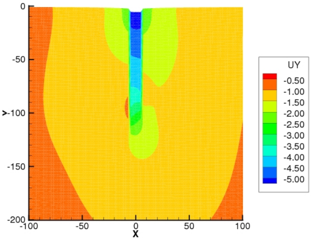


$\tilde{u}_1$	$\tilde{u}_2$	$\tilde{u}_3$
$Q(u) - Q(\tilde{u}_1) = \mathcal{E}_1$	$Q(u) - Q(\tilde{u}_2) = \mathcal{E}_2$	$Q(u) - Q(\tilde{u}_3) = \mathcal{E}_3$
$\lvert\mathcal{E}_1\rvert \leq \gamma_{\text{tol}}$?	$\lvert\mathcal{E}_2\rvert \leq \gamma_{\text{tol}}$?	$\lvert\mathcal{E}_3\rvert \leq \gamma_{\text{tol}}$?

AN EXAMPLE: Nano-indentation

Nano-indentation of a thin aluminium film to study the initial stages of plastic deformation under the action of an indenter.



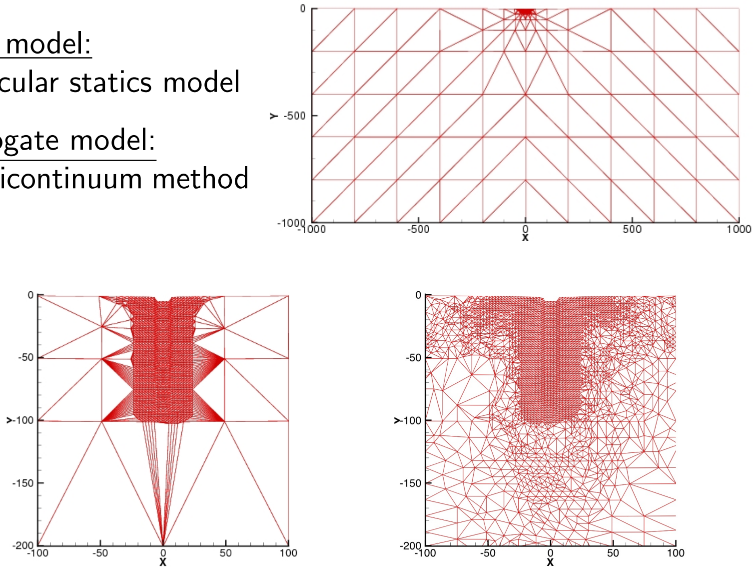


*Tadmor, Miller, Phillips, and Ortiz, *J. Mat. Res.* 14, (1999)
*Phillips, Rodney, Shenoy, Tadmor, and Ortiz, *Model. Simul. Mat. Sci. Eng.* 7 (1999)
*Prudhomme, Bauman, and Oden, *Int. J. Multiscale Comput. Eng.* 4 (2006)

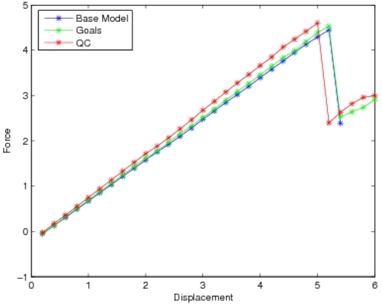
AN EXAMPLE: Nano-indentation

Base model:
Molecular statics model

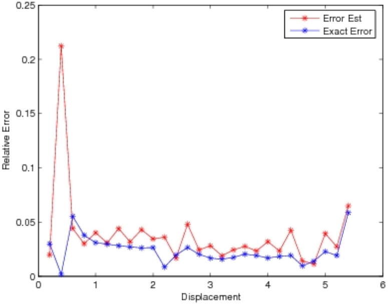
Surrogate model:
Quasicontinuum method



AN EXAMPLE: Nano-indentation



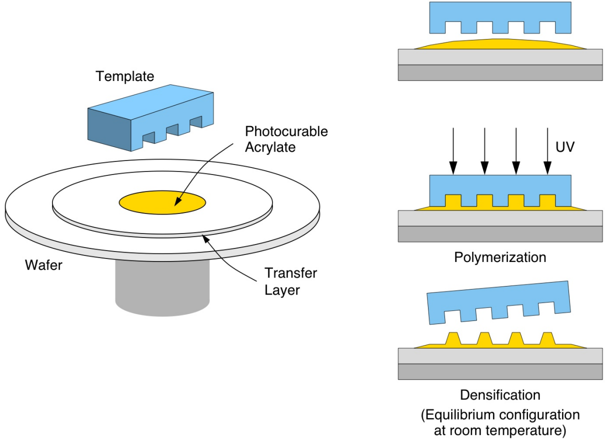
Force vs. displacement curve comparing the evolution of the base, QC, and Goals solutions.



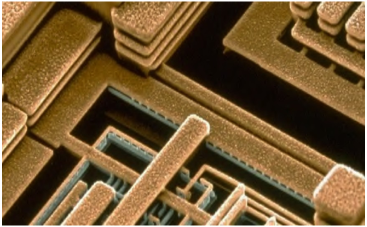
Exact and estimated relative errors for the Goals solution.

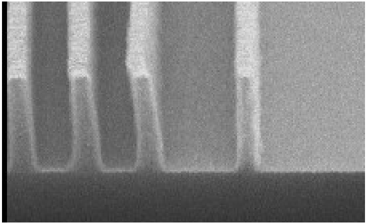
Multi-scale Modeling of a Nano-manufacturing Process

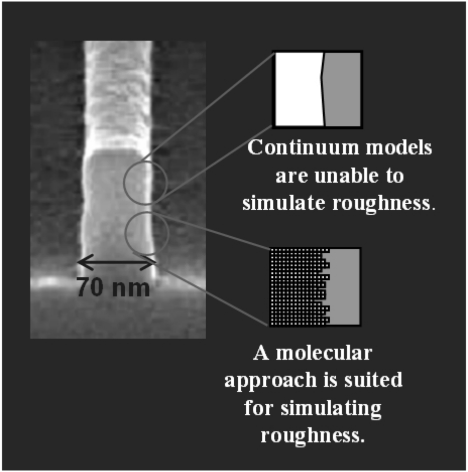
STEP-AND-FLASH IMPRINT LITHOGRAPHY (SFIL)



Multi-scale Modeling of a Nano-manufacturing Process

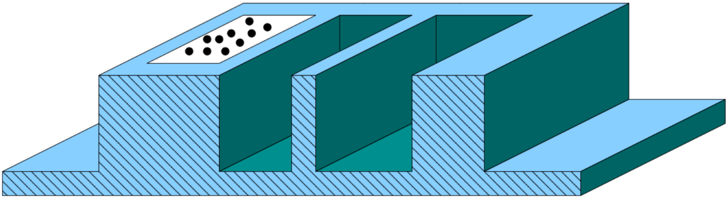






Multi-scale Modeling of a Nano-manufacturing Process

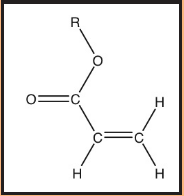
1. Base model
2. Quantity of interest
3. Interface conditions for the surrogate model
4. Error estimation
5. Adaptation



The Base Model: Polymerization Step

The polymer is a mixture of two acrylate-based monomers:

1. M_1 = silicon monoacrylate for etch resistance
2. M_2 = t-Butyl acrylate to maintain low viscosity
3. Photo-initiator I
4. Cross-linker X_L



Acrylate

Initiation:

$$I + h\nu \longrightarrow R_1^\bullet + R_2^\bullet$$

Propagation:

$$M + R^\bullet \longrightarrow MR^\bullet$$
$$M_nR^\bullet \longrightarrow M_{m+1}R^\bullet$$

Termination:

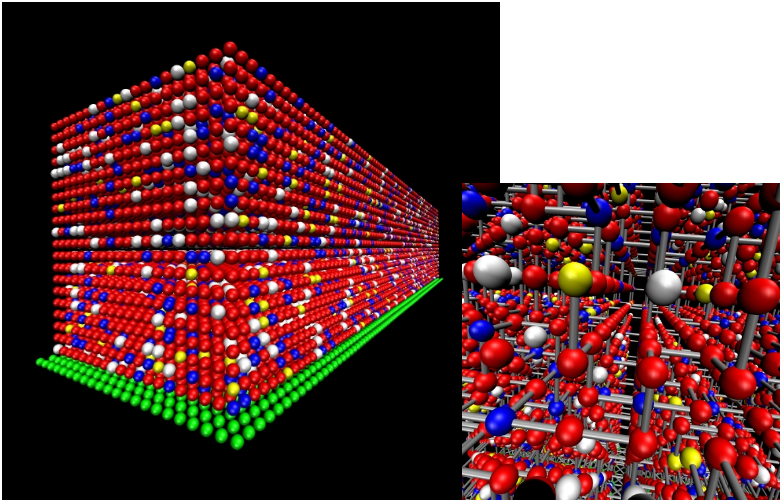
$$M_nR^\bullet + M_mR^\bullet \longrightarrow M_{n+m}$$

Arrhenius Law:

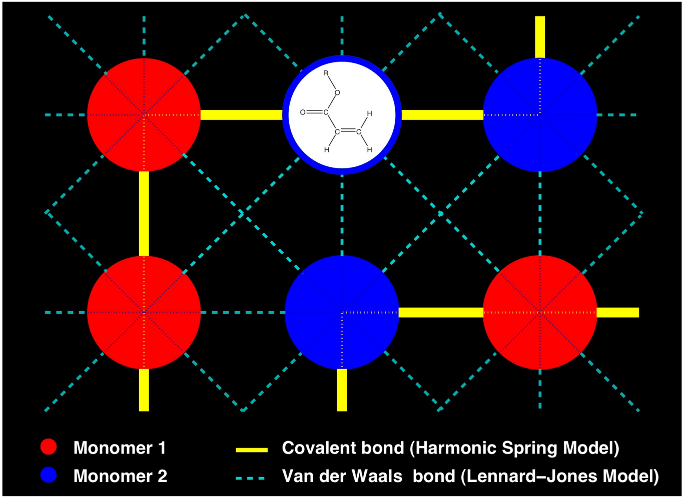
Canonical Ensemble

$$P = Ce^{-E_a/\kappa T} \propto k$$

One Realization of Polymerization Process



Molecular Potentials for Polymers



Calibration by Inverse Analysis

Base Model: Densification Step

Given:

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

Goal:

$$\text{Find } x^* = \arg\min_x E(x)$$

where

$$E(x) = \sum_{i=1}^{N} \sum_{k=1}^{N_i} E_{ik}(x_i, x_k)$$

System of equations:

$$\frac{\partial E(x^*)}{\partial x} = f(x^*) = 0$$

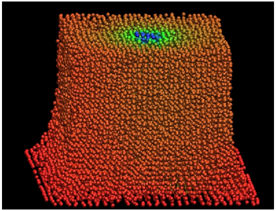
Base Model: Densification Step

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

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

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

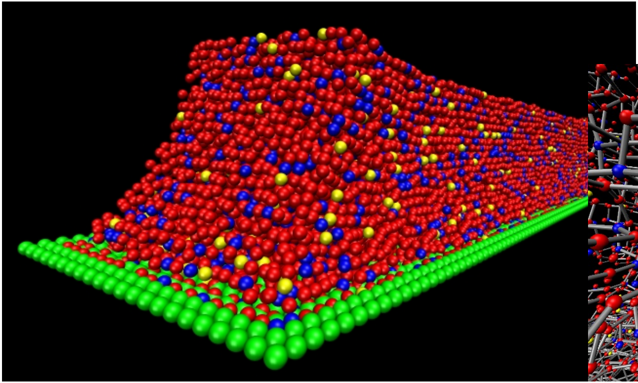
$$Q(u) = \frac{1}{M} \sum_{m=1}^{M} u_m \cdot e_1$$

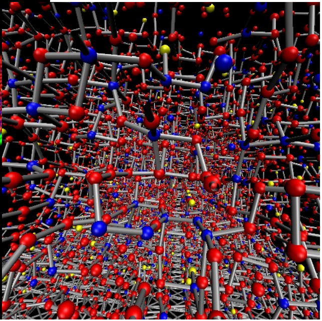


Solver:

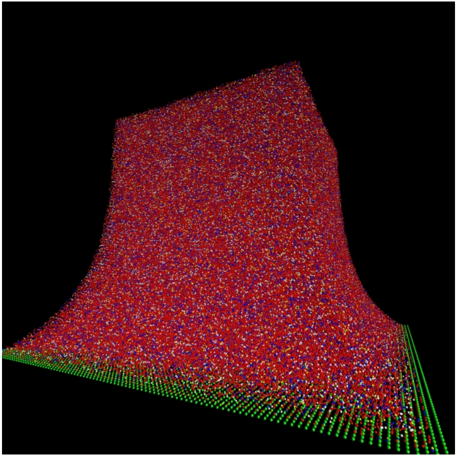
- Inexact Newton Trust Region
- TAO/PETSc. (http://www.mcs.anl.gov/petsc)

Densification of One Realization





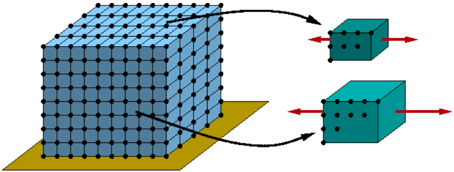
Initial Multi-Processor Computations



100x100x100 particles — 3,000,000 D.O.F.
370 CPU hours on 64 processors — 25000 Newton Iterations

Construction of a Continuum Model

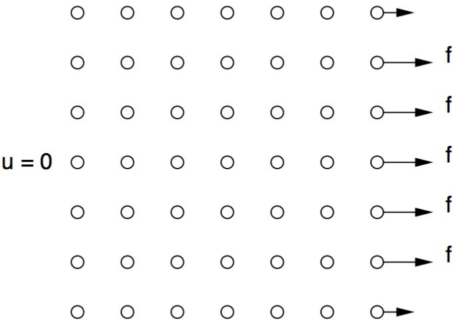
1. **Virtual experiments on RVE's:**
   - Isotropy, homogeneity
   - Must be validated against molecular model
   - Objectivity: frame indifference
2. **Statistical Mechanics of Polymer Networks:**
   - Flory, Treloar, Weiner, Fried.

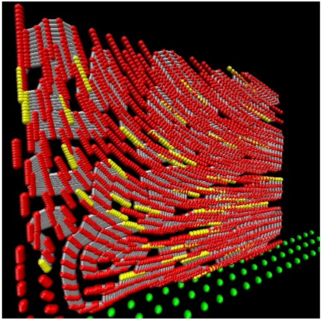


$$\Rightarrow \quad W = \widehat{W}(I_1, I_2, I_3)$$

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

CALIBRATION TESTS

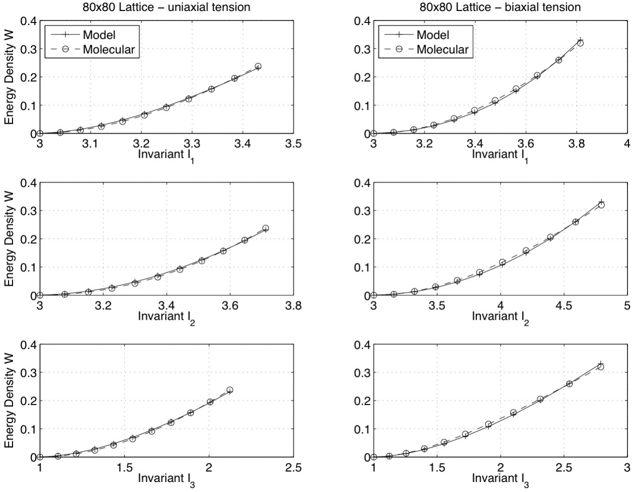




(LEFT) Uni-axial test: the molecules on right side are subjected to forces f and molecules to the left are constrained to zero displacement in x-direction.
(RIGHT) Superposition of 10 incremental loading steps

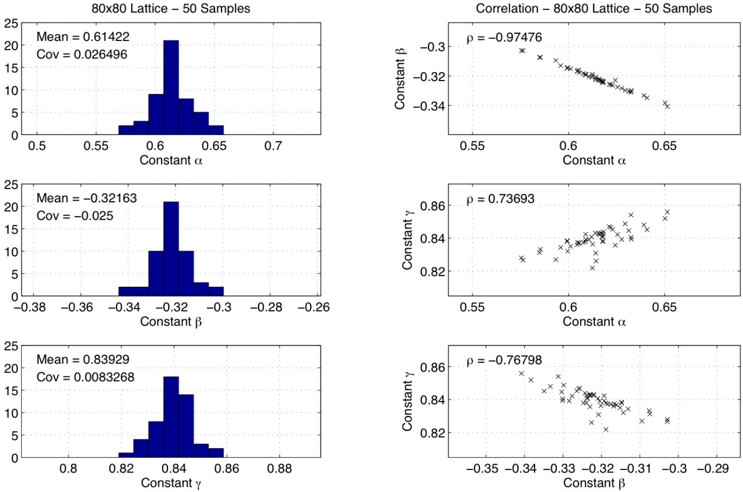
MOONEY-RIVLIN: 80×80 Lattices

$$E_{\text{Molecular System}} = \int_{\Omega} W\,dx$$

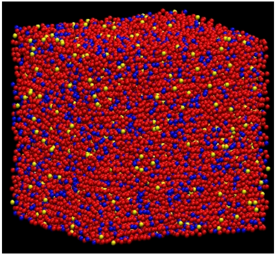


MOONEY-RIVLIN: 80×80 Lattices

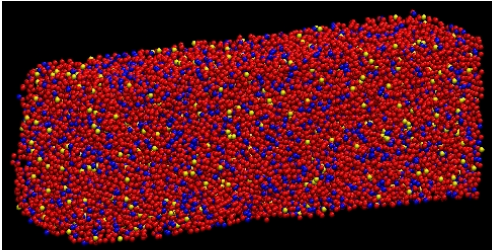
$$E_{\text{Molecular System}} = \int_\Omega W\,dx$$



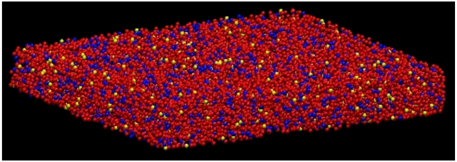
VIRTUAL EXPERIMENTS IN 3D



Relaxation

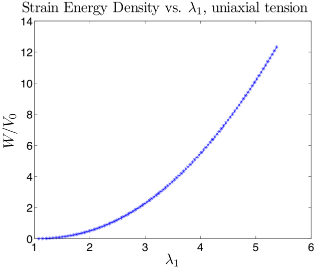


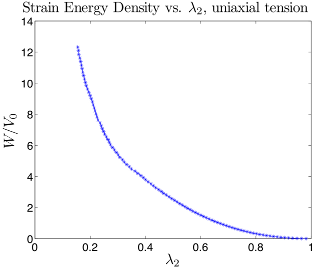
Uniaxial Stretch

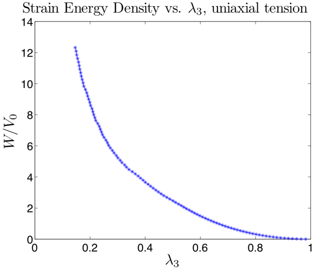


Biaxial Stretch

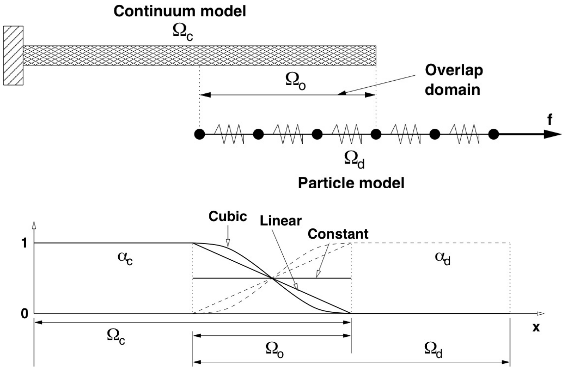
VIRTUAL EXPERIMENTS IN 3D







Model Coupling: The Arlequin Method



Schwarz (1870), Many Domain Decomposition Methods...
Ben Dhia, "Problèmes mécaniques multi-échelles: la méthode Arlequin" CRAS (1998)
Cai, Dryja, & Sarkis, "Overlapping nonmatching grid mortar element methods for elliptic problems" SIAM J. Numer. Anal. (1999)
Xiao & Belytschko, "A bridging domain method for coupling continua with molecular dynamics" IJNME (2004)
Prudhomme & Bauman, "On the application of the Arlequin method to the coupling of particle and continuum models", J. Comput. mechanics (to appear)

The Arlequin Problem

Find $(u, w) \in X$, $\lambda \in M$ such that:

$$\begin{aligned} a\left((u,w),(v,z)\right) + b\left(\lambda,(v,z)\right) &= l((v,z)) \quad \forall (v,z) \in X \\ b\left(\mu,(u,w)\right) &= 0 \quad \forall \mu \in M \end{aligned}$$

where

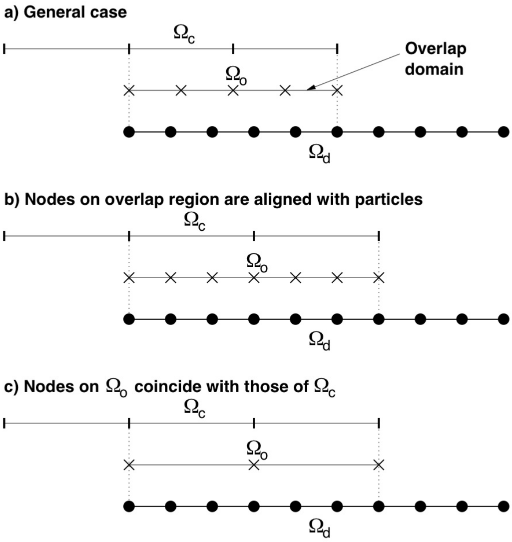
$$a\left((u,w),(v,z)\right) = \int_{\Omega_c} \alpha_c W'(u) v' dx + \sum_{i=1}^{m} \alpha_d E_i'(w_i, w_{i-1})(z_i - z_{i-1})$$

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

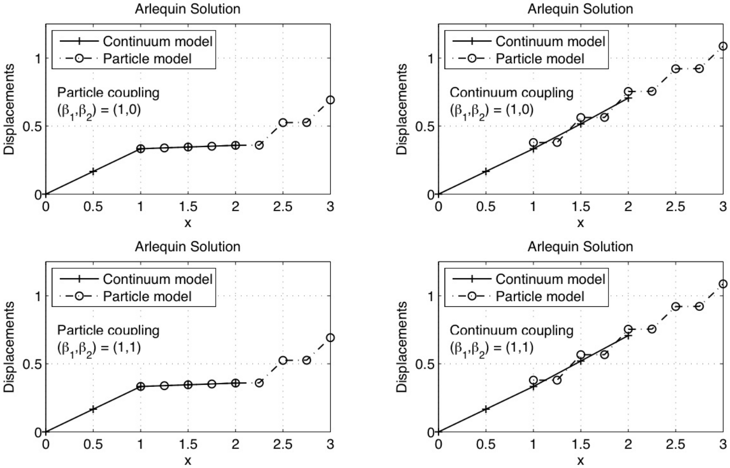
$$l((v,z)) = f z_m$$

Theorem (PB 2007) Let $\alpha_c = \alpha_d = 1/2$ and $\beta_2 > 0$. Then, the above problem is well-posed.

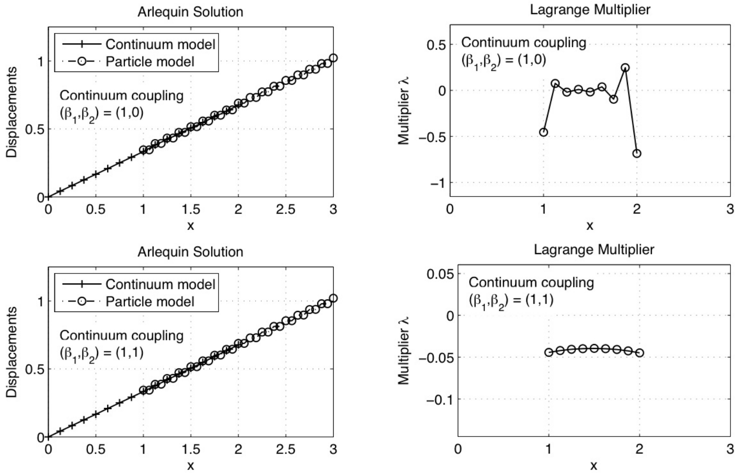
Discretization of Arlequin method



1-D Example: Part. vs Cont. Coupling

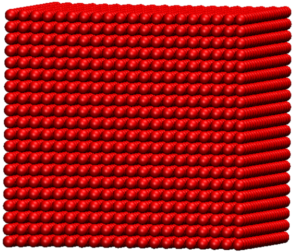


1-D Example: L2 versus H1 Coupling

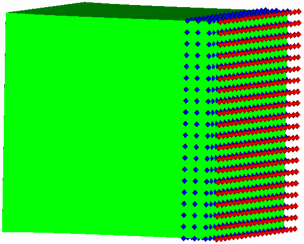


3-D Solution: Uniform Springs

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

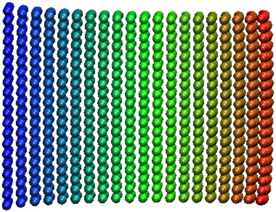


Base Model

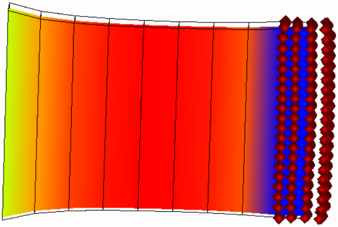


Surrogate Model

3-D Solution: Poor continuum model



Base Model
Colored by Adjoint Solution



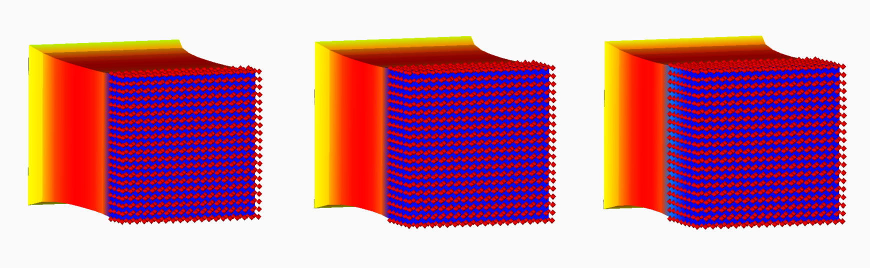
Arlequin Solution
20% Longer

Error Estimation: Uniform springs

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

	Relative error	Effectivity index	Effectivity index
f	$\frac{\lvert(Q(u)-Q(u_0)\rvert}{\lvert Q(u)\rvert}$	$\frac{\lvert\mathcal{R}(u_0,p_0)\rvert}{\lvert Q(u)-Q(u_0)\rvert}$	$\frac{\lvert\mathcal{R}(u_0,p)\rvert}{\lvert Q(u)-Q(u_0)\rvert}$
1	0.0048	0.98	1.02
10	0.1900	0.75	0.85

Error control: Increasing Overlap



$$|R(u_0, p_0)| = 12.3, \quad |R(u_1, p_1)| = 10.3, \quad |R(u_2, p_2)| = 8.59$$

CONCLUDING REMARKS

- Any meaningful analysis must begin with
  1. a specification of the mathematical problem to be solved – the base problem,
  2. the quantities of interest – the target outputs.
- The base model depicts the finest scales and its construction may be an enormous computational problem.
- Surrogate models can depict events at a coarser scale.
- The error in $Q(u_0)$ is always $\approx R(u_0; p)$ so one needs to devise methods for approximating
  1. $R =$ the residual
  2. $p =$ the adjoint solution
  3. Reducing $R(\tilde{u}^h; \tilde{p}^h) =$ the error – the Goals Algorithms.

WHAT'S NEXT

- Parallel implementation of Arlequin method
- Parallel Goals algorithm
- Large-scale applications on multi-processor machines
- Uncertainty quantification and stochastic systems
- Model calibration and validation
- Mathematical foundation of coupling algorithms