ATOMS AND THE CONTINUUM

Coupling Atomistic Simulations and

Continuum Elasticity for

Multiscale Simlations

Noam Bernstein
Center for Computational Materials Science
Naval Research Laboratory
Washington, DC

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

$$V = E(\{\vec{u}\})$$

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)

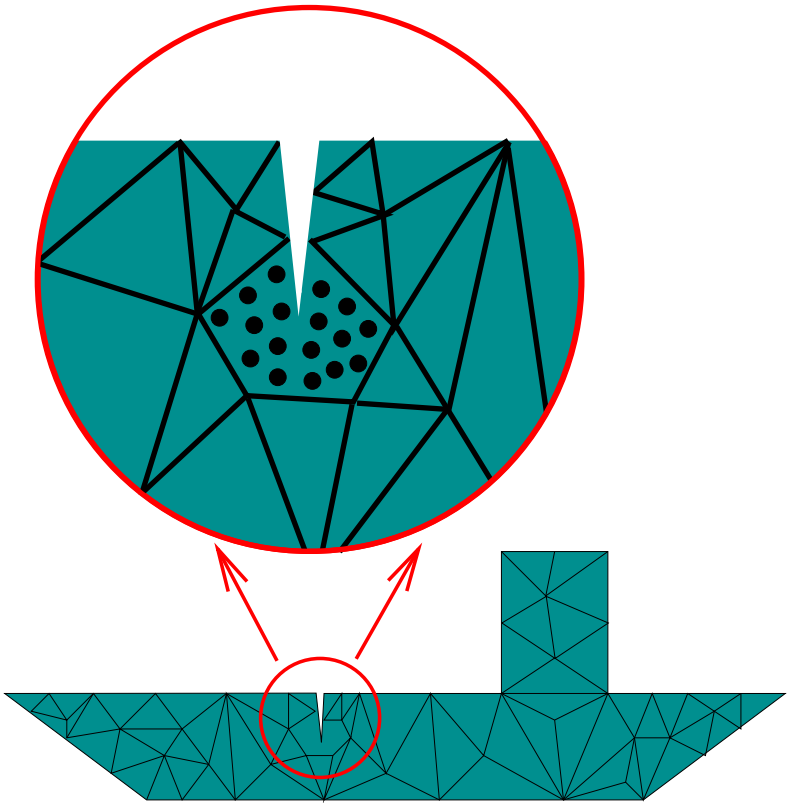
difficulties:

- 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 ($F = ma$)

$$\ddot{\vec{x}}^i = \frac{\partial E(\{\vec{x}\})}{\partial \vec{x}^i}/m^i = \vec{f}^i(\{\vec{x}\})/m^i$$

Integrate $\{\ddot{\vec{x}}\}$ with respect to time
with $\{\dot{\vec{x}}\}$ 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 $c_{\sigma\mu\tau\nu}$

CONTINUUM ELASTICITY

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

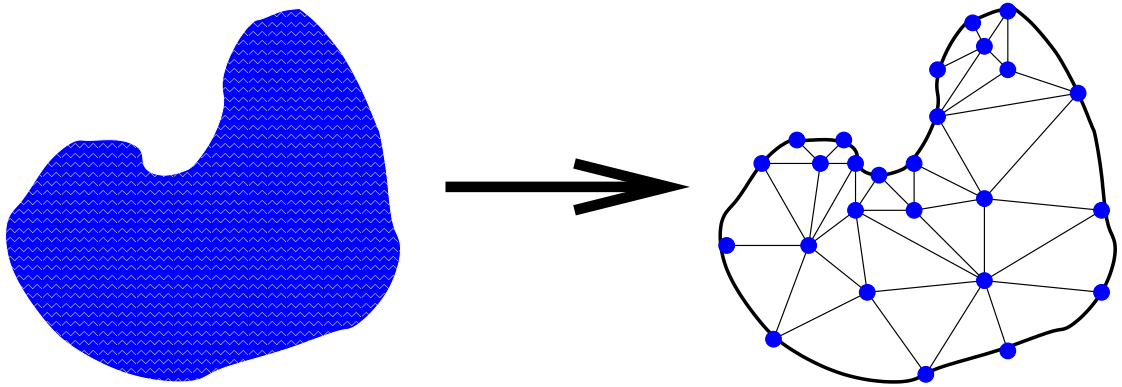
$$U \approx \frac{1}{2} \sum_{\mu\nu\sigma\tau} \int d\vec{r} \left(\frac{\partial}{\partial x_\sigma} u_\mu(\vec{r}) \right) \frac{E_{\sigma\mu\tau\nu}}{\Omega} \left(\frac{\partial}{\partial x_\tau} u_\nu(\vec{r}) \right)$$

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



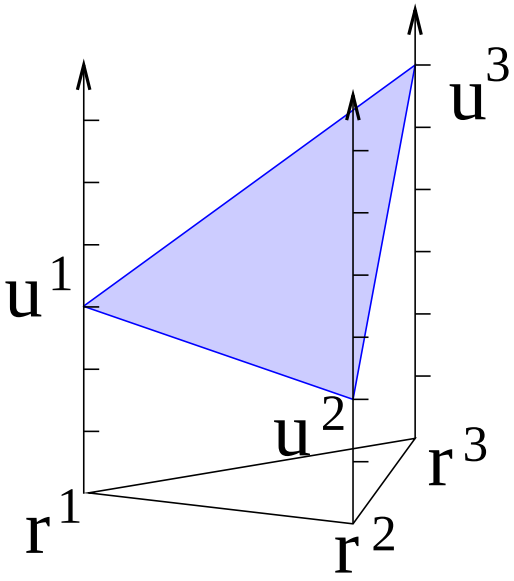
FINITE ELEMENTS

(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_μ ($\mu = x, y$) at each vertex

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



6 equations (u^i_μ, $i = 1 - 3$, $\mu = x, y$), 6 unknowns (α_μ, β_μ, γ_μ)

$$\vec{u}(\vec{r}) = \sum_{i=1}^{3} \mathbf{N}^i(\vec{r})\vec{u}^i$$

where $\mathbf{N}^i(\vec{r}) = \mathbf{I}N^i(\vec{r})$ contains the information about the coefficients

$N^i(\vec{r})$ is linear in x and y

FINITE ELEMENTS CONT'D

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

$$\frac{\partial}{\partial x_\sigma} u_\mu(\vec{r}) = \sum_{i=1}^{3} \frac{\partial}{\partial x_\sigma} N^i(\vec{r}) u_\mu^i = \sum_{i=1}^{3} B_\sigma^i u_\mu^i$$

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

$$\begin{aligned}
U &\approx \frac{1}{2} \sum_{\mu\nu\sigma\tau} \int d\vec{r} \left(\frac{\partial}{\partial x_\sigma} u_\mu(\vec{r}) \right) \frac{E_{\sigma\mu\tau\nu}}{\Omega} \left(\frac{\partial}{\partial x_\tau} u_\nu(\vec{r}) \right) \\
&= \frac{1}{2} \sum_{\mu\nu\sigma\tau} \sum_{\langle ijk \rangle} A_{ijk} \left(\sum_{m \in \{i,j,k\}} B_\sigma^m u_\mu^m \right) E_{\sigma\mu\tau\nu} \left(\sum_{n \in \{i,j,k\}} B_\tau^n u_\nu^n \right) \\
&= \frac{1}{2} \sum_{\mu\nu\sigma\tau} \sum_{\langle ijk \rangle} \sum_{m,n \in \{i,j,k\}} u_\mu^m \left(A_{ijk} B_\sigma^m E_{\sigma\mu\tau\nu} B_\tau^n \right) u_\nu^n
\end{aligned}$$

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

$$U = \sum_{mn\mu\nu} u_\mu^m U_{m\mu n\nu} u_\nu^n$$

Kinetic energy is something like

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

(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

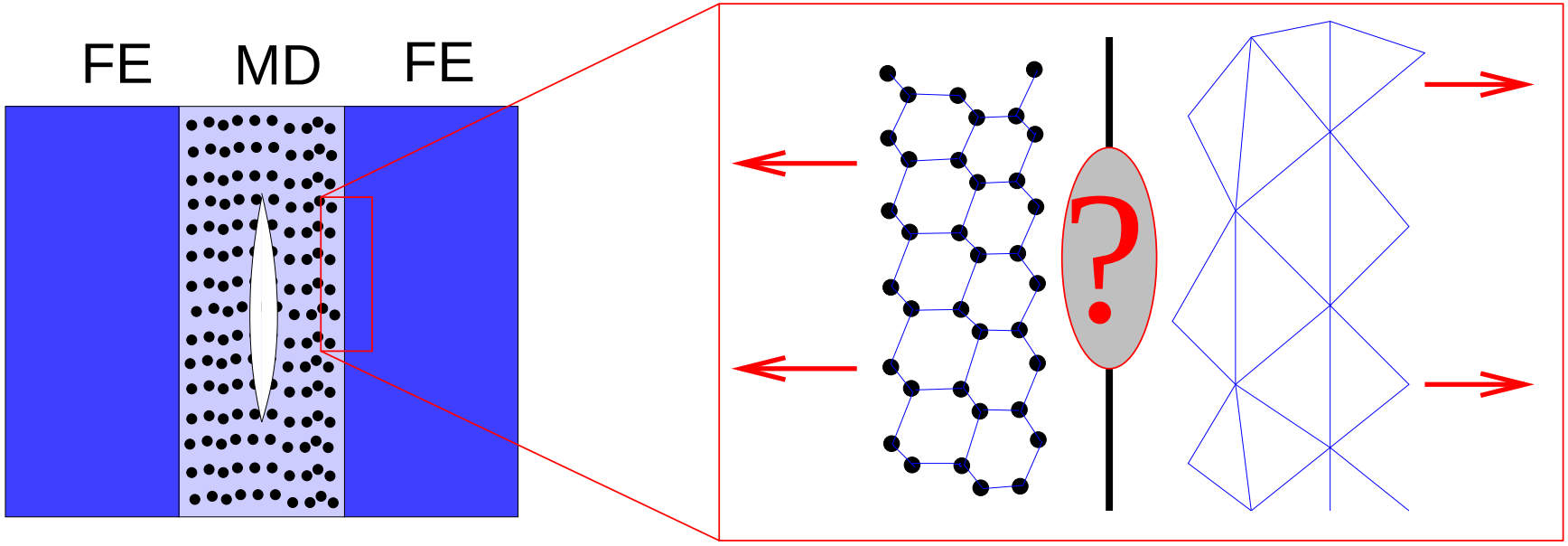
Concepts		
Matter	atoms	continuous distribution
Variables	atomic positions	displacement field
Energy calc.	function of atomic positions	function of displ. field
Assumptions		
Length scale	interatomic dist.	variation much slower than interatomic dist.
Deformation mag.	any atomic pos(?)	small deviation from equilib.
Needs		
Energy calc.	interatomic potential	constitutive law
Mass	mass distribution in element	nuclear masses

A PRACTICAL EXAMPLE OF COUPLING

(Broughton *et al.*, PRB **60**)

Couple 2-D finite elements to empirical-potential MD

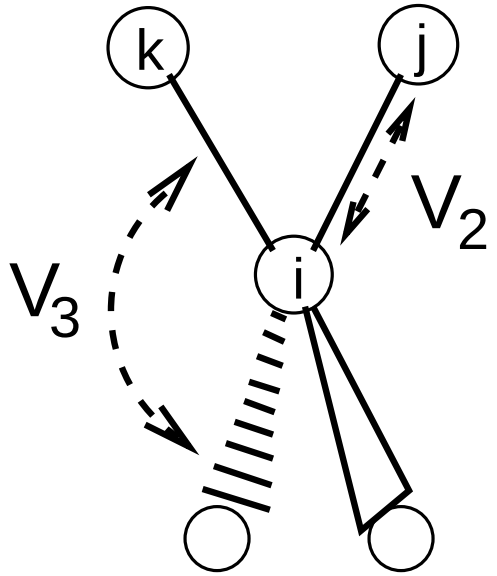
Problem: fracture in silicon single crystal



COUPLING: MOLECULAR DYNAMICS

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

$$V_{\mathrm{SW}} = \sum_{\langle ij \rangle} V_2(\left|r_i - r_j\right|) + \sum_{\langle ijk \rangle} V_3(\theta_{ijk})$$



COUPLING: FINITE ELEMENTS

Finite elements: simplest plausible treatement

- 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

$$V_{\text{tot}} = V_{\text{bulk}}^{\text{MD}} + V_{\text{bulk}}^{\text{FE}} + V_{\text{i'face}}^{\text{MD}} + V_{\text{i'face}}^{\text{FE}}$$

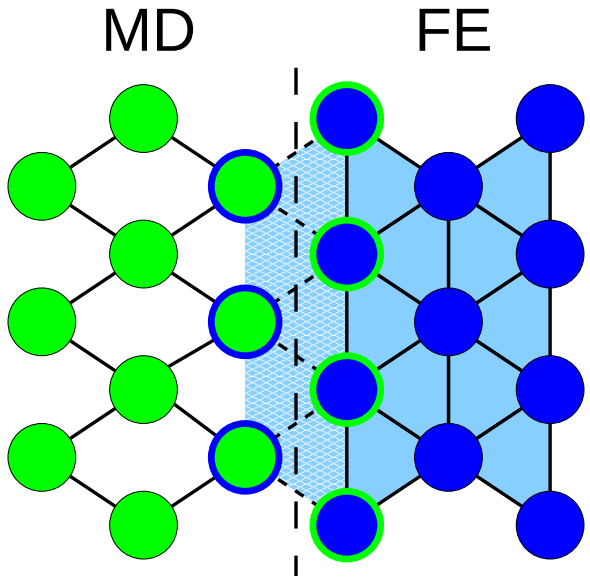
Important coupling details are in the $V_{\text{i'face}}$:

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



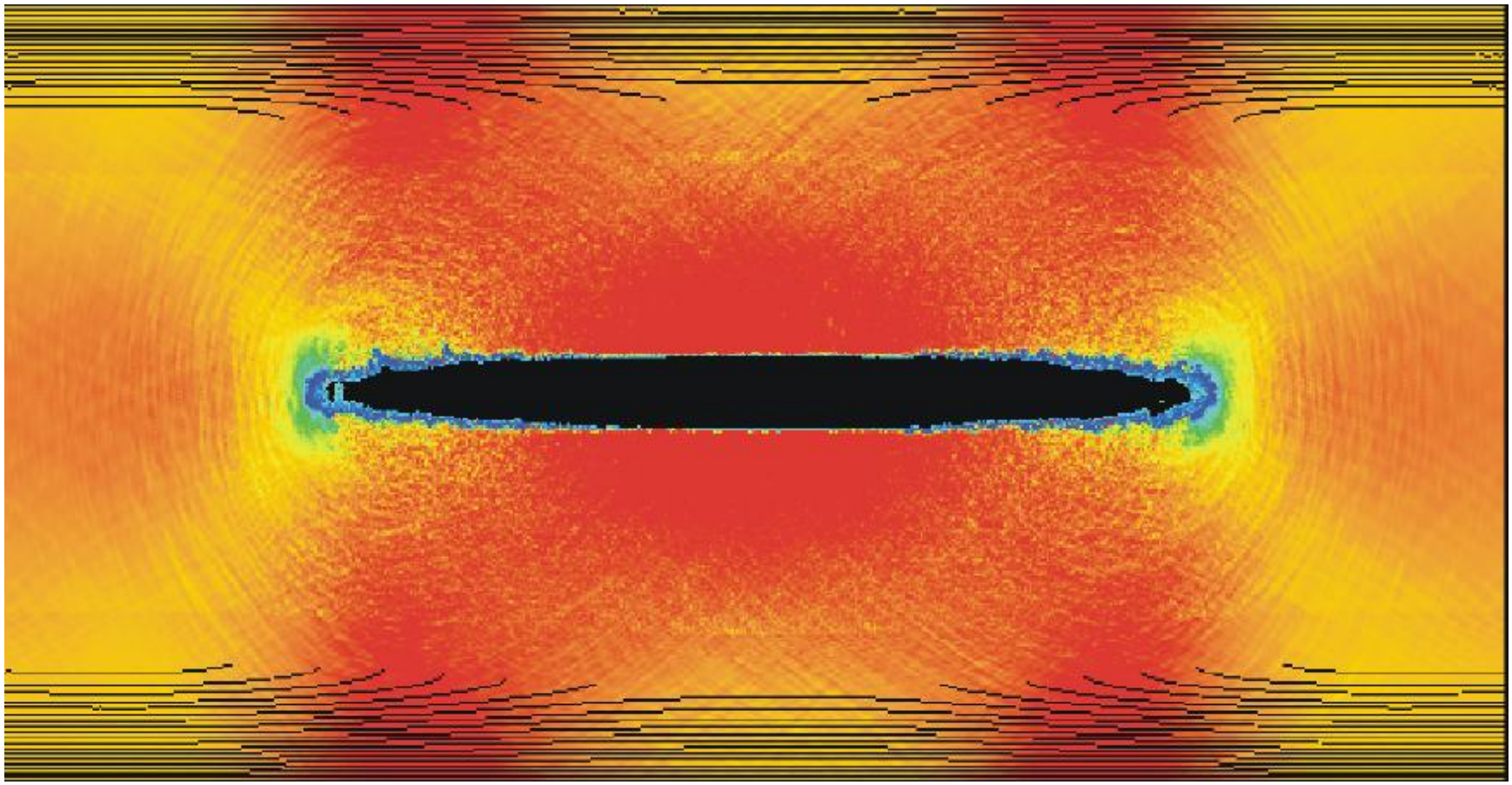
Interactions across boundary are halved

MD	MD/FE	MD/FE	FE
4 bd (E_{SW})	2 bd ($\frac{1}{2}E_{\mathrm{SW}}$)		
	$2\times\frac{1}{2}$ bd ($\frac{1}{4}E_{\mathrm{SW}}$)	$2\times\frac{1}{2}$ bd ($\frac{1}{4}E_{\mathrm{SW}}$)	
	$3\times\frac{1}{2}$ tri ($\frac{1}{4}E_{\mathrm{FE}}$)	$3\times\frac{1}{2}$ tri ($\frac{1}{4}E_{\mathrm{FE}}$)	
		3 tri ($\frac{1}{2}E_{\mathrm{FE}}$)	6 tri (E_{FE})
E_{SW}	$\frac{3}{4}E_{\mathrm{SW}}+\frac{1}{4}E_{\mathrm{FE}}$	$\frac{1}{4}E_{\mathrm{SW}}+\frac{3}{4}E_{\mathrm{FE}}$	E_{FE}

COUPLING: RESULTS

Not rigorously tested, but works OK. . .

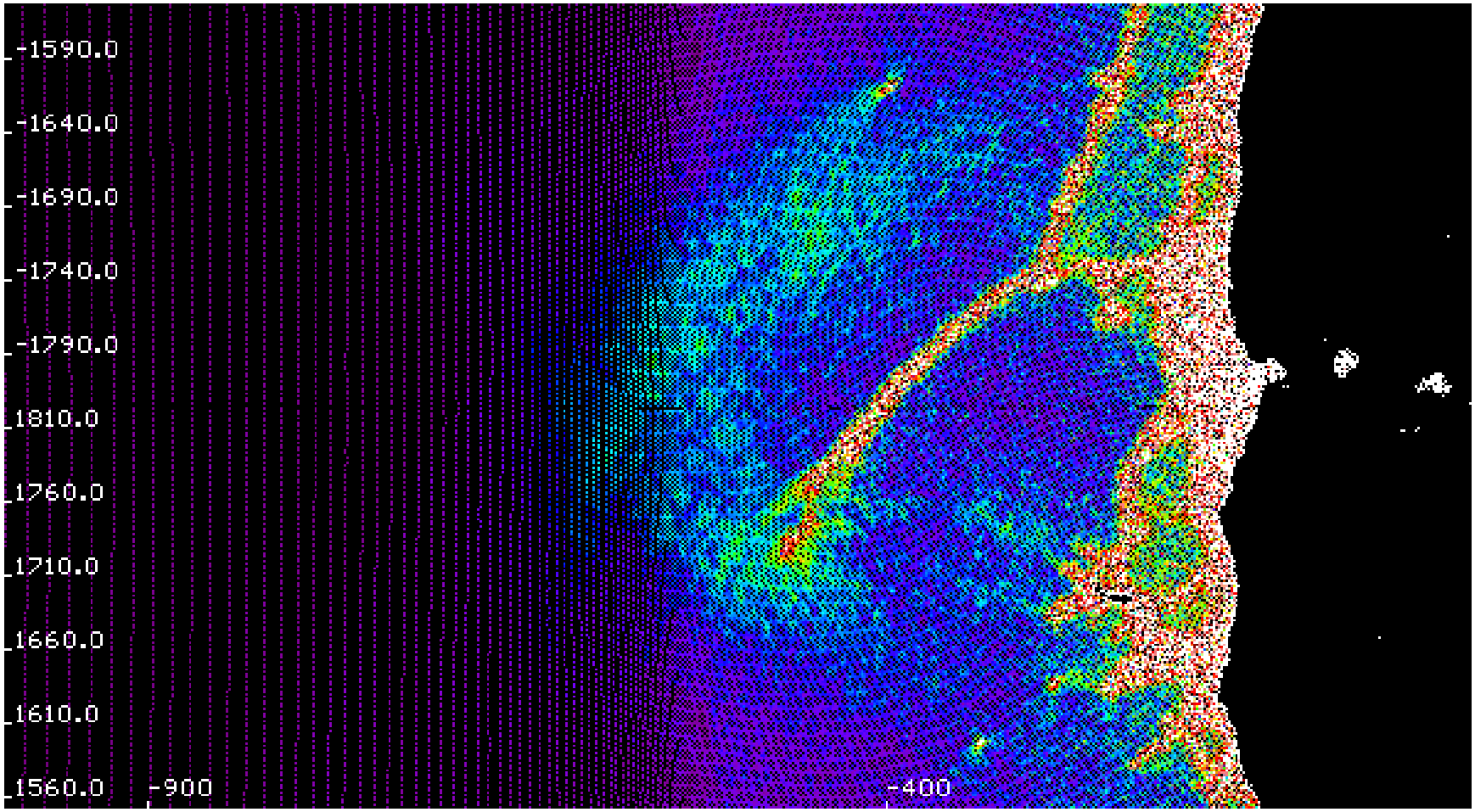
Vibrations emitted from crack go through interface



(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

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