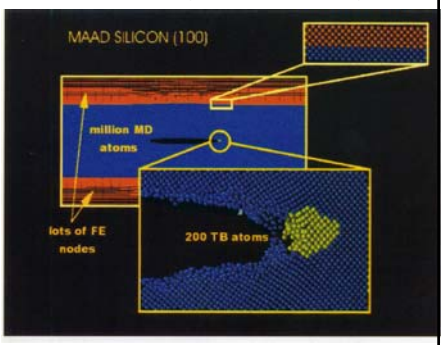
Concurrent Multiscale Modeling
→Increase level of detail with magnitude of strain gradient

Example: Fracture of silicon

- finite-element to treat long-range elastic deformations
- simple potential in nonlinear regions
- detailed electronic calculation where bonds break



Broughton, Abraham, Bernstein and Kaxiras, Phys. Rev. B60, 2391 (1999).

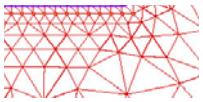
Challenges to Concurrent Modeling

- Fundamentally different descriptions at different scales
  Quantum mechanical – many body electron ground state, nonlocal
  Molecular dynamics – discrete atoms with effective interactions, thermal fluctuations
  Continuum mechanics – continuous displacement or velocity fields related to stress field by effective constitutive laws, no fluctuation
- Need to make sure that descriptions at each scale are consistent
  Effective interactions consistent with electronic energies
  Constitutive law consistent with effective interactions, T, density, …
- Need to treat discontinuity in description at interfaces
  QM/MD – Include effect of electrons in MD region so no sudden truncation of wave functions
  MD/CM – Relate discrete atomic positions to continuum fields
  Requires both coarse- and fine-graining, managing thermal flucts.
  Coupling dynamics complicated by reflection at interfaces
  For fluids have flux across interface – must add/remove atoms

Continuum Description

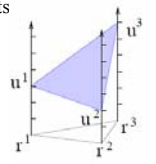
- Represent deformation by displacement field **u** relative to initial positions **R** → Final position **x**(**R**,t) = **R** + **u**(**R**,t)
- Energy can only depend on derivatives of u & rotationally invariant Lagrangian strain $E_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}\right]$
  Usually assume nonlinear term can be ignored – bad for rubber
- Elastic free energy $F = \frac{1}{2}\int d^d x K_{ijkl} E_{ij} E_{kl}$
  Elastic constants K related to phonons in q→0 limit
- Stress $\sigma_{ij} = \sigma_{ji} = \frac{\partial F}{\partial E_{ij}} = K_{ijkl} E_{kl}$
- Dynamic equation with external force **f:** $\nabla_j \sigma_{ij} + f_i = \rho(\frac{\partial}{\partial t} + v \bullet \nabla) v_i$
  In steady state and absence of external force $\nabla_j \sigma_{ij} = 0$

Finite Element Method



Variational approximation to energy
Divide space into elements
Approximate energy by interpolating field in element in terms of values (derivatives) at vertices (edge centers).
Follow dynamics of displacement of vertices = nodes
OR minimize energy subject to nodal displacements

Example:
Linear triangular elements – 3 vertices i=1,3
Fit vertex displacements to linear form
$u^i_\mu = \alpha_\mu + \beta_\mu x^i + \gamma_\mu y^i$
Solve for coefficients and invert to get
$\mathbf{u}(\mathbf{r}) = \Sigma_i N^i(\mathbf{r}) \mathbf{u}^i$ where $N^i(\mathbf{r})$ is linear in **r**,
depends on shape through α,β – called shape functions



Finite Element cont.

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

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

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

(courtesy of N. Bernstein)

Dynamics with Finite Elements

We have a potential energy

$$U = \sum_{mn\mu\nu} u^m_\mu U_{m\mu n\nu} u^n_\nu$$

Kinetic energy is something like

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

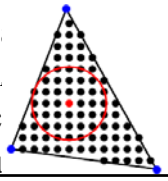
(Choice: what to use for $\rho(\vec{r})$?)

So we can write a Hamiltonian $H = U + T$, and get forces that are conjugate to displacements

(courtesy of N. Bernstein)

Approaches to Finding Constitutive Laws

- Assume linear elasticity or other simple form and fit to atomistic results. Better quality fit, smaller atomistic region.
- Local Quasicontinuum Method – Nodes coincide with "rep
  Calculate energy in eleme
  assuming part of infinite c
  corresponding strain – fu



Approaches to Finding Constitutive Laws

- Coarse Grained MD (Broughton, Rudd)
  Integrate out small scale degrees of freedom in advance
  Retain KE, approximate entropy
- Curtarolo and Ceder
  Replace springs between eliminated atoms by effective springs between remaining atoms (a la Migdal-

What Happens at MD/FEM Interface?

One approach – Refine FEM to atomic scale near MD boundary
Transition between descriptions at sharp interface

1D example MD ● , FEM ○

● ● ● ● ● ● ○ ○ ○ ○ ○ ○

i= -5 -4 -3 -2 -1 0 1 2 3 4 5 6

What Happens at MD/FEM Interface?

- Alternative approach
  Finite elements larger than interaction range – local
  Use overlap region so sharp interfaces outside region of interest
- 1D example MD ● , FEM ○

● ● ● ● ● ● ● ●

○ ○ ○ ○ ○

i= -5 -4 -3 -2 -1 0 1 2 3 4 5 6

- Two descriptions provide boundary conditions for each other at outer edge of overlap
- More to come ….

Reflections in Dynamic Simulations

Most of above methods consider quasi-static limit

Change in representation or resolution
→ reflect short wavelength phonons

Want to dissipate waves smaller than element, allow transmission of longer waves

For linear systems can use effective Greens function to remove entire exterior

$$m\ddot{x}_i(t) = -\frac{\partial V}{\partial x_i} + \int_0^t d\tau \sum_{j=1}^{N} \beta_{ij}(t)\dot{x}_j(t-\tau) + \sum_{j=1}^{N} \beta_{ij}(t)x_j(0) + R_i(t)$$

where $\beta_{ij}(t)$ represents coupling between internal atoms mediated by external atoms, R = random force from ext.

Cai et al. PRL 85, 3213 (2000) → β from simulation of entire ext.

Huang and E, PRL 87, 135501 (2001)

→ Simple analytic approximation for short lengths and times
Minimizes reflections and transmission of q=0 modes that want

What's been studied?

Quasicontinuum perhaps most widely used
Dislocations, Indentation – micrometer scale solids,
Cracks, Grain Boundaries
Review: Miller & Tadmor, J. Comp. Aided Mater. Design 9, 203 (2002)

MAAD and DCET – quantum treatments near crack tips

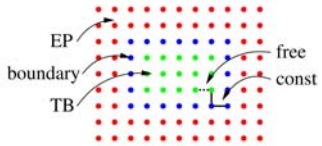
DCET

(No finite elements continuum, just molecular dynamics)

TB forces from constrained electronic Green's function

Mechanical coupling:

- EP atoms: included in EP calculation, forces from EP
- TB atoms: included in TB calculation, forces from TB
- boundary atoms: included in both calculations, forces from EP

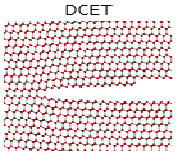


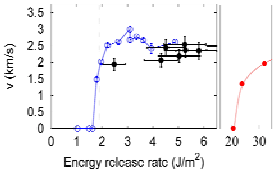
No well defined total energy. (Bernstein Europhys. Lett. 2001)

(courtesy of N. Bernstein)

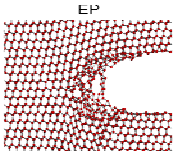
BRITTLE FRACTURE

DCET





EP



Blue: sim.
Black: exper. (Hauch *et al.* PRL **82**)
Red: EP (approx.)
Vertical line: Griffith crit. for brittle fracture

Onset approximately at Griffith criterion

Limiting speed is ≈ 1/2 Rayleigh speed

(courtesy of N. Bernstein)