ATOMS AND THE CONTINUUM

Coupling Atomistic Simulations and

Continuum Elasticity for

Multiscale Simlations

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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

OTHER MESH REFINING ATTEMPTS

Hoover *et al.* (Comput. Phys. **6**, 1992) (very sketchy)
Kohlhoff *et al.* (Phil. Mag. A **64**, 1991)

Molecular dynamics: embedded atom

$$U = \sum_i F(\rho_i) + \sum_{ij} V(r_{ij})$$

where

$$\rho_i = \sum_j \phi(r_{ij})$$

and $F(\rho)$ is nonlinear, and long ranged.

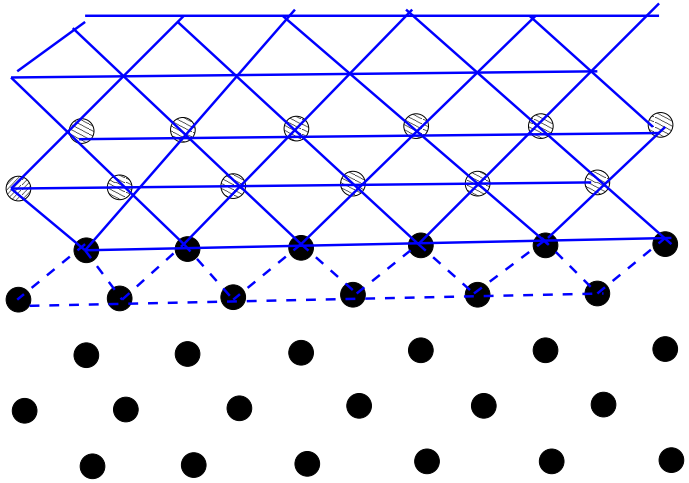
Finite elements: nonlinear elasticity, matched elastic constants

Application: quasistatic fracture in BCC metals

OTHER MESH REFINING ATTEMPTS CONT'D

Refine mesh to atomic size

Two zones, each a boundary condition to the other



Type	contribute to which calc.?	feel which forces?
black atoms	MD	MD
grey atoms	MD	FE
dashed elems.	FE	MD
solid elems.	FE	FE

Not conservative – no well defined total energy

- Forces don't sum to zero
- Energy not conserved during dynamic simulation

IMPROVED CONSTITUTIVE LAWS

What's missing from conventional finite elements?

- variation of mass matrix (lumped vs. distributed)
- variation of stiffness matrix (atomistic vs. bulk)
- accounting for missing deg. of freedom (temperature)
- effects of extreme non-linearity

Several approaches to address subsets:

- coarse-grained molecular dynamics
- quasicontinuum method

COARSE-GRAINED MD CONCEPT

(Rudd and Broughton Phys. Rev. B **58** 1998)

Concept: define a set of finite element equations that are explicitly derived from an atomistic empirical potential description

Assume continuum field is mean of atomistic description, i.e.

$$\vec{u}^j = \sum_\mu f_{j\mu} \vec{u}^\mu$$

$\vec{u}^\mu$ is an atomic displacement
$\vec{u}^j$ is a finite element node displacement
$f_{j\mu}$ is a weight function (related to interpolation/shape function N)

Define quantities (displacement, momentum, energy, etc.) as thermodynamic averages over atomic D.O.F. that obey constraint

COARSE-GRAINED MD TOTAL ENERGY

Given some MD Hamiltonian H_{MD}, define CG energy as

$$E\left(\{\vec{u}^k, \dot{\vec{u}}^k\}\right) = \int d\vec{x}^\mu d\vec{p}^\mu H_{\mathsf{MD}} e^{-\beta H_{\mathsf{MD}}} \Delta / Z$$

where Δ is the constraint

$$\Delta = \prod_j \delta\left(\vec{u}^j - \sum_\mu \vec{u}^\mu f_{j\mu}\right) \delta\left(\dot{\vec{u}}^j - \sum_\mu \vec{p}^\mu f_{j\mu}/m_\mu\right)$$

and Z is the partition function

Results (for a harmonic Hamiltonian):

$$E\left(\{\vec{u}^k, \dot{\vec{u}}^k\}\right) = U_{\mathsf{int}} + \frac{1}{2}\sum_{jk}\left(M_{jk}\dot{\vec{u}}^j\dot{\vec{u}}^k + \vec{u}^j K_{jk}\vec{u}^k\right)$$

where U_{int} is the energy of the missing DOF

$$U_{\mathsf{int}} = 3(N - N_{\mathsf{node}})kT$$

COARSE-GRAINED MD MATRICES

Deriving FE from MD+thermodynamics is nice, but what about details?

$$M_{jk} = m \left(\sum_{\mu} f_{j\mu} f_{k\mu} \right)^{-1}$$

and

$$K_{jk} = \left(\sum_{\mu} f_{j\mu} D^{-1}_{\mu\nu} f_{k\mu} \right)^{-1}$$

(note: $D_{\mu\nu}$ is singular. . .)

How to choose weight functions $f_{j\mu}$?

COARSE-GRAINED MD WEIGHT FUNCS.

Weight functions tell us how we're coarse graining
Equivalent in conventional FEM: shape functions $N^i(\vec{r})$

Reminder: FEM definition

$$\vec{u}(\vec{r}) = \sum \vec{u}^j N^j(\vec{r})$$

From atomistics: best fit displacement field minimizes

$$\chi^2 = \sum_\mu |\vec{u}^\mu - \vec{u}(\vec{r}^\mu)|^2 = \sum_\mu \left| \vec{u}^\mu - \sum_j \vec{u}^j N^j(\vec{r}^\mu) \right|^2$$

Best fit FE field with $\vec{u}^j = \sum_\mu f_{j\mu} \vec{u}^\mu$ and

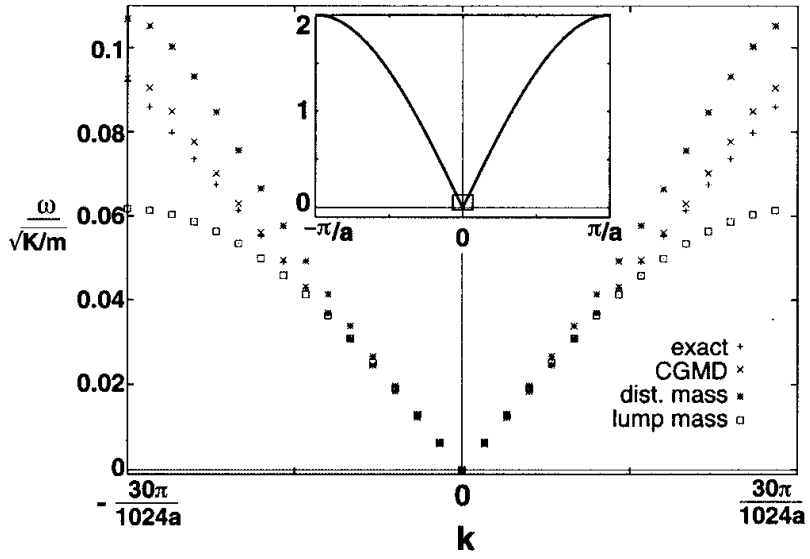
$$f_{j\mu} = \sum_k \left(\sum_\nu N^j(\vec{r}^\nu) N^k(\vec{r}^\nu) \right)^{-1} N^k(\vec{r}^\mu)$$

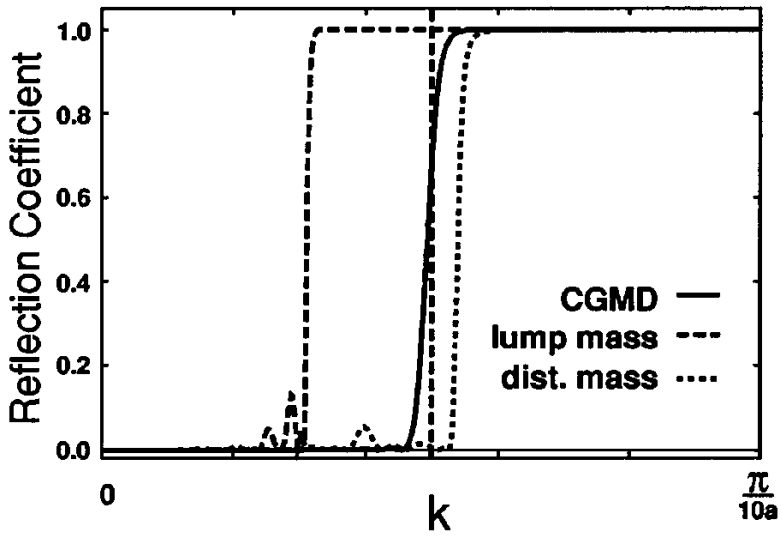
Recipe: $N^j(\vec{r}) \Rightarrow f_{j\mu} \Rightarrow$ (with $D_{\mu\nu}$) M_{jk} and K_{jk}

COARSE-GRAINED MD RESULTS

1-D chain with harmonic springs
incommensurate coarse grained mesh

- Phonon spectrum error $< 6\%$
  Conventional FEM $> 18\%$ (worst at zone edge)
- Reflection coefficient through CG region
  Nice transition from to 0 to 1 at correct wavelength
  Conventional FEM shows wavelength shift, little peaks





(by permission from Rudd and Broughton, Phys. Rev. B **58**, p. R5893 (1998).)

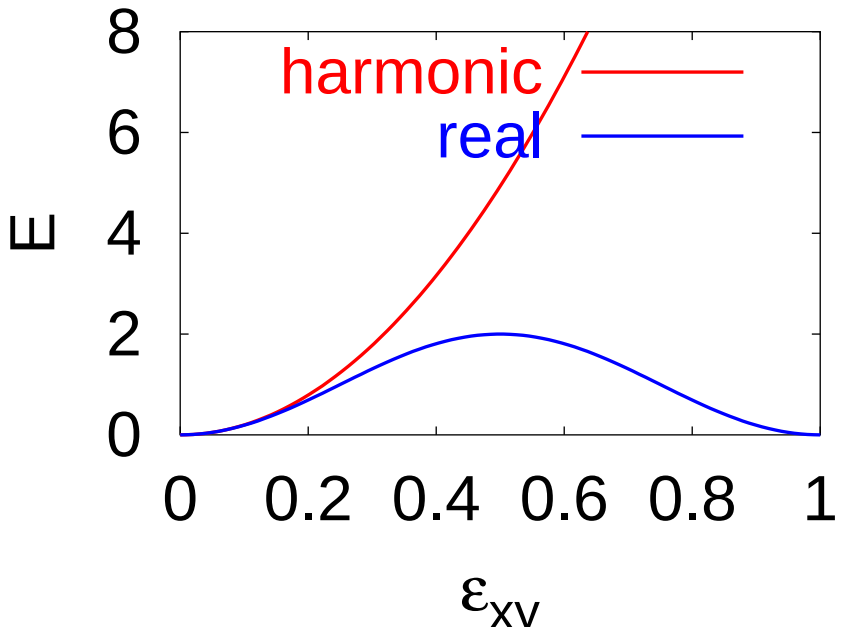
QUASI-CONTINUUM METHOD CONCEPT

Concept: standard finite elements with explicitly atomistic constitutive model

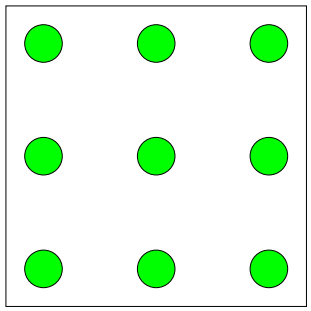
Conventional approach: elasticity

- small deformation - quadratic
- maybe few higher order terms

Real materials: inelastic (very)



ε=0.0



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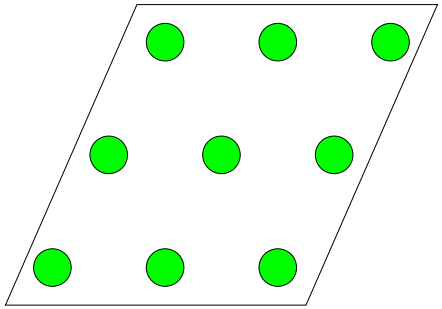

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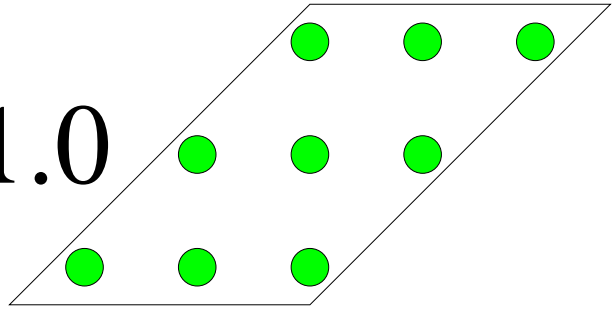
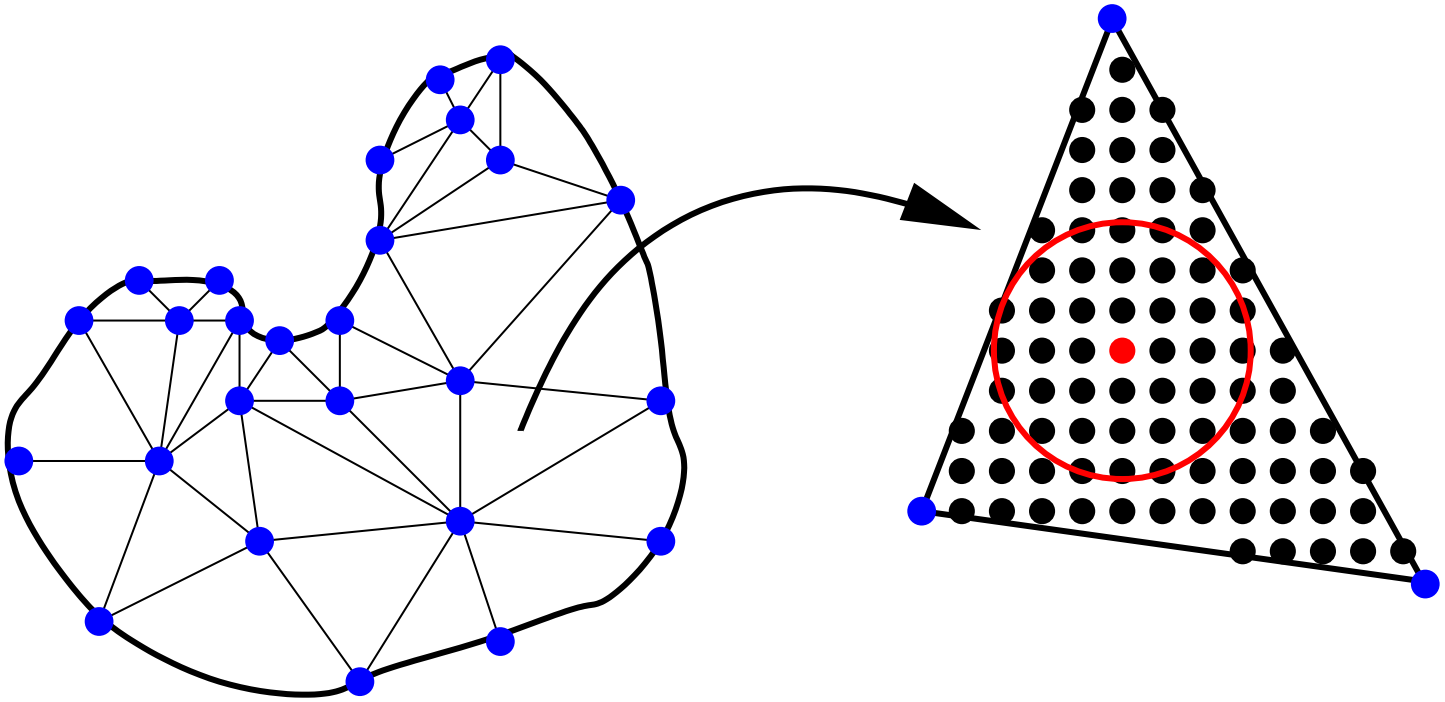


LOCAL QUASI-CONTINUUM



For each element:

- Construct deformation gradient for this element
- Pick representative atom in center of element
- Calc. energy per atom using atomistic model
- Assign energy to element

LOCAL QUASI-CONTINUUM ISSUES

Advantages:

- Include underlying periodicity
- Phase transformations

Missing effects:

- Multi-atom unit cells [fix by relaxing internal DOF]
- Rapidly varying displacement fields
- Interactions between elements (phase boundaries)
- Finite temperatures
- Dynamics (no prescription for mass)

QUASI-CONTINUUM AND COMPLEX LATTICES

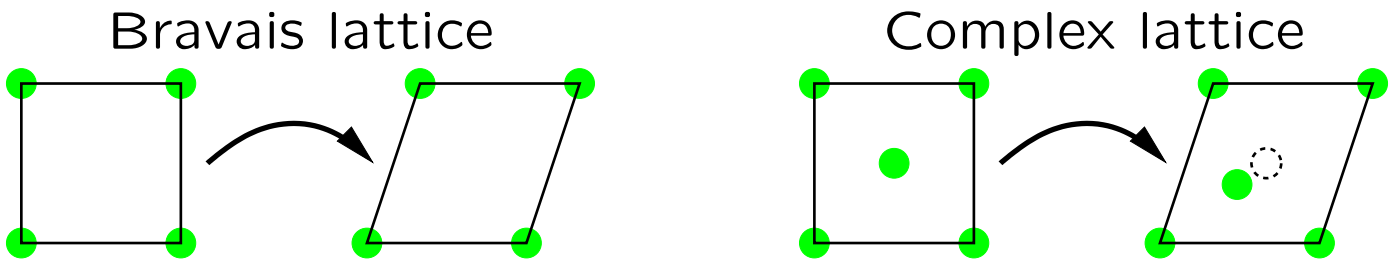
Displacements $\vec{u}$ determine deformation gradient F_{iJ}

For Bravais lattices, F_{iJ} is everything (Cauchy-Born)

$$x_i = F_{iJ} x_J$$

For complex lattices, additional internal DOF

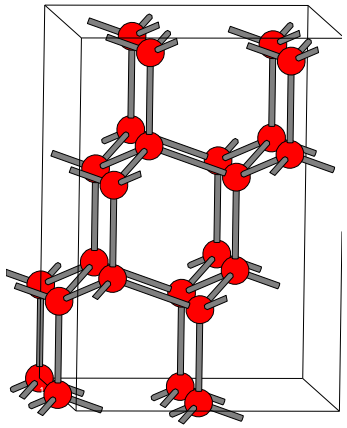
E.g. for a shear F_{iJ}



Explicitly minimize w.r.t. internal DOF

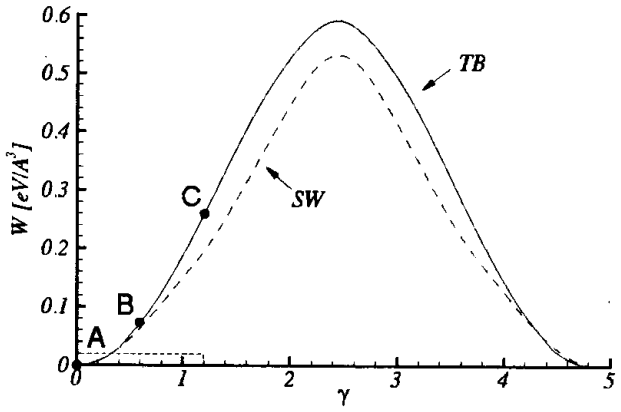
QC COMPLEX LATTICE EXAMPLE

Silicon:
diamond structure
2 atoms per unit cell

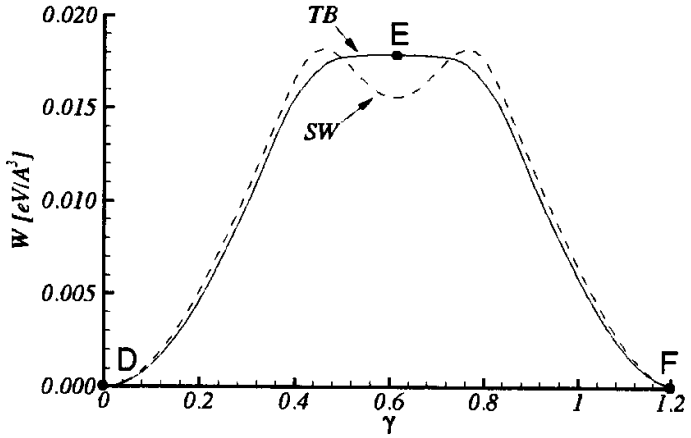


Energy vs. shear:

No relaxation



With Relaxation

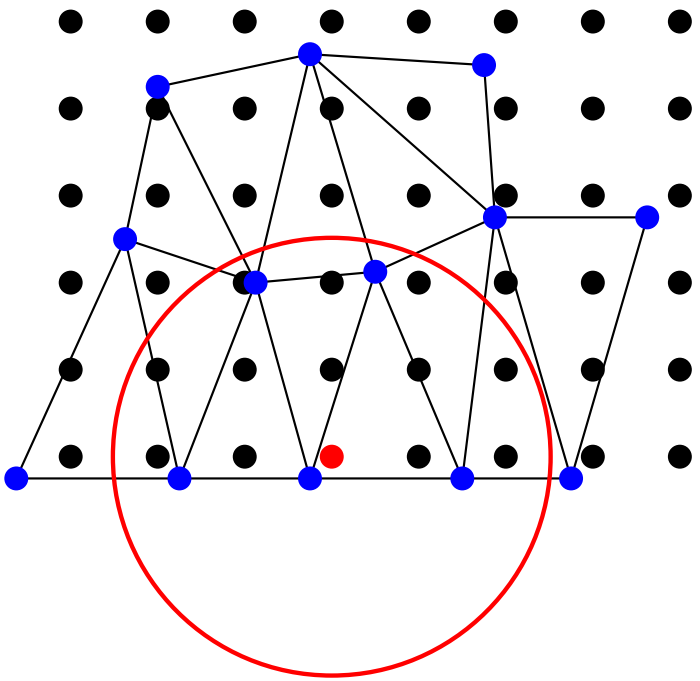


(by permission from Tadmor *et al.*, Phys. Rev. B **59**, p. 235 (1999).)

Big difference in energetics, allows for phase transformation

NON-LOCAL QUASI-CONTINUUM

Like local QC, except environment of representative atom depends on several nearby elements



Fix for:

- Rapidly varying displacement fields
- Interactions between elements:
  - phase boundaries
  - free surfaces
- Arbitrary local disorder
  - grain boundaries
  - dislocation cores

Reproduces MD in limit of one atom per element

QUASI-CONTINUUM RESULTS AND ISSUES

Results

- Dislocations
- Crack - grain boundary interactions
- Nanoindentation (metals and Si)

Issues

- Dynamics and finite temperatures
- Boundary between local and non-local:
  - Atoms in local elements don't feel nearby non-local atoms
  - Non-local atoms do feel nearby local elements
  - No well defined energy, forces don't balance

COUPLING: WHERE DO WE STAND?

MD - well understood, computationally expensive

FEM - well understood, computationally cheap

Coupling - connect disparate concepts (atoms vs. fields)

Mesh refining:

- One possible way for short range potentials
  Details would vary for each potential
- What to do about non 2- or 3-body potentials?
- Not all prescriptions conserve energy
- Constitutive laws must vary with scale

PROGRESS: VARIABLE CONSTITUTIVE LAWS

Coarse-grained MD

- Thermodynamically motivated
- Prescription for dynamics (mass matrix)
- Only small deviation from equilibrium

Quasicontinuum

- Full blown nonlinearity (large deviation from equil.)
- No dynamics worked out yet
- Problems matching local to non-local

BIGGER ISSUES: TEMPERATURE

Temperature:

- What do we do when temperature varies?
  (CGMD derived for equilibrium)
  - T dependent constitutive law
    (little MD sim. for each QC cell?)
  - Solve heat transport problem on FE mesh
- What about missing deg. of freedom?
  - Add dissipative terms (less ad hoc than Broughton et al.)
  - Need to account for
    atomic vibrations conversion into FE temperature
    and
    FE temperature causing atomic vibrations

BIGGER ISSUES: TIME SCALE

Atoms move one time scale of 1 / Debye frequency

Elements move at $1/\sqrt{LY/\rho}$

Variable time step time integration?

How much can FE help anyway?

$$l = vt$$

v is speed of sound, t is time scale

l is distance that information could propagate

t is limited by MD region, how big does the system ever need to be?

BIGGER ISSUES: OTHER CONTINUA

Fields that aren't mass distributions, e.g.
Continuum electrodynamics?

Probably straightforward
Need potentials that interact with fields

Fluids?

Much harder – need to mesh very different concepts

Solid mechanics: atomic positions $\Leftrightarrow$ displacement fields

- Deterministic atomic positions (neglecting dynamics)

Fluid mechanics: atomic positions/velocities vs. flow/potential fields

- Stochastic atomic positions (even for statics)

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