ATOMS AND THE CONTINUUM

Coupling Atomistic Simulations and Continuum Elasticity for Multiscale Simulations

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OUTLINE

• Introduction
  – (Brief) Overview of Molecular Dynamics
  – Continuum Elasticity - Concepts and Basic Equations
  – Overview of Finite Element Method
  – Atomistics vs. Continuum

• Approaches to coupling
  – Mesh Refining
  – Coarse Grained MD
  – Quasi-Continuum Method

• Outstanding Issues
  – Variable Constitutive Laws
  – Temperature/Vibrations
  – Fluids
MOLECULAR DYNAMICS

“Microscopic Reality”

- Matter is made out of atoms
- Electrons mediate interactions

Central Assumptions

- Atomic nuclei are classical objects
- Electrons give effective interaction potential
  (computed explicitly or approximated implicitly)

Relevant variables

- Atomic trajectories \( \{\vec{x}(t)\} \)
- Potential energy

\[ V = E(\{\vec{x}\}) \]
CONTINUUM ELASTICITY

“Macroscopic Reality”

- Matter is continuous
- Changes in shape cost energy

Central Assumptions

- Matter described by a classical mass distribution
- Total energy is a function of the deformation

Relevant variables

- Displacement $\mathbf{u}(\mathbf{r})$ or strain tensor $\mathbf{\epsilon}(\mathbf{r})$ field
- Potential energy

\[
V = E(\{\mathbf{u}\})
\]
ATOMISTIC VS. CONTINUUM: COSTS AND BENEFITS

Atomistics
positions:
• computationally expensive: few DOF per atom
• describe any deformation, crystal lattice
• energy expression either inaccurate or slow

difficulties:
• computational expense
• fast energy expression

Continuum
displacement field:
• computationally cheap: few DOF per (large) element
• only small deformation from equilibrium is easy
• energy expression very fast and accurate (within constraining assumptions)

difficulties:
• missing degrees of freedom (temperature)
• constitutive law for large deformation (plasticity, phase transformations)
WHY COUPLE?

Can treat very large systems
accuracy where needed
not too much wasted effort

• Most of system treated efficiently, accurately
• Put in computationally expensive technique only where needed: bond breaking, phase transformation
MOLECULAR DYNAMICS EQUATIONS

How do we compute trajectories as a function of time?

Potential Energy:

\[ V = \sum_{ij}^{N} f_{2}(\vec{x}^{ij}) + \sum_{ijk}^{N} f_{3}(\vec{x}^{ij}, \vec{x}^{jk}, \vec{x}^{ik}) \]

Kinetic Energy (in terms of velocity \( \dot{x} \) or momentum \( p = m\dot{x} \)):

\[ T = \frac{1}{2} \sum_{i}^{N} m^{i}(\dot{x}^{i})^{2} = \frac{1}{2} \sum_{i}^{N} (p^{i})^{2} / m^{i} \]

Hamiltonian:

\[ H = V + T \]

Newton’s eqns. of motion (\( F = ma \))

\[ \ddot{x}^{i} = \frac{\partial E(\{\vec{x}\})}{\partial \dot{x}^{i}} / m^{i} = \tilde{f}^{i}(\{\vec{x}\}) / m^{i} \]

Integrate \( \{\ddot{x}\} \) with respect to time with \( \{\dot{x}\} \) and \( \{\vec{x}\} \) as initial conditions
ELASTICITY FROM ATOMISTICS

(following Ashcroft and Mermin)

Hooke’s law: at equilibrium, energy depends quadratically on atomic positions through the dynamical matrix $\mathbf{D}$

$$U = -\frac{1}{4} \sum_{\vec{R} \vec{R}'} \left[ \vec{u}(\vec{R}') - \vec{u}(\vec{R}) \right] \mathbf{D}(\vec{R} - \vec{R}') \left[ \vec{u}(\vec{R}') - \vec{u}(\vec{R}) \right]$$

When $\vec{u}$ varies much more slowly than $\mathbf{D}(\vec{r})$, then

$$\vec{u}(\vec{R}') \approx \vec{u}(\vec{R}) + (\vec{R}' - \vec{R}) \cdot \nabla \vec{u}(\vec{R})$$

So

$$U \approx \frac{1}{2} \sum_{\vec{R} \mu \nu \sigma \tau} \left( \frac{\partial}{\partial x_\sigma} u_\mu(\vec{R}) \right) E_{\sigma \mu \tau \nu} \left( \frac{\partial}{\partial x_\tau} u_\nu(\vec{R}) \right)$$

where

$$E_{\sigma \mu \tau \nu} = -\frac{1}{2} \sum_{\vec{R}} R_\sigma D_{\mu \nu}(\vec{R}) R_\tau$$

is closely related to the usual elastic constants $c_{\sigma \mu \tau \nu}$
CONTINUM ELASTICITY

Since $\vec{u}(\vec{r})$ is varying slowly, define a continuous field

$$U \approx \frac{1}{2} \sum_{\mu\nu\sigma\tau} \int d\vec{r} \left( \frac{\partial}{\partial x_\sigma} u_\mu(\vec{r}) \right) \frac{E_{\sigma\mu\tau\nu}}{\Omega} \left( \frac{\partial}{\partial x_\tau} u_\nu(\vec{r}) \right)$$

How do we work with this equation?

I.e. how do we

- Calculate $U$ given a displacement field $\vec{u}(\vec{r})$?
- Solve for equilibrium $\vec{u}(\vec{r})$ given some boundary conditions?
- Calculate time evolution of displacement field?

Finite elements: represent the continuous field on a mesh
FINITE ELEMENTS

(not quite following Zienkiewicz and Taylor)

Divide our region in elements, interpolate field in element as a function of values (derivatives) at vertices (edge centers).

In 2-D, for triangular elements:

Three vertices $i = 1 - 3$

Displacement $u^i_\mu \ (\mu = x, y)$ at each vertex

\[ u^i_\mu = \alpha_\mu + \beta_\mu x^i + \gamma_\mu y^i \]

6 equations ($u^i_\mu, \ i = 1 - 3, \ \mu = x, y$), 6 unknowns ($\alpha_\mu, \ \beta_\mu, \ \gamma_\mu$)

\[ \vec{u}(\vec{r}) = \sum_{i=1}^{3} N^i(\vec{r}) \vec{u}^i \]

where $N^i(\vec{r}) = I N^i(\vec{r})$ contains the information about the coefficients $N^i(\vec{r})$ is linear in $x$ and $y$
FINITE ELEMENTS CONT’D

Equations involve stuff like \( \frac{\partial}{\partial x_\sigma} u_\mu(\vec{r}) \)

\[
\frac{\partial}{\partial x_\sigma} u_\mu(\vec{r}) = \sum_{i=1}^{3} \frac{\partial}{\partial x_\sigma} N^i(\vec{r}) u^i_\mu = \sum_{i=1}^{3} B^i_\sigma u^i_\mu
\]

Since \( N^i(\vec{r}) \) is linear in position, \( \frac{\partial}{\partial x_\sigma} N^i(\vec{r}) \) is constant

Easy to evaluate relevant integrals over the element analytically

\[
U \approx \frac{1}{2} \sum_{\mu\nu\sigma\tau} \int d\vec{r} \left( \frac{\partial}{\partial x_\sigma} u_\mu(\vec{r}) \right) \frac{E_{\sigma\mu\tau\nu}}{\Omega} \left( \frac{\partial}{\partial x_\tau} u_\nu(\vec{r}) \right)
\]

\[
= \frac{1}{2} \sum_{\mu\nu\sigma\tau} \sum_{\langle ijk \rangle} A_{ijk} \left( \sum_{m\in\{i,j,k\}} B^m_\sigma u^m_\mu \right) E_{\sigma\mu\tau\nu} \left( \sum_{n\in\{i,j,k\}} B^n_\tau u^n_\nu \right)
\]

\[
= \frac{1}{2} \sum_{\mu\nu\sigma\tau} \sum_{\langle ijk \rangle} \sum_{m,n\in\{i,j,k\}} u^m_\mu \left( A_{ijk} B^m_\sigma E_{\sigma\mu\tau\nu} B^n_\tau \right) u^n_\nu
\]

Transformed the equation in terms of \( \vec{u}(\vec{r}) \) into a (messy) linear equation in terms of \( \vec{u}^i \)
DYNAMICS WITH FINITE ELEMENTS

We have a potential energy

\[ U = \sum_{m\mu\nu} u^m_\mu U^m_{\mu\nu n} u^n_\nu \]

Kinetic energy is something like

\[ T = \frac{1}{2} \left( \int d\vec{r} \rho(\vec{r}) [\dot{u}(\vec{r})]^2 \right) \]

\[ \approx \frac{1}{2} \sum_{\langle ijk \rangle} \int_{\text{tri}} d\vec{r} \rho(\vec{r}) \left( \sum_{m \in \{i,j,k\}} N^m(\vec{r}) \dot{u}^m \right) \left( \sum_{n \in \{i,j,k\}} N^n(\vec{r}) \dot{u}^n \right) \]

\[ = \frac{1}{2} \sum_{\langle ijk \rangle} \sum_{m \in \{i,j,k\}} \sum_{n \in \{i,j,k\}} \dot{u}^n \left[ \int_{\text{tri}} d\vec{r} \rho(\vec{r}) N^n(\vec{r}) N^m(\vec{r}) \right] \dot{u}^m \]

(Choice: what to use for \( \rho(\vec{r}) \)?)

So we can write a Hamiltonian \( H = U + T \), and get forces that are conjugate to displacements.
## MD VS. FE

### Concepts

<table>
<thead>
<tr>
<th>Matter</th>
<th>atoms</th>
<th>continuous distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variables</td>
<td>atomic positions</td>
<td>displacement field</td>
</tr>
<tr>
<td>Energy calc.</td>
<td>function of atomic positions</td>
<td>function of displ. field</td>
</tr>
</tbody>
</table>

### Assumptions

<table>
<thead>
<tr>
<th>Length scale</th>
<th>interatomic dist.</th>
<th>variation much slower than interatomic dist.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deformation mag.</td>
<td>any atomic pos(?)</td>
<td>small deviation from equilib.</td>
</tr>
</tbody>
</table>

### Needs

<table>
<thead>
<tr>
<th>Energy calc.</th>
<th>interatomic potential</th>
<th>constitutive law</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass</td>
<td>mass distribution in element</td>
<td>nuclear masses</td>
</tr>
</tbody>
</table>
A PRACTICAL EXAMPLE OF COUPLING

(Broughton et al., PRB 60)

Couple 2-D finite elements to empirical-potential MD

Problem: fracture in silicon single crystal
COUPLING: MOLECULAR DYNAMICS

- Constant energy, volume, MD
- velocity Verlet time integrator
- Stillinger-Weber (SW) empirical interatomic potential

\[ V_{SW} = \sum_{\langle ij \rangle} V_{2}(|r_i - r_j|) + \sum_{\langle ijk \rangle} V_{3}(\theta_{ijk}) \]
COUPLING: FINITE ELEMENTS

Finite elements: simplest plausible treatment

- 2-D, plane strain (z-strain is 0)
- triangular elements
- isotropic linear elasticity

To couple to atomistics, pick approximations that allow FE to go to atomic limit (sort of)

- elastic constants from SW
- velocity Verlet time integrator
- Refine mesh to atomic dimensions at interface
- ”Lumped mass” - mass concentrated at vertices
COUPLING: THE INTERFACE

Refine mesh to atomic dimensions

Identify positions of atoms with displacement at element vertices

Hamiltonian description:

specify a single total energy, derive eqn’s of motion

\[ V_{\text{tot}} = V_{\text{MD}}^{\text{bulk}} + V_{\text{FE}}^{\text{bulk}} + V_{\text{i′face}}^{\text{MD}} + V_{\text{i′face}}^{\text{FE}} \]

Important coupling details are in the \( V_{\text{i′face}} \):

Define an interface plane between two atomic planes

FE elements at interface weighted by 1/2

SW interactions across interface weighted by 1/2
**COUPLING: THE INTERFACE**

![Diagram of MD and FE interactions]

Interactions across boundary are halved

<table>
<thead>
<tr>
<th>MD</th>
<th>MD/FE</th>
<th>MD/FE</th>
<th>FE</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 bd ( (E_{SW}) )</td>
<td>2 bd ( (\frac{1}{2}E_{SW}) )</td>
<td>2 bd ( (\frac{1}{2}E_{SW}) )</td>
<td>( E_{FE} )</td>
</tr>
<tr>
<td>( 2 \times \frac{1}{2} ) bd ( (\frac{1}{4}E_{SW}) )</td>
<td>( 2 \times \frac{1}{2} ) bd ( (\frac{1}{4}E_{SW}) )</td>
<td>( 3 \times \frac{1}{2} ) tri ( (\frac{1}{4}E_{FE}) )</td>
<td>( 6 ) tri ( (E_{FE}) )</td>
</tr>
<tr>
<td>( 3 \times \frac{1}{2} ) tri ( (\frac{1}{4}E_{FE}) )</td>
<td>( 3 \times \frac{1}{2} ) tri ( (\frac{1}{4}E_{FE}) )</td>
<td>( 3 ) tri ( (\frac{1}{2}E_{FE}) )</td>
<td>( E_{FE} )</td>
</tr>
</tbody>
</table>

\[
E_{SW} = \frac{3}{4}E_{SW} + \frac{1}{4}E_{FE}
\]

\[
\frac{1}{4}E_{SW} + \frac{3}{4}E_{FE}
\]

\[
E_{FE}
\]
COUPLING: RESULTS

Not rigorously tested, but works OK...

Vibrations emitted from crack go through interface

(by permission from Broughton et al., Phys. Rev. B 60, p. 2391 (1999).)
COUPLING: RESULTS 2

Shock wave emitted from crack tip
SUBTLETIES

Limitations:

- dimensionality
- potentials with very different form:
  potentials without 2 & 3 body terms (e.g. embedded atom)
  quantum-mechanics: can’t assign energy to individual atoms

Definite problems:

- Temperature - what about short wavelength vibrations that aren’t represented by big finite elements?
- Missing / double counted energy terms at interface
- Lumped mass bad for big elements
- Bulk elastic constants don’t apply to individual atoms
BIBLIOGRAPHY

