Coupling of MD with Continuum Mechanics via a Bridging Scale Approach

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Examples of Multi-Scale Phenomena in Solids

Fracture/Failure of Solids

Nanoscale Devices
Poncharal et al., Science 283:1513

Film Growth

Nanoindentation

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Concurrent Multiscales: Motivation

- Molecular dynamics simulations are limited to small domains (~$10^6-10^8$ atoms) and small time frames (~nanoseconds)
  - Experiments, even on nano-systems, involve much larger systems over longer times
- Continuum models are good, but not always adequate
  - Problems in fracture and failure of solids require improved constitutive models to describe material behavior
  - Molecular dynamics is required in regions of high deformation or discontinuity
- Multiple scale nature of these problems calls for a combined molecular dynamics/continuum mechanics approach
Concurrent Multiple Scales: Goals

• Method for coupling molecular dynamics to finite element or meshfree computations in concurrent simulations
  – Simulation of time dependent, finite temperature problems
• True “coarse scale” discretization in continuum
  – No meshing down to atomic scale
  – Subcycling time-stepping algorithms to take advantage of multiple time scales
    • don’t want to be limited to nano time scale everywhere in the domain
• Easy implementation
  – Re-use of existing MD and continuum codes
  – Easily parallelizable algorithms
Concurrent Coupled Simulations

- Molecular dynamics to be used in region of interest
  - near crack/shear band tip
  - inside shear band
  - at area of large deformation
  - around dislocations
  - etc.
- Finite elements/meshless “coarse scale” defined *everywhere* in domain
  - not just overlap/handshake region
- Bridging scale used to ensure FEM gives correct coarse scale behavior
2-Part Strategy for Multiscale Coupling

- First, formally define exactly what is simulated at each scale
  - decompose total solution into coarse and fine scales
  - “bridging scale” used to represent the part of the total solution common to both simulations
    - provides coupling between the two simulations
- Second, eliminate fine scale degrees of freedom analytically outside of region of interest
  - use molecular dynamics (MD) only where necessary
  - use bridging scale decomposition to further define coupling between simulations
    - constitutive law in pure coarse scale region
    - boundary conditions on MD region
Coarse-Fine Decomposition

• Fields like displacement are decomposed into coarse and fine scales:
  \[ u = \bar{u} + u' \]

• Coarse scale is represented by smooth basis functions associated with nodes, e.g. finite element shape functions:
  \[ \bar{u}(x_\alpha) = \sum_l N_l(x_\alpha) d_l \quad \text{matrix notation} \quad \bar{u} = Nd \]
  
  – nodal degrees of freedom minimize mass-weighted error norm:
  \[ E = (u - Nd)^T M_A (u - Nd) \]
  \[ \frac{dE}{dd} = 0 \Rightarrow d = (N^T M_A N)^{-1} N^T M_A u \]
  
  – This leads to a definition of the coarse scale in terms of a projection matrix:
  \[ \bar{u} = Pu \]
  \[ P = N(N^T M_A N)^{-1} N^T M_A \]
Coarse-Fine Decomposition

- Once coarse scale is defined, fine scale is “everything else”:

\[
\mathbf{u}' = \mathbf{u} - \bar{\mathbf{u}} = \mathbf{u} - \mathbf{Pu} = (\mathbf{I} - \mathbf{P})\mathbf{u} \equiv \mathbf{Qu}
\]
Concurrent Multiscale Solution

- Use FEM for the coarse scale, MD for the fine scale in the decomposition:
  \[ \tilde{\mathbf{u}} = \mathbf{Nd} \quad \rightarrow \quad \text{solve } \mathbf{d} \text{ using FEM} \]
  \[ \mathbf{u}' = (\mathbf{I} - \mathbf{P})\mathbf{q} \quad \rightarrow \quad \text{solve } \mathbf{q} \text{ using MD} \]

- With our choice of projection operator, kinetic energy separates completely into coarse and fine scales:
  \[ K_E = \frac{1}{2} \mathbf{d}^T \mathbf{M} \mathbf{d} + \frac{1}{2} \mathbf{q}^T \tilde{\mathbf{M}} \mathbf{q} \]

- Coupling between scales is only through the forcing term
  - Final momentum equations become:
    
    \begin{align*}
    \text{Coarse scale:} & \quad \mathbf{M} \ddot{\mathbf{d}} = \mathbf{Nf} (\tilde{\mathbf{u}} + \mathbf{u}') \\
    \text{Fine scale:} & \quad m_\alpha \ddot{q}_\alpha = f_\alpha (\tilde{\mathbf{u}} + \mathbf{u}')
    \end{align*}

Coarse Scale Modeling

- Coarse scale equation can be related to usual finite element treatment by approximating summations over atoms as domain integrals:

\[
\sum_j M_{ij} \ddot{d}_j = f_i (\bar{u}, u')
\]

where

\[
M_{ij} = \int_\Omega \rho(x) N_i(x) N_j(x) dx
\]

- The nodal force depends on the coarse scale only through the deformation gradient \( \mathbf{F} \):

\[
f_i = -\frac{\partial U}{\partial \mathbf{d}_i} = -\sum_\alpha \frac{\partial W_\alpha}{\partial \mathbf{d}_i} \Delta V_\alpha
\]

\[
= -\sum_\alpha \frac{\partial F^T_\alpha}{\partial \mathbf{d}_i} \frac{\partial W_\alpha}{\partial \mathbf{F}_\alpha} \Delta V_\alpha \approx -\int_\Omega N_{i,x}(x) \mathbf{P}^K(x) dx
\]
Fine Scale Boundary Conditions

• We want to avoid grading the coarse mesh down to the atomic lattice scale at the boundary
  – expensive
  – too much information
  – limits coarse scale time step
• Information passes from a fine MD lattice directly into a coarse scale mesh
  – small-scale energy can’t be represented on the coarse scale, has nowhere else to go
  – leads to internal reflection of small scale waves
• Proper boundary treatment requires accounting for fine scale dynamics that are not simulated directly
  – correct boundary treatment falls out automatically from bridging scale decomposition
    • linearize in the fine scales at the boundary
MD Boundary Condition

\[ \ddot{q}_1(t) = M_A^{-1}f^*_1(t) + \int_{0}^{t} \theta(t - \tau) a'_2(\tau) d\tau + R_1(t) \]
\[ a'_2(t) = M_A^{-1}f^*_2(t) - \ddot{u}_2(t) \]

Region 1: MD + FEM
Region 2: FEM only (+ “ghost atoms”)

where \( f^*(t) \) are forces computed using just the coarse scale displacements outside MD region (e.g. through “ghost atoms”)

- The total forcing term consists of three major parts:
  - The standard interatomic force computed in MD simulation by assuming displacements of all atoms just outside the boundary are given by the coarse scale
  - A time history-dependent dissipation at the boundary (similar to a damping term)
  - A random forcing term at the boundary
    - the form of this term can be related to the temperature of the solid:
      \[ \langle R_i(t)R_j(0) \rangle = -\delta_{ij} \beta(t) k_B T \]
Example Problem: 1D Harmonic Chain
Effects of BC’s on Internal Wave Reflection

\[ \dot{q}_\alpha = \sum I N_l(x_\alpha) \dot{d}_l \]

\[ \ddot{q}_1(t) = M_A^{-1} f_1^* (t) + \int_0^t \theta(t - \tau) a_2^*(\tau) d\tau \]
Energy Transfer out of MD Region

The graph shows the normalized MD region energy as a function of $(k/m_a)^{1/2}t$ for different boundary conditions:

- **Multiscale with matched velocity BC**
- **Multiscale with simple damped BC**
- **Multiscale with correct BC**
- **Full MD**
Energy Transfer out of MD Region: Nonlinear Potential
Damping Kernels in Multiple Dimensions

- Damping kernel can be easily computed for any regular crystal lattice across a planar boundary
  - periodicity allows spatial Fourier transform
  - unit cells can be indexed \((l,m,n)\) in 3D, or \((l,m)\) in 2D
  - boundary condition obtained by solving for atoms just outside boundary \((l=1)\) in terms of atoms just inside boundary \((l=0)\)
  - final boundary condition has form of time history integration with spatial coupling along boundary:

\[
\mathbf{f}_{m}^{1 \rightarrow 0}(t) = \sum_{m'=-\infty}^{\infty} \int_{0}^{t} \theta_{m-m'} \left( t - \tau \right) \mathbf{u}_{0,m'}(\tau) d\tau
\]

- note that \(\mathbf{u}\) and \(\mathbf{f}\) are vectors containing all dof’s in the unit cell, and \(\theta\) is a matrix coupling them
Damping Kernels in 3D: Carbon Structures
2D Multiscale Wave Propagation

Energy Transfer Rates:
No BC: 35.47%
N_{crit} = 0: 90.94%
N_{crit} = 1: 92.85%
N_{crit} = 2: 93.34%
N_{crit} = 4: 95.27%
Full MD: 100%

Harold Park, Northwestern University
Problem Description:

- LJ 6-12 potential, $\sigma=\varepsilon=1$
- Nearest neighbor interactions
- 90000 atoms, 1800 finite elements (900 in coupled region)
  - 100 atoms per finite element
- $\Delta t_{fe} = 40\Delta t_{md}$
- Ramp velocity BC on FEM
- Full MD = 180,000 atoms
Summary: Coupled MD/FEM

- Bridging scale decomposition allows concurrent simulation of fine scale using MD and coarse scale using FEM
  - bridging scale projection provides a unique decomposition of total solution for separation into coarse and fine scales
  - coarse scale mesh need not correspond to atomic lattice for coupling
  - subcycling can be used to take advantage of the different time scales in the coarse and fine regions
  - coarse scale equations and boundary conditions follow directly from the multi-scale formulation

- Future work:
  - study of approximations in boundary conditions
    - truncations of summations/integrals, approximations to kernel function
  - determination of most accurate/efficient integration of coarse scale region near MD boundary
  - development of coupled energy equation to track fine scale energy
    - time averaging as part of coarse scale projection