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Multiscale Modeling of the Mechanical Responses of Solids

Lecture 1: Length Scales

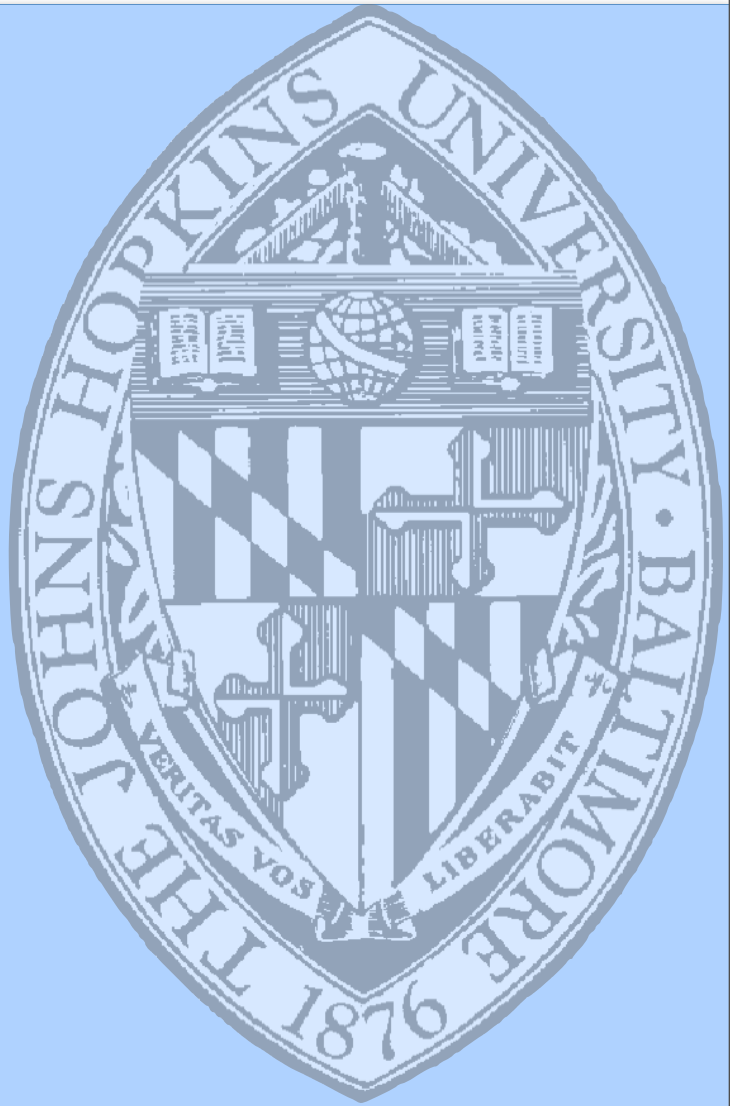
Michael L. Falk

Johns Hopkins University

Materials Science and Engineering;

Mechanical Engineering;

Physics and Astronomy



Who am I? What do I do?

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Associate Professor, Johns Hopkins

Computational Materials Science

MSE in Computer Science

PhD in Theoretical Condensed Matter Physics

I use a variety of computational methods to understand how stress affects material structure and properties. I have particular interests in plasticity and failure in amorphous solids.

Primary methodologies: molecular dynamics (MD) plus some kinetic Monte Carlo (KMC). Developing new approaches to extended time scale MD (hyperdynamics) for application to modeling friction.

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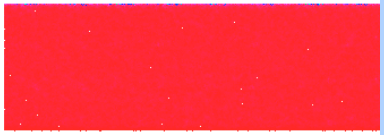

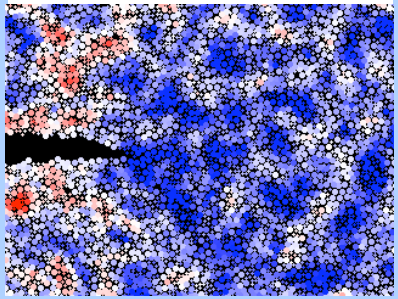

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What I will discuss in this lecture ...

- General overview of classes of problems in mechanics of materials.
- Review of some simulations techniques used to study solids at different length scales.
- Four case studies to illustrate the challenges of modeling at various scales.
- Hierarchical versus concurrent modeling.
- Discussion of the Quasicontinuum Method and related techniques.
- Limitations of this class of concurrent methods.

Scientific Questions in Mechanics

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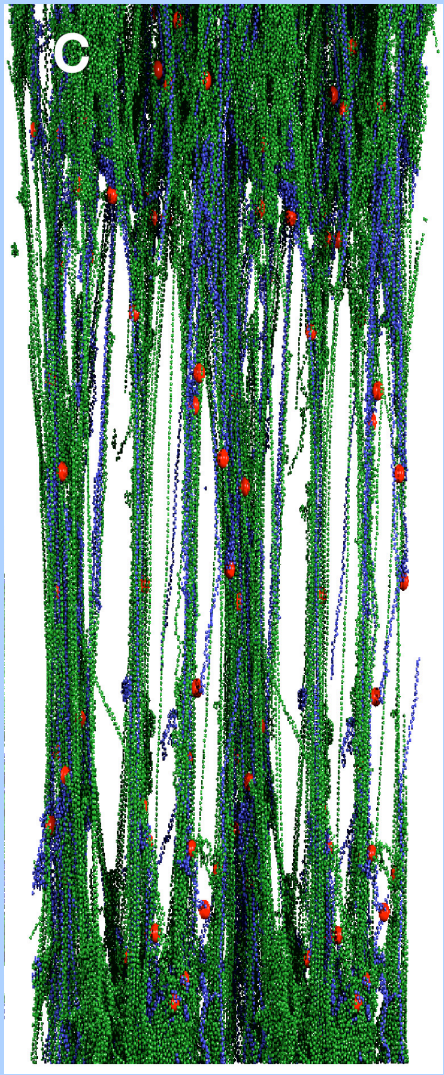
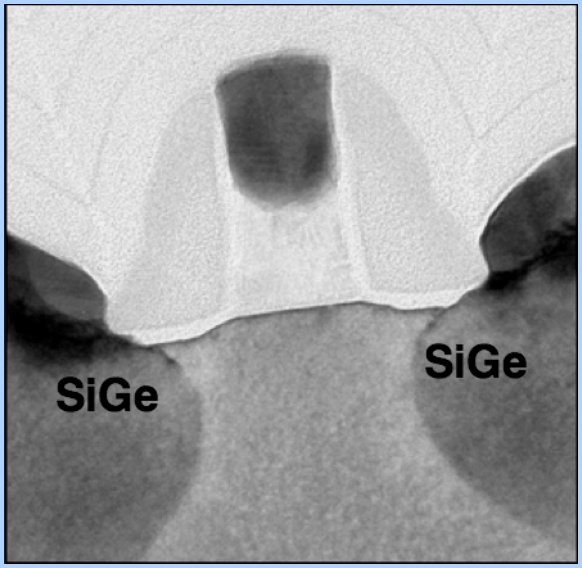
- **The field of mechanics of materials is quite broad, and it is difficult to provide an overview.**
  - What sets the toughness of amorphous polymers when they craze?
  - How do we design superalloy microstructure to enhance high temperature reliability?
  - How do stresses affect the processability and reliability of semiconductors?
  - What surface treatments will be most effective in reducing friction?



Crazing in polymer simulated by Mark Robbins and Joerg Rottler

Problems in Elasticity

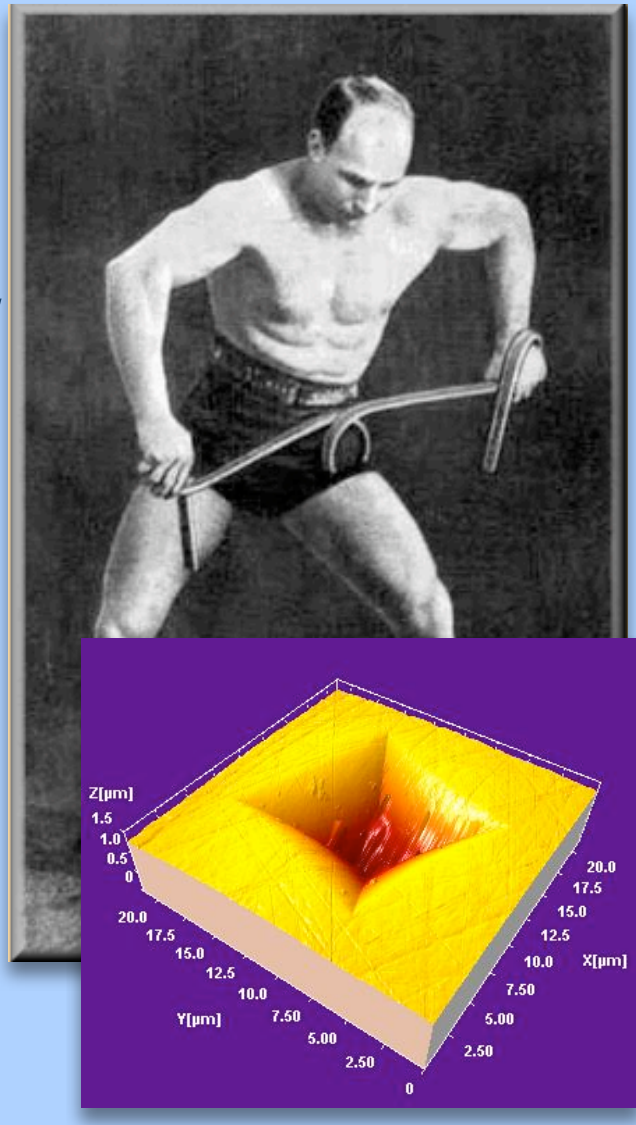
- Problems in solid mechanics can be categorized into a few general classes based on the nature of the physics involved.
- **Elasticity**: reversible response of a solid material to an applied stress.
- Complexity can arise due to geometry, material response or heterogeneity of properties.
- **Example:** Stresses in semiconductor devices can influence electron transport, cause pattern formation during crystal growth, drive motion of dopant atoms.



From: S. Tyagi, An Advanced low power, high performance, strained channel 65nm technology, 2005 IEEE International Electron Devices Meeting (IEDM) December 5–7, 2005

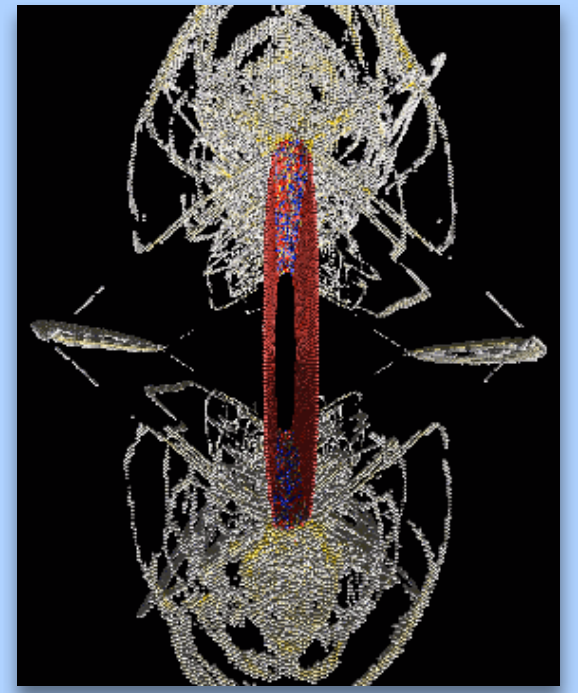
Problems in Plasticity

- When stresses become high enough, they induce irreversible deformation known as **plasticity** or **plastic flow**.
- Such deformation is typically mediated by defects in the structure.
- Plasticity can lead to instabilities that can result in failure.
- **Example:** Crystalline metals typically exhibit hardening, a process whereby the material becomes "stronger" as it is progressively deformed.



Problems in Failure

- Any material subjected to high enough stresses for long enough will eventually fail.
- Failure is catastrophic and typically local, but involves elastic and/or plastic processes.
- This could be due to a plastic instability (shear banding), a pre-existing flaw that grows (fracture), gradual shape change (creep), the formation of bubbles (cavitation), or other mechanisms.
- **Example:** Fracture in copper involves significant blunting of the crack tip due to plasticity.



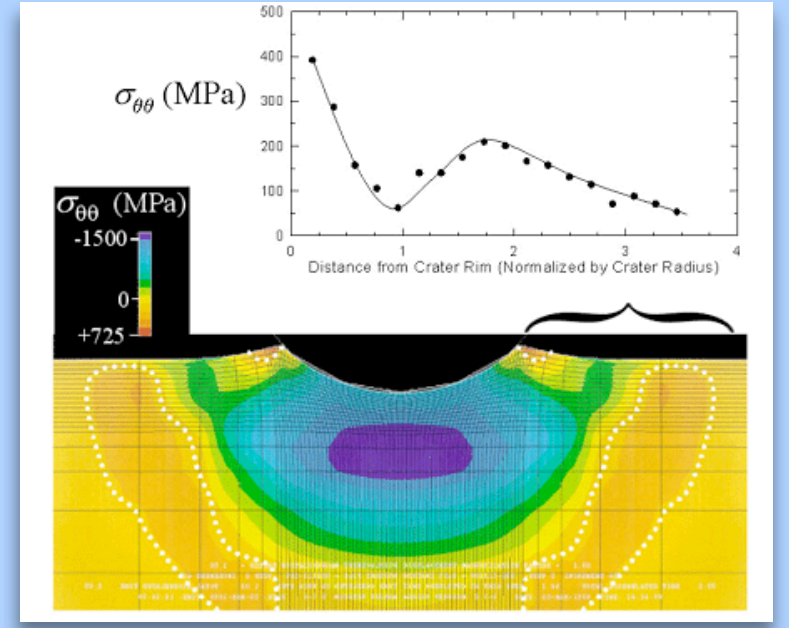
Simulation of a crack tip in copper performed by Zhou, Holian and Lomdahl at Los Alamos National Laboratory

Methods for Modeling

- **There are numerous approaches to simulation of these various problems.**
  - Continuum Methods (i.e. finite element elasticity)
  - Mesoscale Methods (i.e. phase field)
  - Empirical Atomistic Methods
  - Ab Initio Atomistic Methods

Continuum Mechanics

- The workhorse of solid mechanics.
- Typically scale free.
- All information about the smaller scales are incorporated via constitutive "laws".
- Boundary value problems are constructed.
- Frameworks: direct dynamics (force based) or variational (energy based) methods.



FEM analysis of foreign object damage on a turbine blade performed by Boyce, Mehta, Peters and Ritchie

Mesoscale Methods

- One scale down from the continuum methods are a host of methods used to account for microstructure and its evolution.
- Phase field models evolve one or more order parameters, describing various phases and the boundaries between them, according to the dictates of a free energy functional.
- Also in this class are lattice models like the Potts model and Ising model that reduce microstructure to sites that can take on a restricted number of values.

Phase field simulation of crystal growth by James Warren, NIST.

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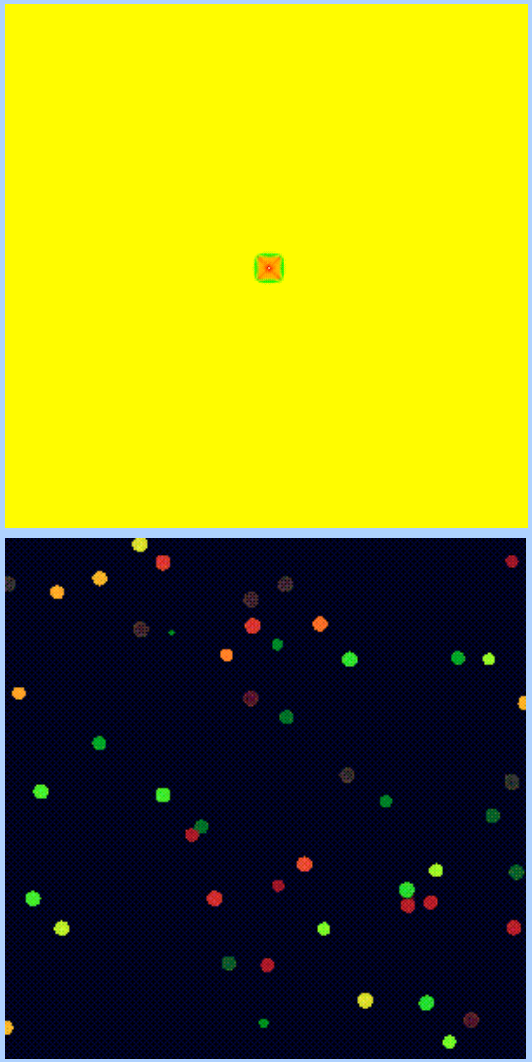
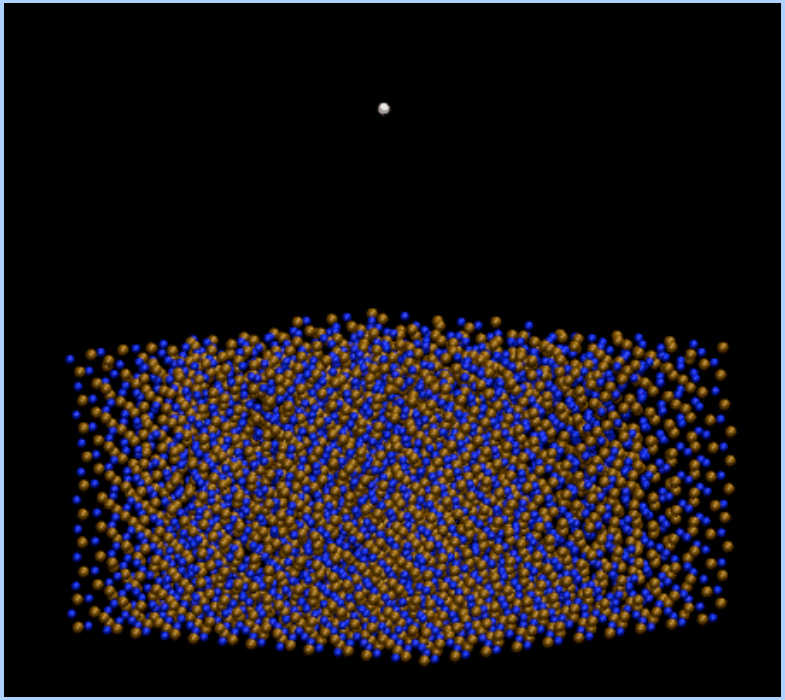


Phase field simulation of crystal growth by James Warren, NIST.

Empirical Molecular Simulation

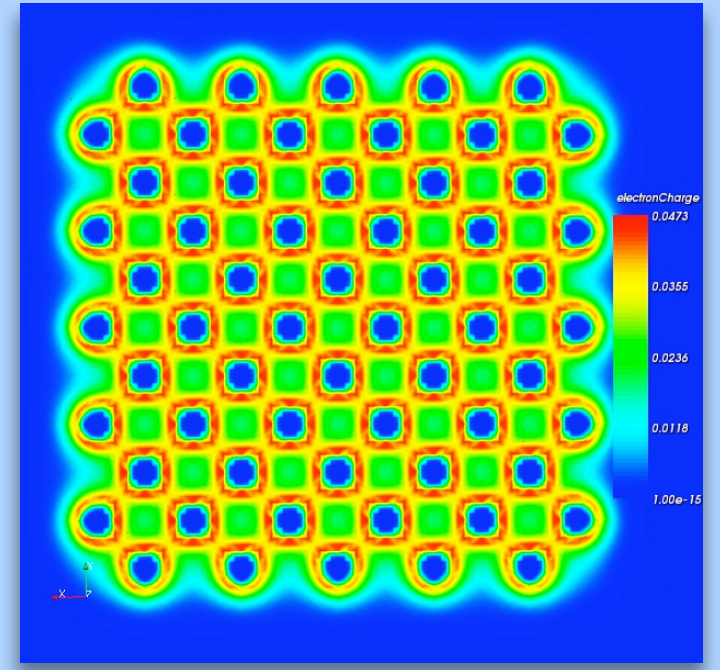
- We can attempt to directly resolve interactions of atoms or super-atomic units.
- To first approximation one may employ an **empirical potential** to describe the energy of the system in terms of particle coordinates.
- The structures that result can be explored through energy minimization, equilibrium statistics (Monte Carlo) or by numerically integrating Newton's equations (Molecular Dynamics).
- In MD vibrations naturally account for important aspects of heat and sound.



MD simulation of sputtering of BN by Xe ions by Yim, Boyd and Falk.

Ab Initio Simulation

- We can also attempt to explicitly account for electronic degrees of freedom.
- This typically involves approximating the ground state electron density subject to the ionic positions (DFT).
- Provides higher fidelity than empirical methods, and reveals information about electronic properties.
- Severely limits the size and time scales from ~10^6 atoms for 10^{-7} s using empirical methods to ~10^2 atoms for 10^{-9} s using DFT.



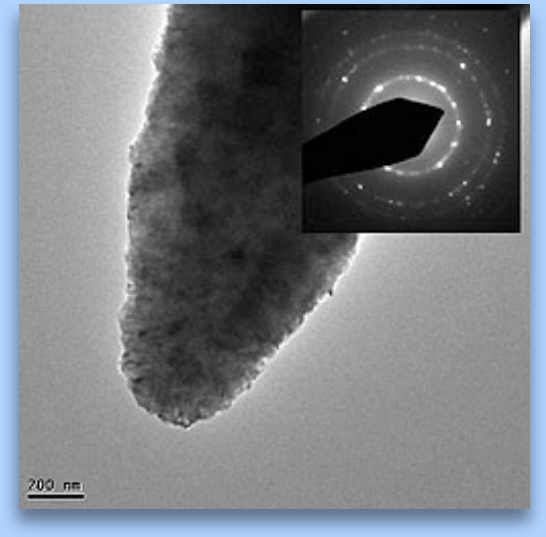
Ab initio calculation of an aluminum cluster by Gavini, University of Michigan.

Four Case Studies

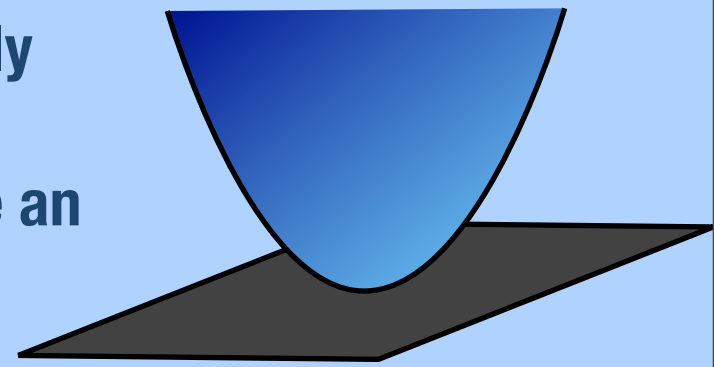
- I will primarily focus on empirical molecular simulation and continuum methods, because these are the most widely used methods in the context of mechanics.
- There is a tension between the purveyors of atomistics (typically physicists) and those of continuum methods (typically mechanicians).
- Each method has its claim to necessity. Oftentimes neither presents a complete picture.
- Four examples where neither result is entirely satisfactory
  - Surfaces in Contact (elastic contact)
  - Crystal Plasticity
  - Dynamic Crack Branching (failure)
  - Shear Bands in Metallic Glass(failure/plasticity)

Tips in Contact: Continuum

- What happens when a tip is brought in contact with a surface?
- This is a crucial problem for understanding friction and other surface properties and measurements.
- Continuum solutions exist: Hertz solutions, Johnson-Kendall-Roberts (JKR) model and subsequent theories.
- A finite element simulation of this is fairly straightforward, but is it an accurate depiction, particularly for a situation like an atomic force microscope (AFM)?



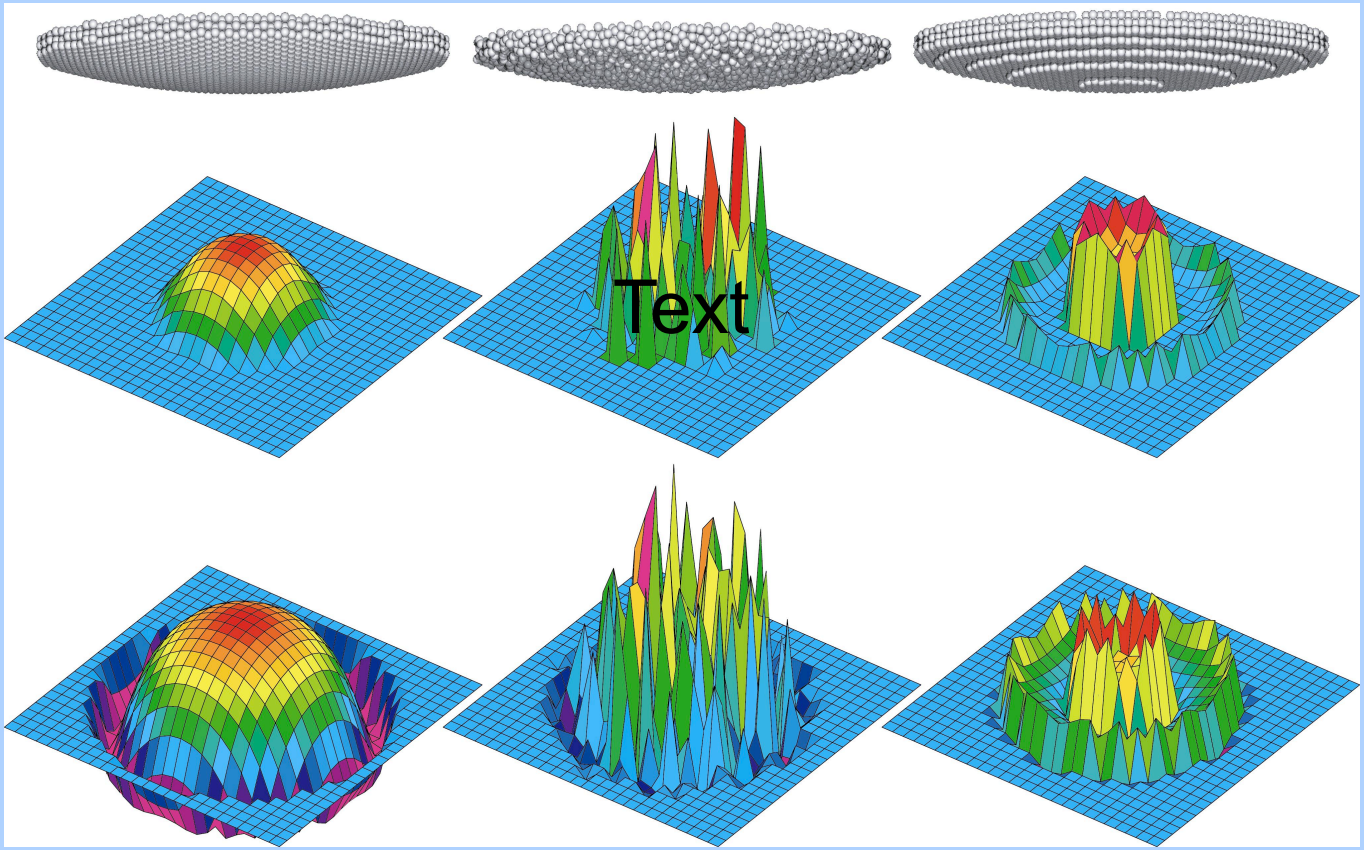
Nanocrystalline diamond AFM tip
Robert Carpick, U Penn



Tips in Contact: Atomistics

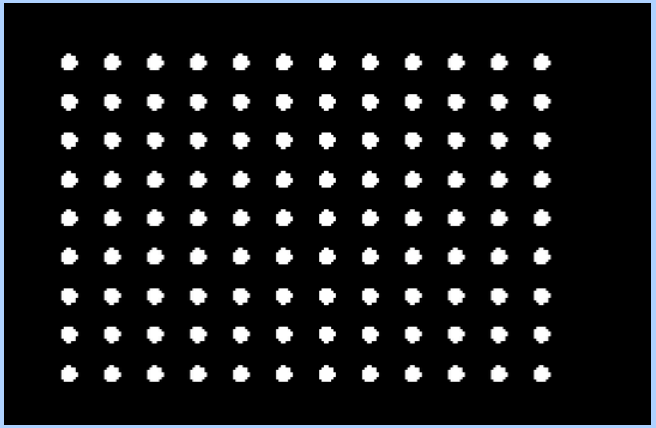
- **Pressure Distribution for a Sphere on a Flat**

Luan & Robbins, Nature 435, 929 (2005)



Crystal Plasticity: Continuum

- Plastic flow in crystals occurs due to the motion of dislocation defects.
- Since dislocations move along particular slip planes, single crystals exhibit anisotropic plastic flow.
- Continuum theories exist for crystal plasticity.
- Glide can be easily accounted for, but dislocation nucleation and interaction must be put in by ad hoc methods.
- Also continuum theories are scale free, but size effects are observed in experiment.



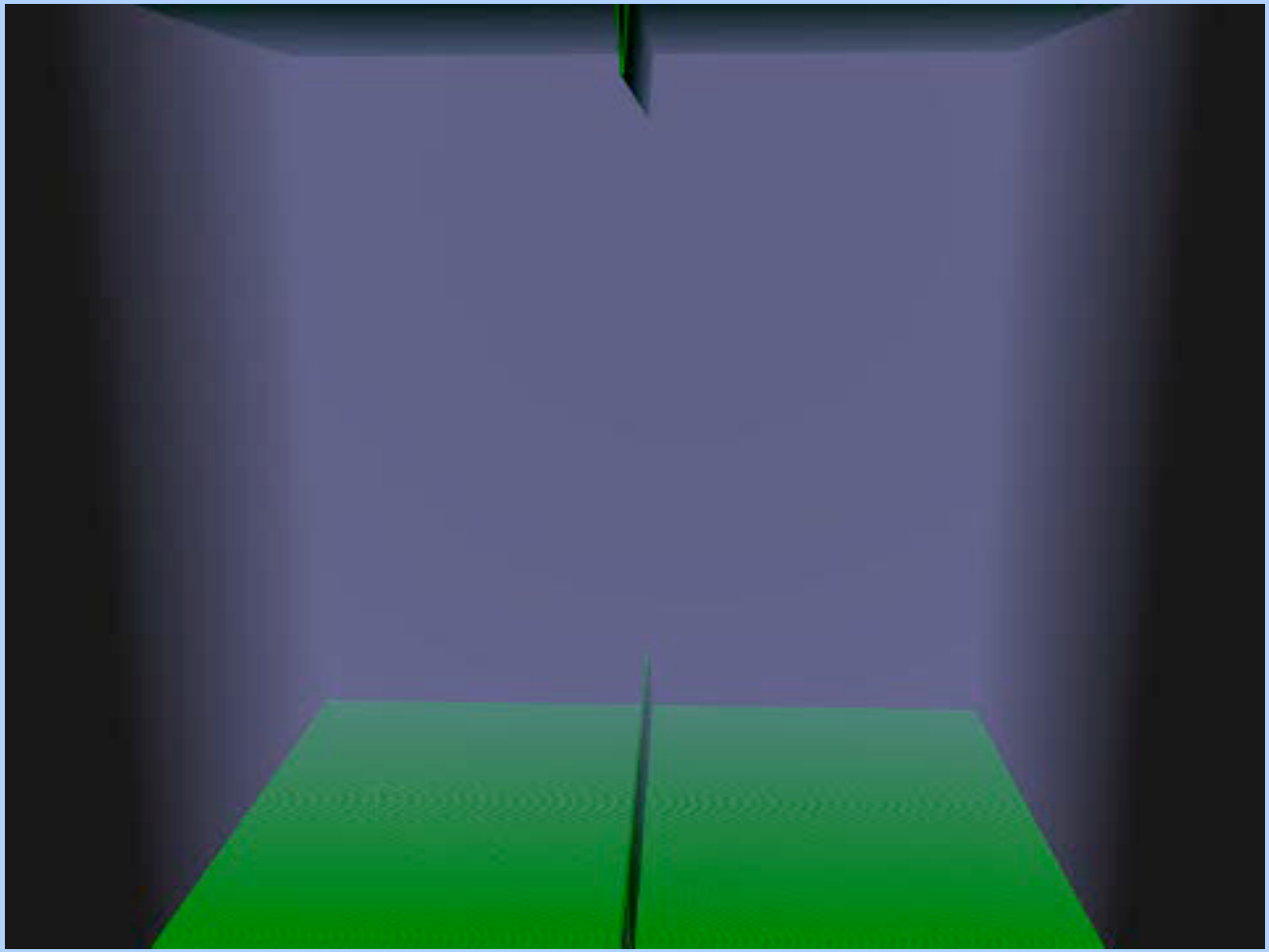
M Jessell, P Bons & P Rey 2002
Microstructures Online
http://www.virtualexplorer.com.au/special/meansvolume/contribs/jessell/

Crystal Plasticity: Atomistics

- **Atomistic simulation gives ample detail**

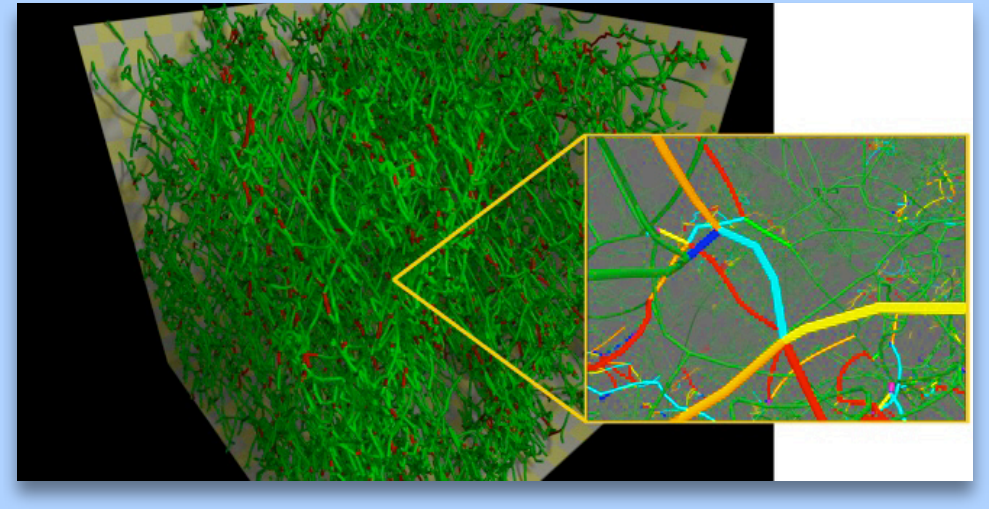
Abraham F. F. et al., Proc. Nat. Acad. Sci., 99, 5783-5787 (2002).

- **10^9 atoms**
- **$2x10^5$ steps ~nanoseconds**
- **40,000 CPU hrs**
- **LJ potential**
- **4 days on "White" at LLNL**
- **0.3μ on a side**

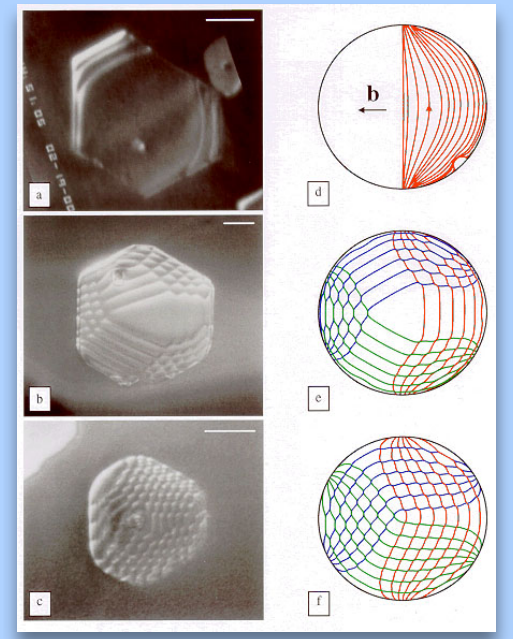


Crystal Plasticity: Mesoscale

- One could argue that most computation time is wasted simulating atoms not participating in deformation.
- Dislocation dynamics models only simulate the dislocations, but need information from lower scales to handle dislocation crossing events and nucleation.



Dislocation structures in Mo run using ParaDis by Meijie Tang at LLNL

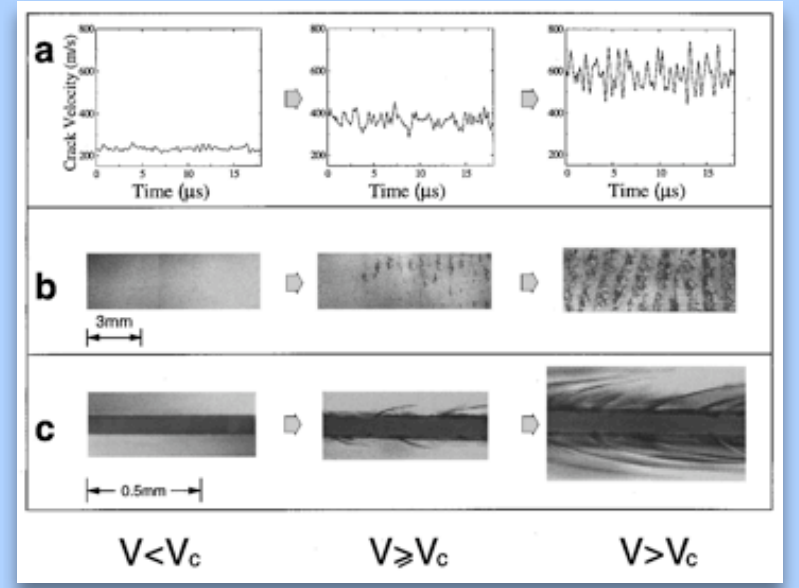


Dislocation simulations of strain induced slip in $MoSi_2$ islands by K Schwarz, IBM

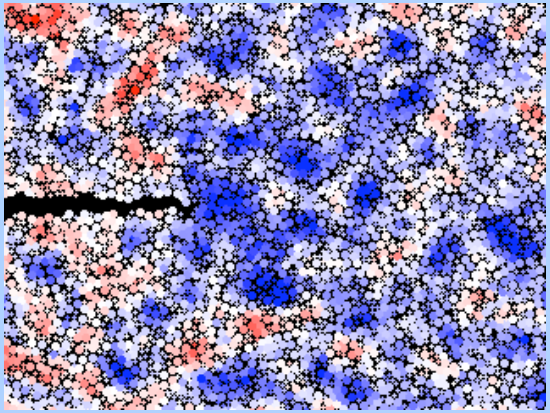
Crack Branching: Experiment

A personal cautionary tale...

- Crack branching is of scientific and practical interest because it is not understood why fast moving cracks spawn daughter cracks.
- I had studied fracture atomistically in glassy materials, but the sizes available to us were too limited to follow the crack for long enough to observe branching phenomena.
- However there was an intersting continuum model...



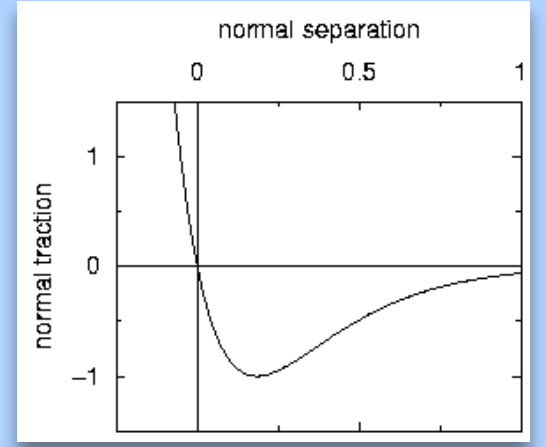
Crack branching in PMMA by J Fineberg and E Sharon, Hebrew U

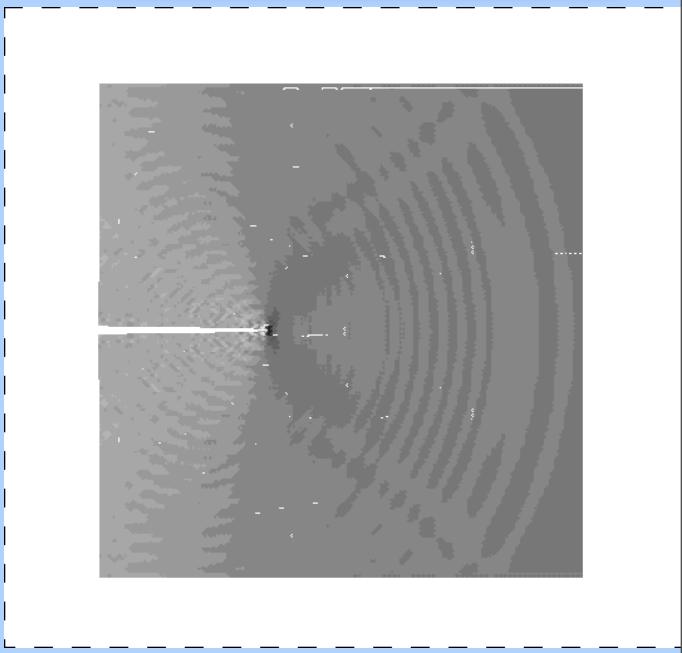


Brittle fracture in amorphous solids, M. Falk

Crack Branching: Continuum

- Xu and Needleman had proposed a continuum model in which cohesive zones were placed between all elements.
- The results showed branching at speeds near the Rayleigh wave speed.
- My job was to reimplement this, confirm the result and use these simulations to better understand the physics.





Crack Branching: Trouble!

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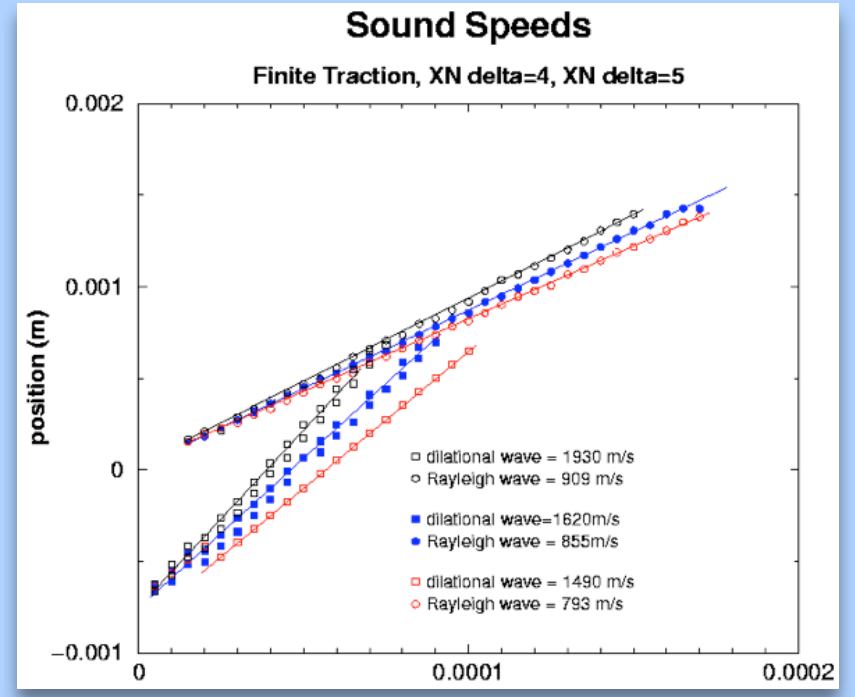
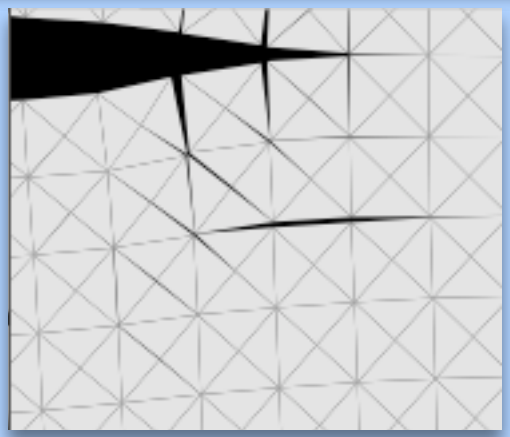
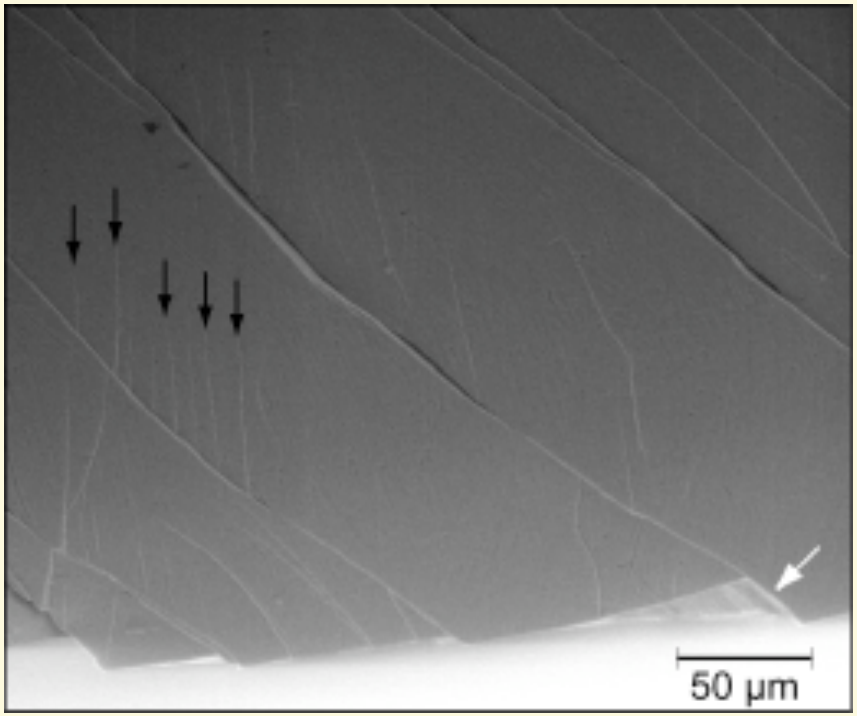
- In quantifying the sound speed, I noticed mesh dependence.
- The introduction of the cohesive law was systematically changing the stiffness of the mesh.
- It could be mathematically shown that you could not simultaneously resolve the cohesive zone near the tip and have elasticity dominated by the elements.
- Even introducing a stiff cohesive zone did not solve the problem. The near tip region disintegrated!



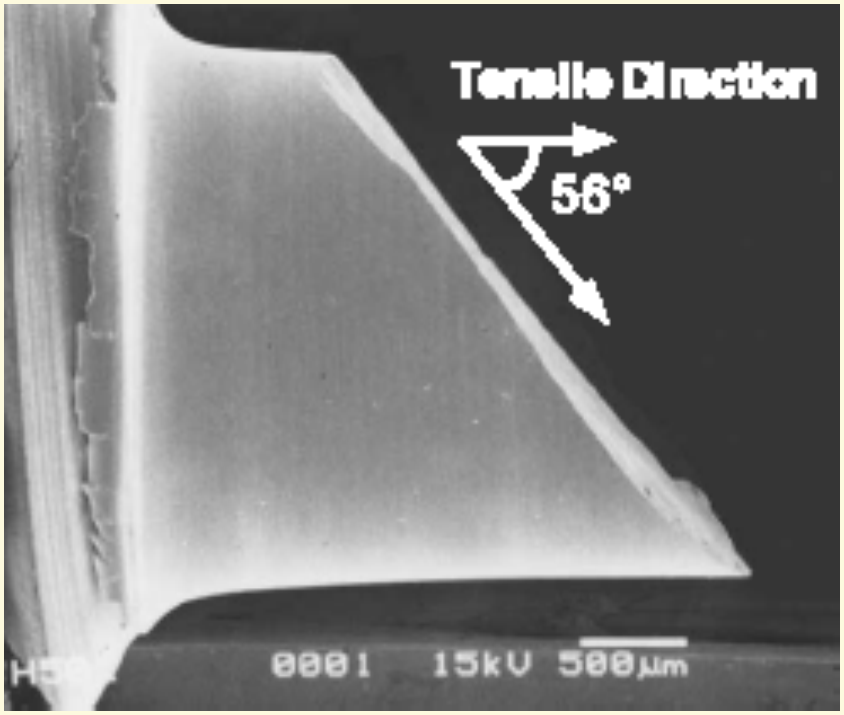


Shear Bands: Experiment

Metallic glasses failure by plastic instability



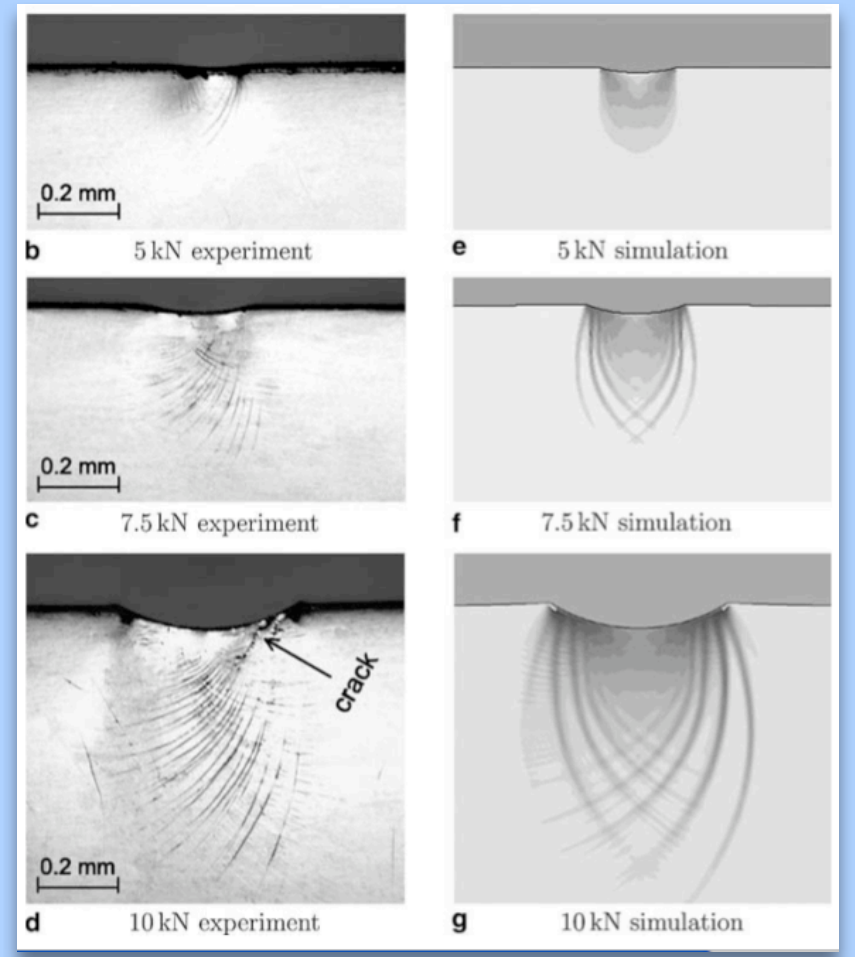
Electron Micrograph of Shear Bands Formed in Bending Metallic Glass
Hufnagel, El-Deiry, Vinci (2000)



Quasistatic Fracture Specimen
Mukai, Nieh, Kawamura, Inoue, Higashi (2002)

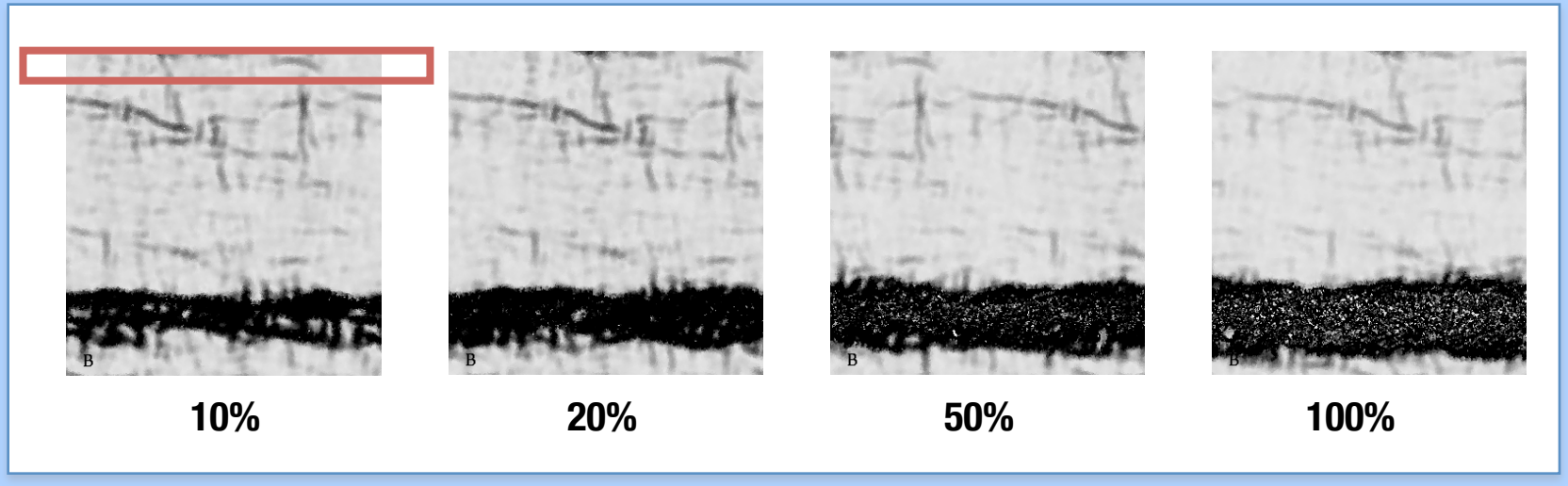
Shear Bands: Continuum

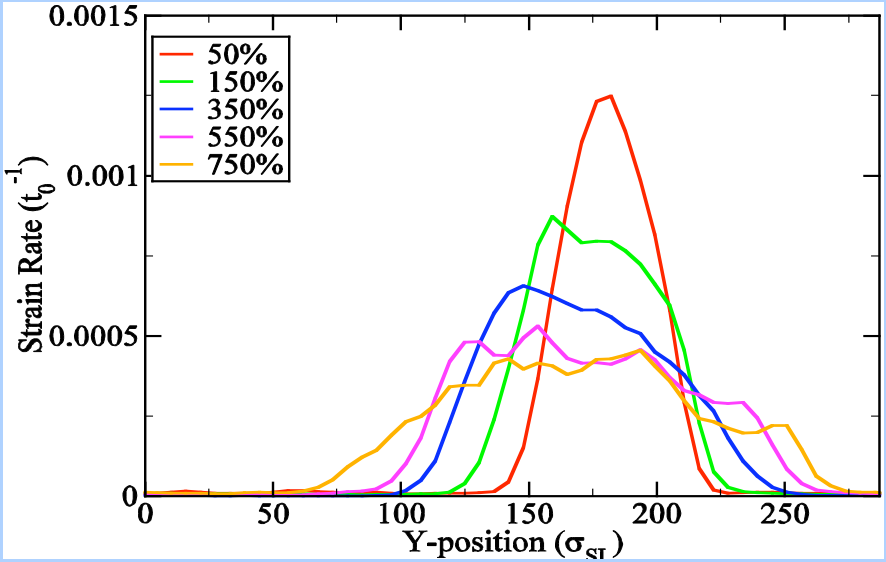
- Constitutive laws have been developed for modeling shear banding in metallic glass.
- These constitutive laws soften, ie stress decreases with increasing strain, and thus undergo an instability.
- However, the short length scale cutoff for the instability is set by the mesh length scale.
- Thus the results become mesh dependent.

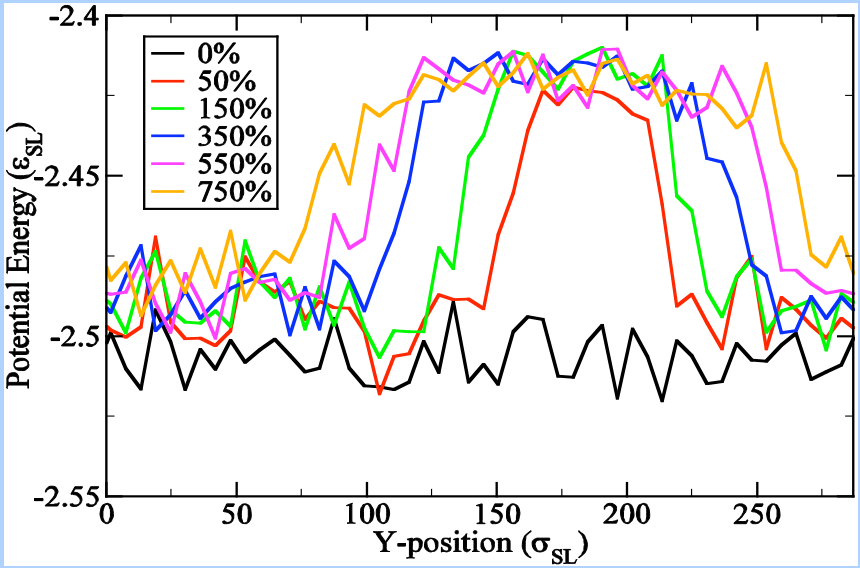


Experiment and finite element simulation
by C Su and L Anand, MIT

Shear Bands: Atomistics

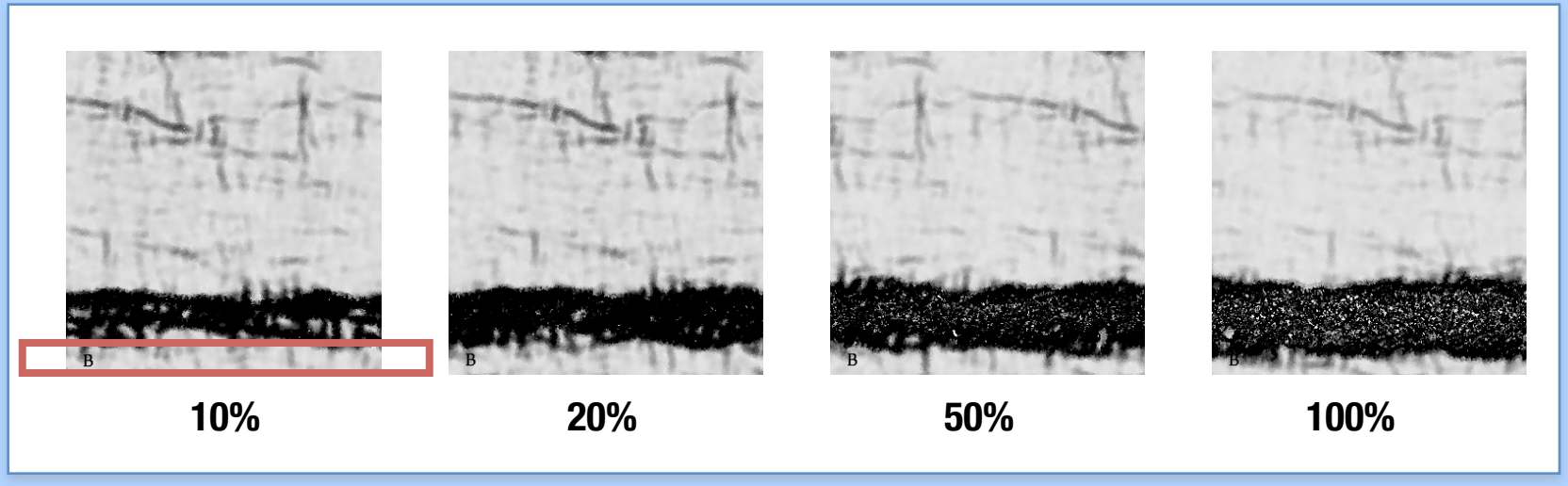


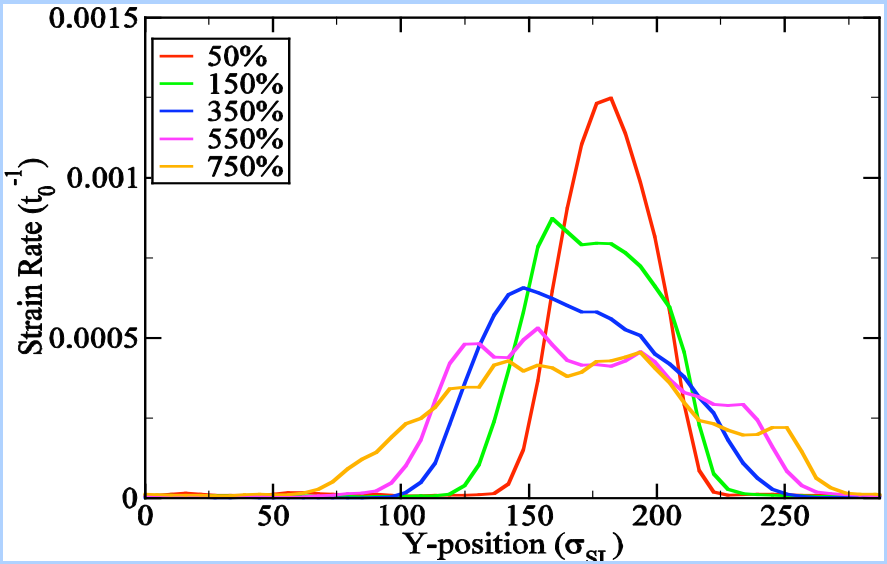


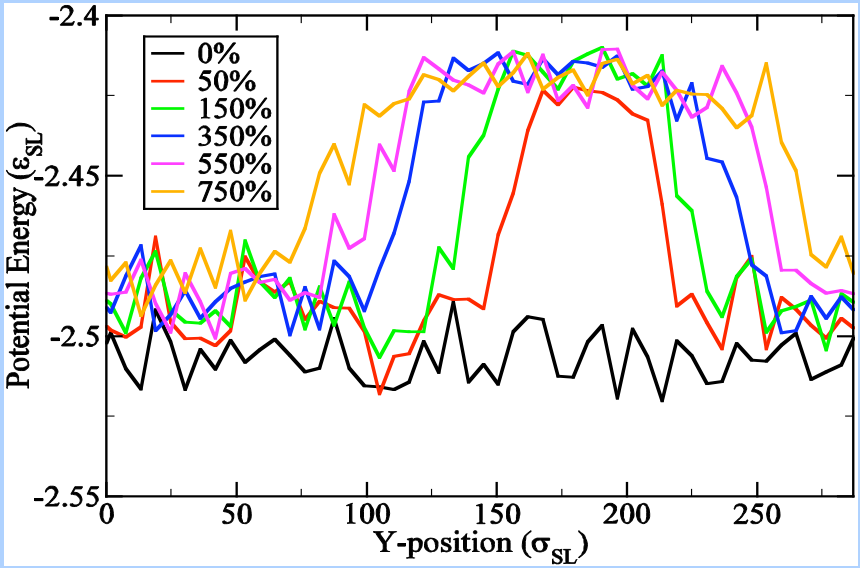


Y Shi, MB Katz, H Li, MLF, PRL, 98, 185505 (2007)

Shear Bands: Atomistics







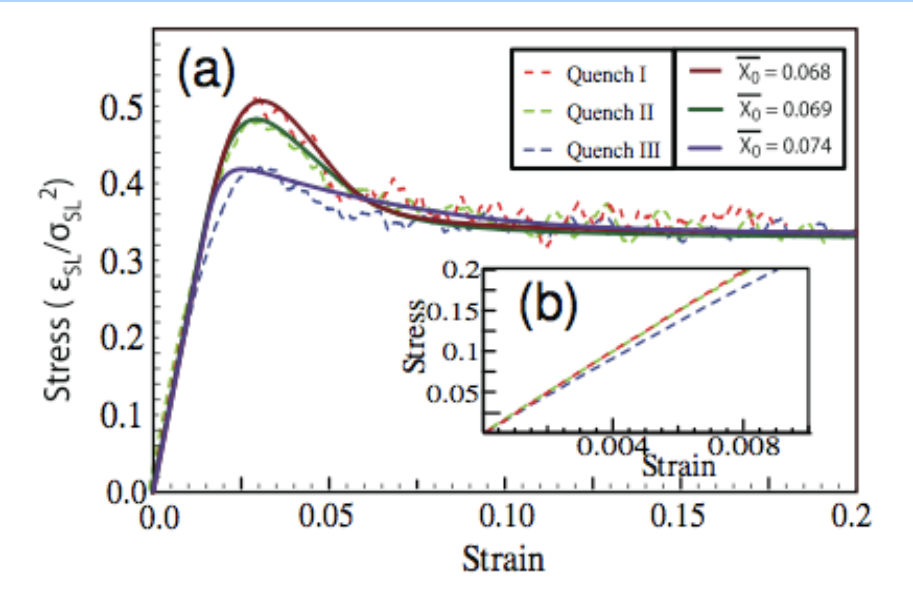
Y Shi, MB Katz, H Li, MLF, PRL, 98, 185505 (2007)

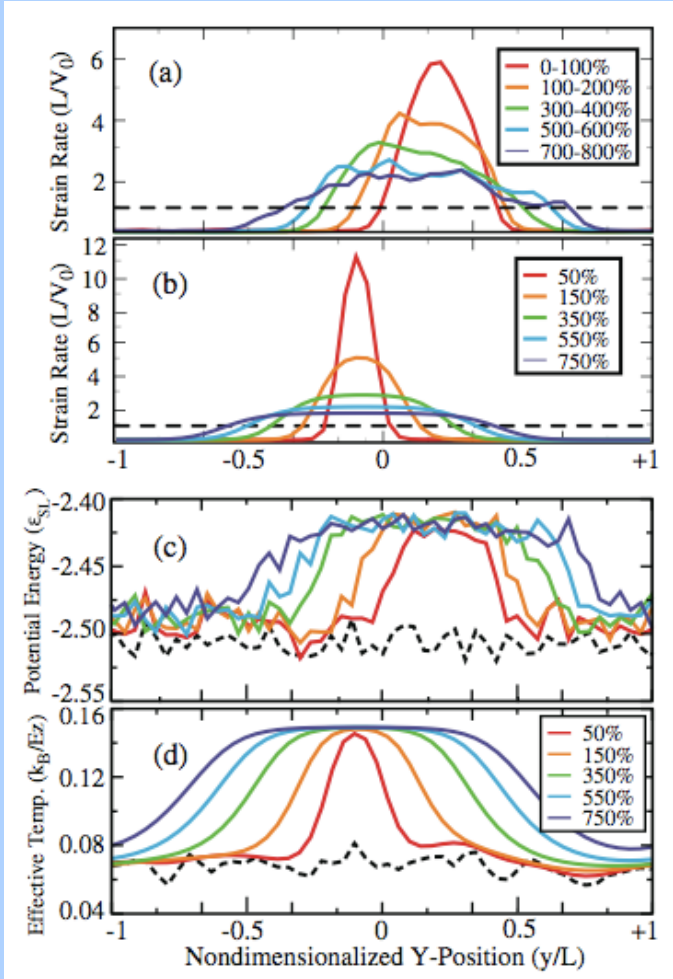
Validating Constitutive Theory

- **We can then develop and test a constitutive law that includes a length scale**

$$\dot{\varepsilon}_{ij}^{pl} = e^{-1/\chi} f_{ij}\left(s_{kl}\right)$$

$$\partial_t \chi - D\partial_x^2 \chi = \frac{2 s_{ij} \dot{\varepsilon}_{ij}^{pl}}{c_0}\left(\chi_\infty - \chi\right)$$





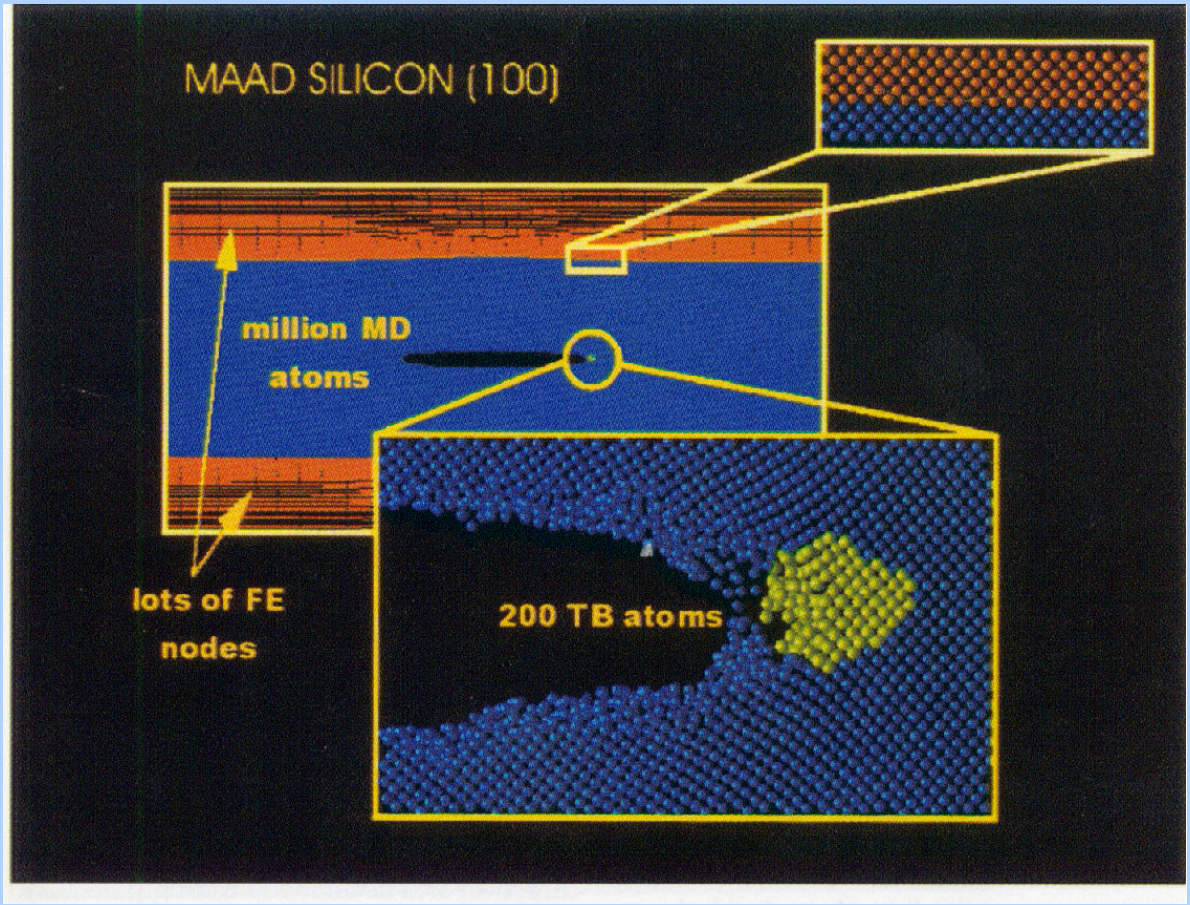
Comparison of theory and atomistics by M Lisa Manning and JS Langer, PRE, 76, 056106(2007)

Hierarchical vs. Concurrent

- This is an example of a **hierarchical** approach to passing information up length scales (atomistics to continuum).
- Simulations are done at each scale independently and cross-validated in overlapping scales.
- New approaches are being developed to model on different scales **concurrently**.
- In such approaches atomistics and continuum (for example) are integrated into a common framework.
- This way continuum calculations can provide boundary conditions for atomistic calculations in particular regions of interest.

Example: Fracture of Silicon

- One appropriate context is fracture of brittle materials, where the process zone is very small.
- Reliable bonding at tip (Tight Binding)
- Atomistic plasticity near tip region (MD)
- Continuum (FEM) boundary condition
- 3 Fundamentally different descriptions



Concurrent FEM/MD/TB simualtion of fracture of silicon by Broughton, Abraham, Bernstein and Kaxiras, Phys. Rev. B60, 2391 (1999)

Challenges of Concurrent Models

- How do you decide where to resolve atomic scale details?
- How do you pass information back and forth without introducing artifacts?
- How do you incorporate not just the atoms, but the underlying physics that arises from atomic dynamics motion?

Atomistic-Continuum Coupling

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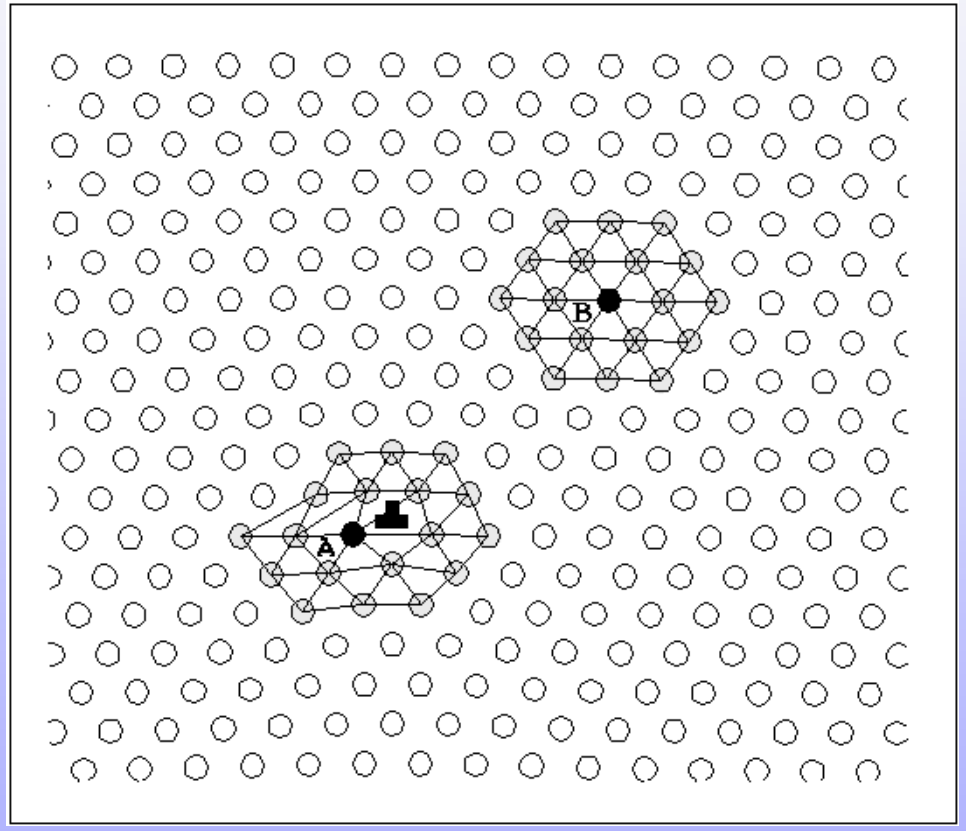
Method	Acronym	Key references	Continuum model	Handshake	Coupling boundary condition	Governing formulation
Quasicontinuum	QC	[45, 53] section 4.1	Cauchy–Born	None	Strong compatibility	Energy-based
Coupling of length scales	CLS	[44] section 4.2	Linear elasticity	None	Strong compatibility	Energy-based
Bridging domain	BD	[60] section 4.3	Cauchy–Born	Linear mixing of energy	Weak compatibility (penalty)	Energy-based
Bridging scale method	BSM	[39, 59] section 4.4	Cauchy–Born	None	Weak/stong mix (least-squares fit)	Energy-based
Composite grid atomistic continuum method	CACM	[10] section 4.5	Linear elasticity	None	Weak compatibility (average atomic positions)	Iterative energy-based (two energy functionals)
Cluster-energy quasicontinuum	CQC(m)-E	[15] section 4.6	Averaging of atomic clusters	None	Strong compatibility	Energy-based
Ghost-force corrected quasicontinuum	QC-GFC	[46] section 4.7.1	Cauchy–Born	None	Strong compatibility	Energy-based with dead load GFC
Ghost-force corrected cluster-energy QC	CQC(m)-GFC	[15] section 4.7.2	Averaging of atomic clusters	None	Strong compatibility	Energy-based with dead load GFC
Finite-element/ atomistics Method	FEAt	[25] section 6.1	non-linear, nonlocal elasticity	None	Strong compatibility	Force-based
Coupled atomistics and discrete dislocations	CADD	[47, 48] section 6.1	Linear elasticity	None	Strong compatibility	Force-based
Hybrid simulation method	HSM	[28] section 6.2	Non-linear elasticity	atomic averaging for nodal B.C.	Weak compatibility (average atomic positions)	Force-based
Concurrent AtC coupling	AtC	[4, 5, 19, 35] section 6.3	Linear elasticity	Linear mixing of stress and atomic force	Strong compatibility	Force-based
Ghost-force corrected concurrent AtC coupling	AtC-GFC	unpublished section 6.3.1	Linear elasticity	Linear mixing of stress and atomic force	Strong compatibility	Force-based
Cluster-force quasicontinuum	CQC(m)-F	[24] section 6.4	Averaging of atomic clusters	None	Strong compatibility	Force-based

Miller and Tadmor, "A unified framework and performance benchmark of fourteen multiscale atomistic/continuum coupling methods," Modeling and Simulation in Materials Science and Engineering, Vol. 17, 053001 (2009)

I will discuss Quasi-continuum.

I refer you to this paper if you wish to learn about the similarities and differences of other models.

Quasicontinuum Philosophy

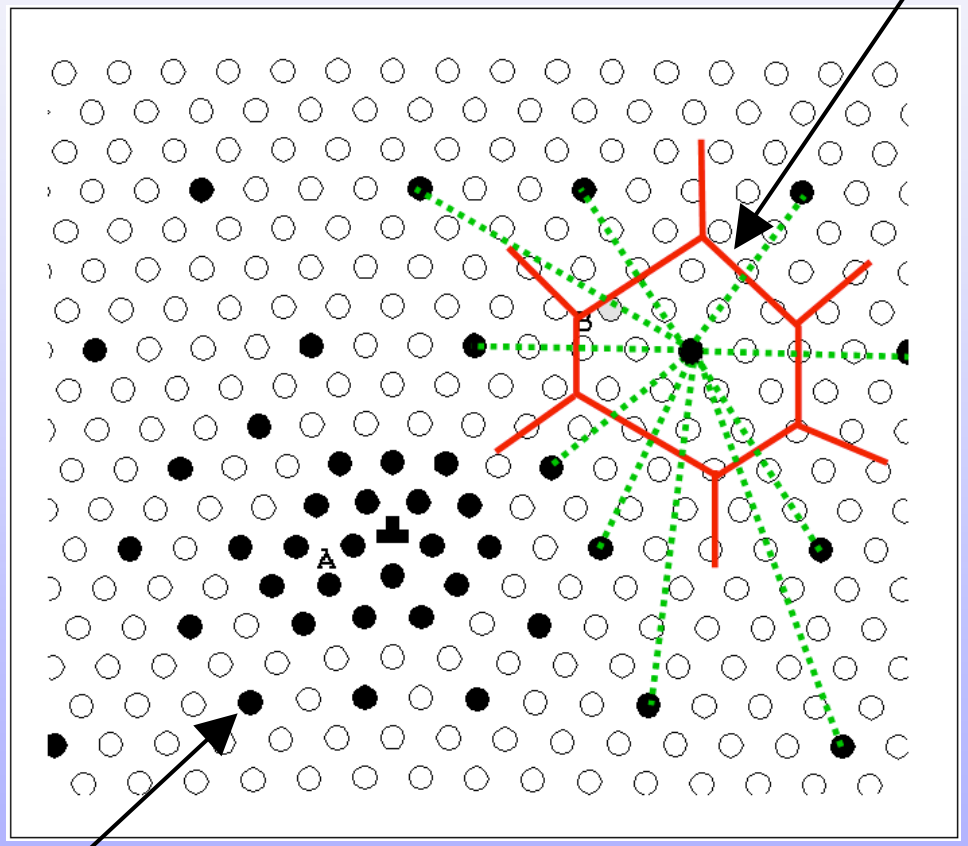


- Environment of core atom A is highly distorted and non-uniform.
- At the same time, far atom B sees a nearly homogeneous environment.
- Many atoms in the vicinity of B experience environments very similar to it, while each atom near A is unique.

REF: Tadmor, Ortiz and Phillips, *Phil. Mag. A*, **73**, 1529-1563 (1996).
Shenoy, Miller, Tadmor, Rodney, Phillips, Ortiz, *JMPS*, **47**, 611 (1999).

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Representative Atoms



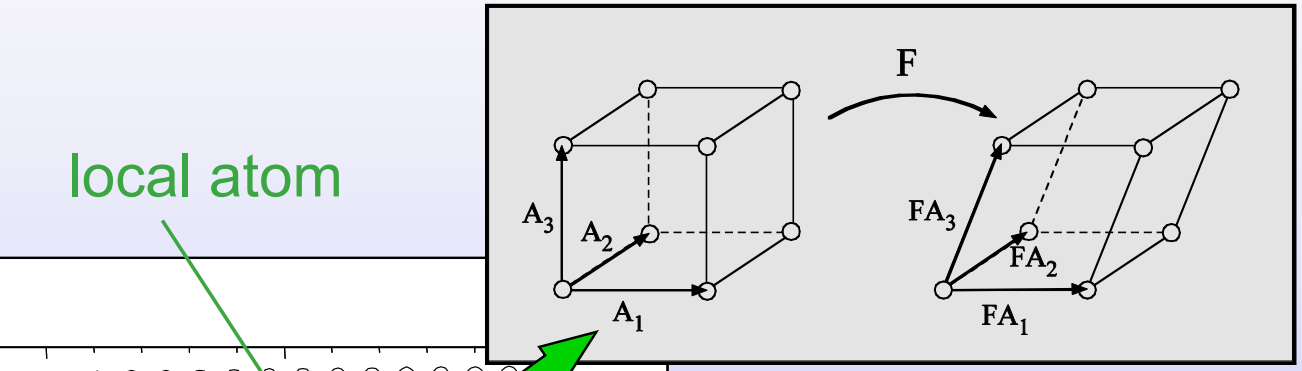
$$E_{\text{tot}} = \sum_{i=1}^{N} E_i$$

$$E_{\text{tot}} \approx \sum_{i=1}^{N_R} n_j E_j$$

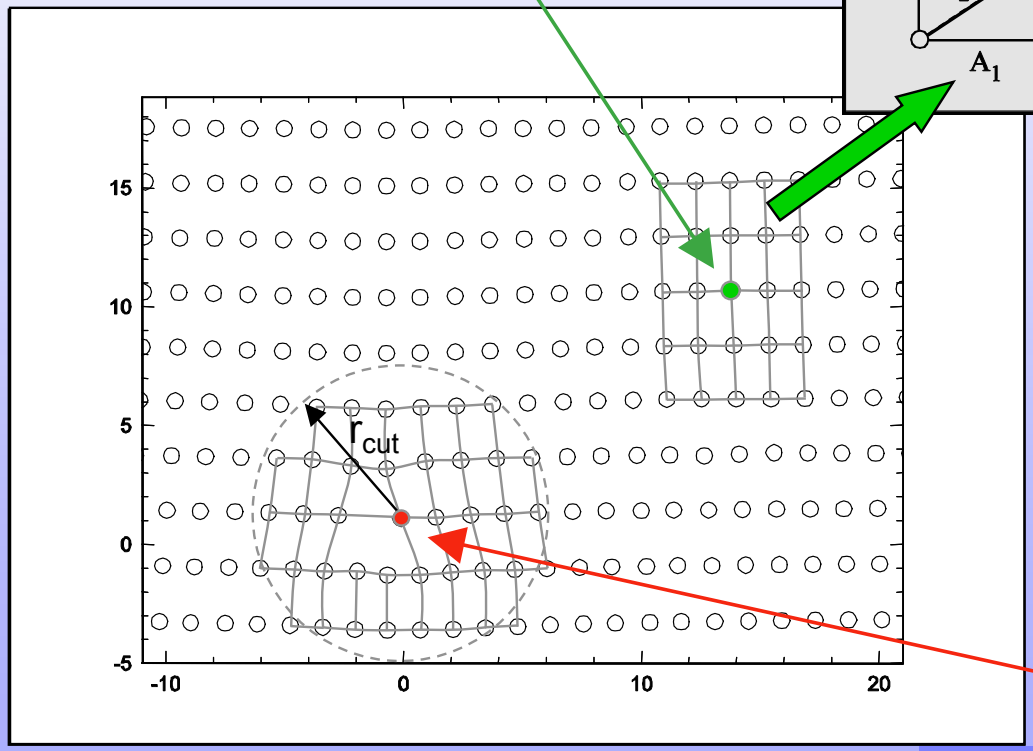
where N_R << N
is the number of
Representative Atoms

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Local vs Non-Local Representation



local atom



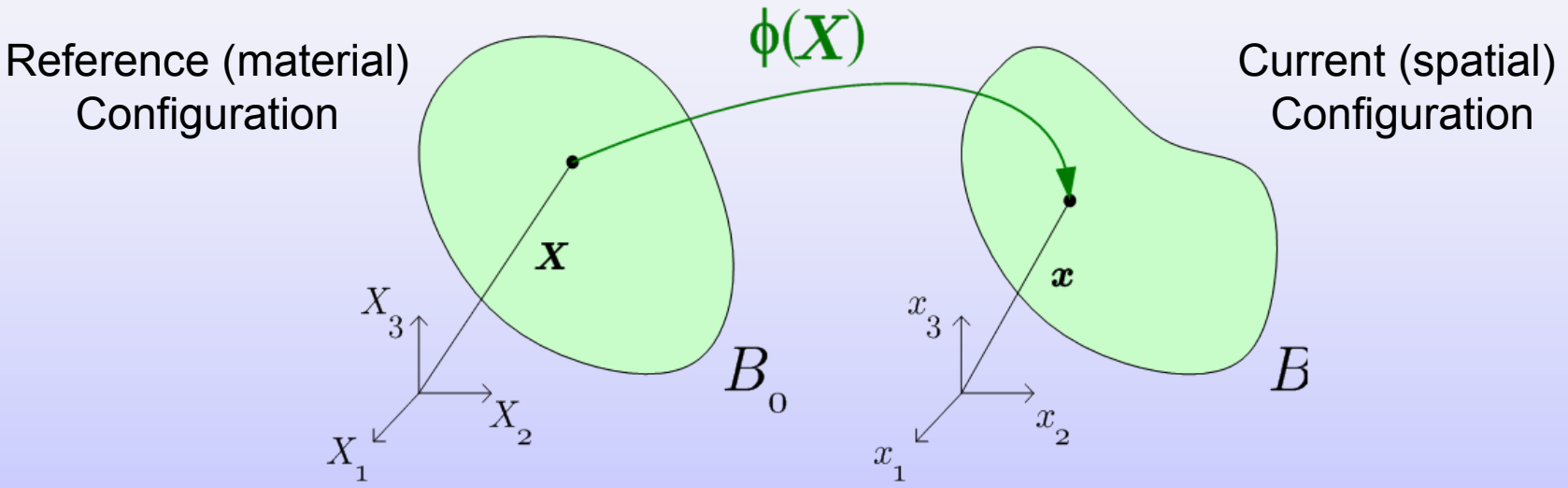
Cauchy-Born Rule

$$E_i^{NL} = \frac{1}{2}\sum_{j \neq i} \phi(r_{ij}) + U_i(\rho_i)$$

nonlocal atom

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Kinematics: Deformation Mapping



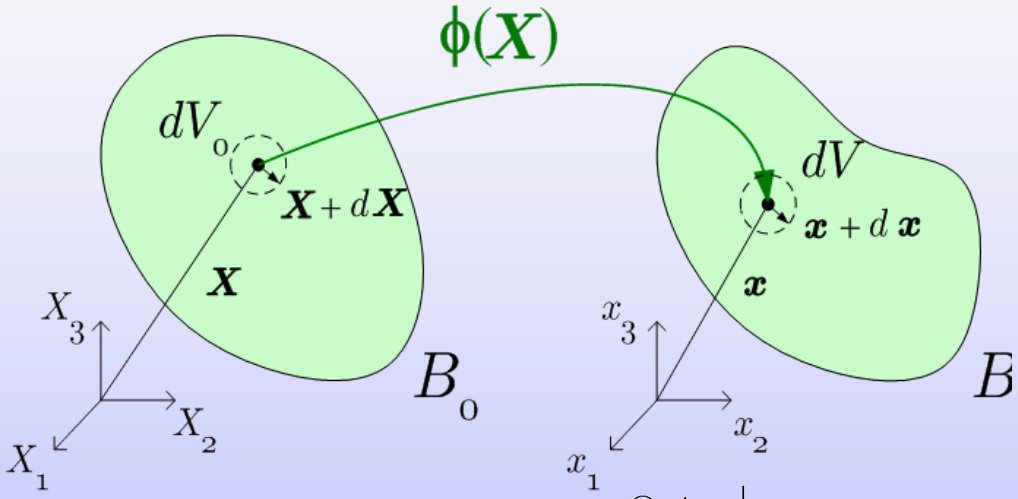
$$x_i = \phi_i(X_1, X_2, X_3)$$

Deformation Mapping

Convention: Capitals letters → reference config
Small-case → current config

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Kinematics: Deformation Gradient



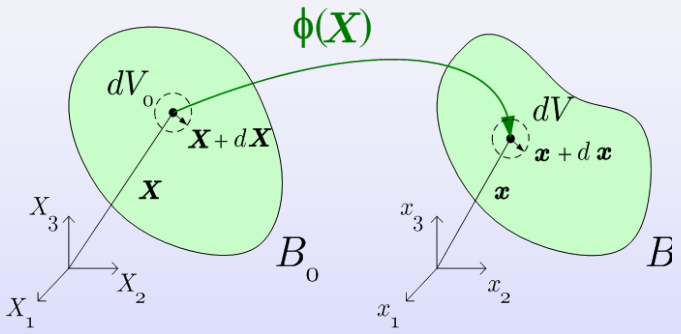
$$x_i + dx_i = \phi_i(\mathbf{X}+d\mathbf{X}) \approx \underbrace{\phi_i(\mathbf{X})}_{x_i} + \underbrace{\left.\frac{\partial \phi_i}{\partial X_J}\right|_{\mathbf{X}}}_{F_{iJ}} dX_J + \text{h.o.t.}$$

F_{iJ} ≡ Deformation Gradient

$$dx_i = F_{iJ} dX_J; \quad F_{iJ} = \frac{\partial \phi_i}{\partial X_J} = \frac{\partial x_i}{\partial X_J}$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Kinematics: Deformation Gradient



$$dx_i = F_{iJ} dX_J; \quad F_{iJ} = \frac{\partial \phi_i}{\partial X_J} = \frac{\partial x_i}{\partial X_J}$$

$(*)$

Notes:

•Eq $(*)$ exactly characterizes the deformation in the infinitesimal vicinity of $\mathbf{X}$.

•If ϕ is homogeneous, $\mathbf{F}$ exactly characterizes the deformation everywhere:

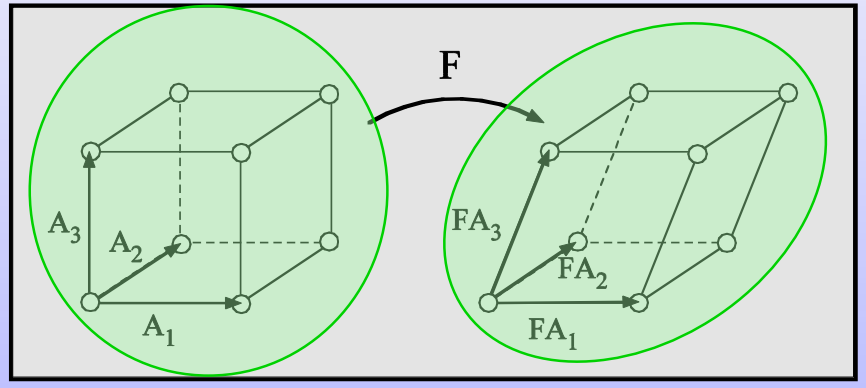
$$\mathbf{x} = \mathbf{F}\mathbf{X} + \mathbf{C}$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Cauchy-Born Rule

Cauchy-Born Rule: *Atoms are mapped according to the continuum deformation field.*

Point in Reference Configuration



Point in Current Configuration

$$W(\mathbf{F}) = \frac{1}{\Omega_0} E_{\text{atom}}(\mathbf{F})$$

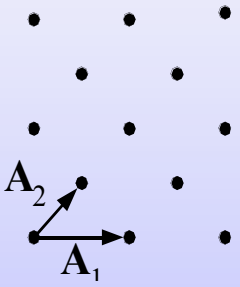
strain energy density

atomic volume

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Cauchy-Born Rule

➔ The coordinates of the atoms in the reference configuration are defined in terms of a simple Bravais lattice:

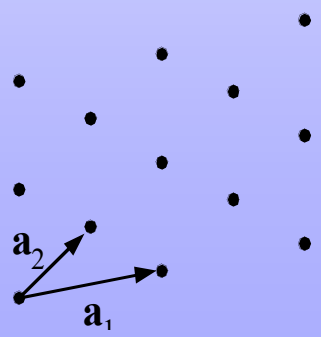


$$\mathbf{X}(\mathbf{m}) = m_i \mathbf{A}_i$$

Triplet of integers

Bravais Vectors

➔ According to the Cauchy-Born rule, the coordinates in the current configuration are:



$$\begin{aligned} \mathbf{x}(\mathbf{m}) &= \mathbf{F}\mathbf{X}(\mathbf{m}) \\ &= m_i(\mathbf{F}\mathbf{A}_i) \\ &= m_i \mathbf{a}_i \end{aligned}$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Cauchy-Born Rule

➔ In a simple Bravais lattice all atoms are equivalent.

➔ The EAM strain energy density of an atom in the deformed lattice is:

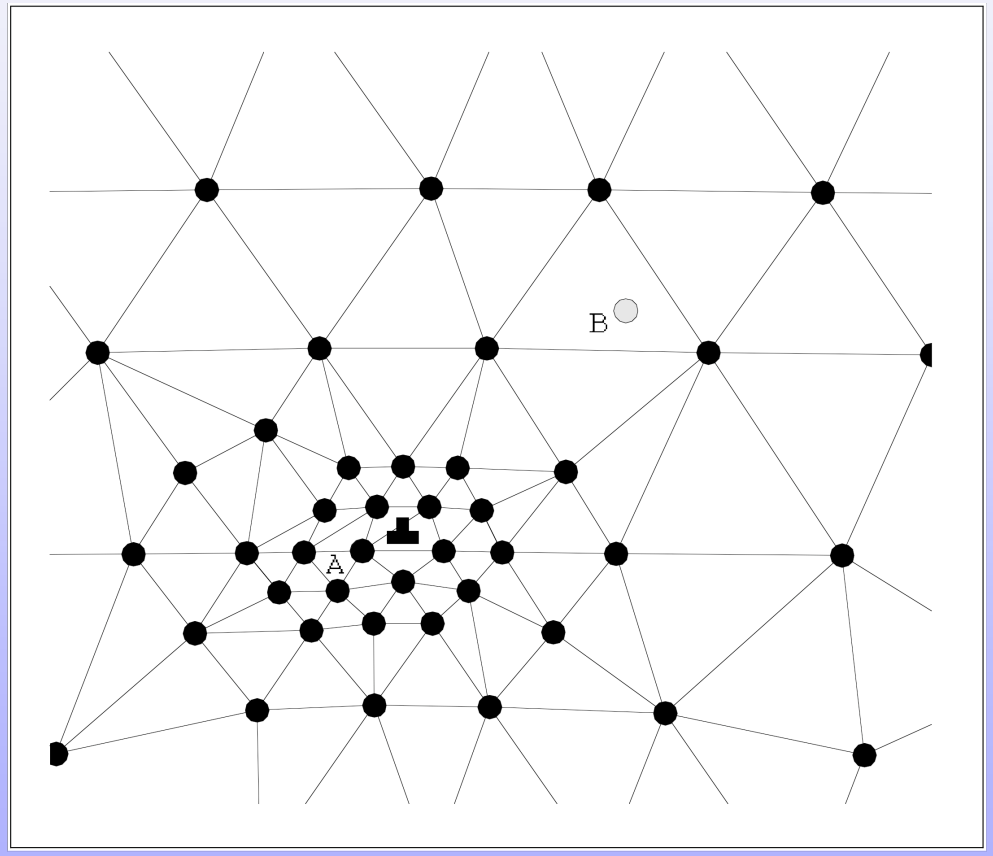
$$W(\mathbf{F}) = \frac{1}{\Omega_0}\left\{\frac{1}{2}\sum_{\mathbf{m}}\phi(r^{\mathbf{m}}) + U\left(\sum_{\mathbf{m}} f(r^{\mathbf{m}})\right)\right\}$$

where $r^{\mathbf{m}} = |\mathbf{x}(\mathbf{m})| = |\mathbf{F}\mathbf{X}(\mathbf{m})|$

NOTE: *The above expression is only correct for simple Bravais lattices.*
For complex Bravais lattices, off-site atom shuffles must be accounted for.
See: Tadmor et al., *Phys. Rev. B*, **59**, 235-245 (1999).

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Finite Element Formulation



- Define FEM mesh with nodes corresponding to rep atoms.

- Coordinates of non-rep atoms obtained through FEM interpolation:

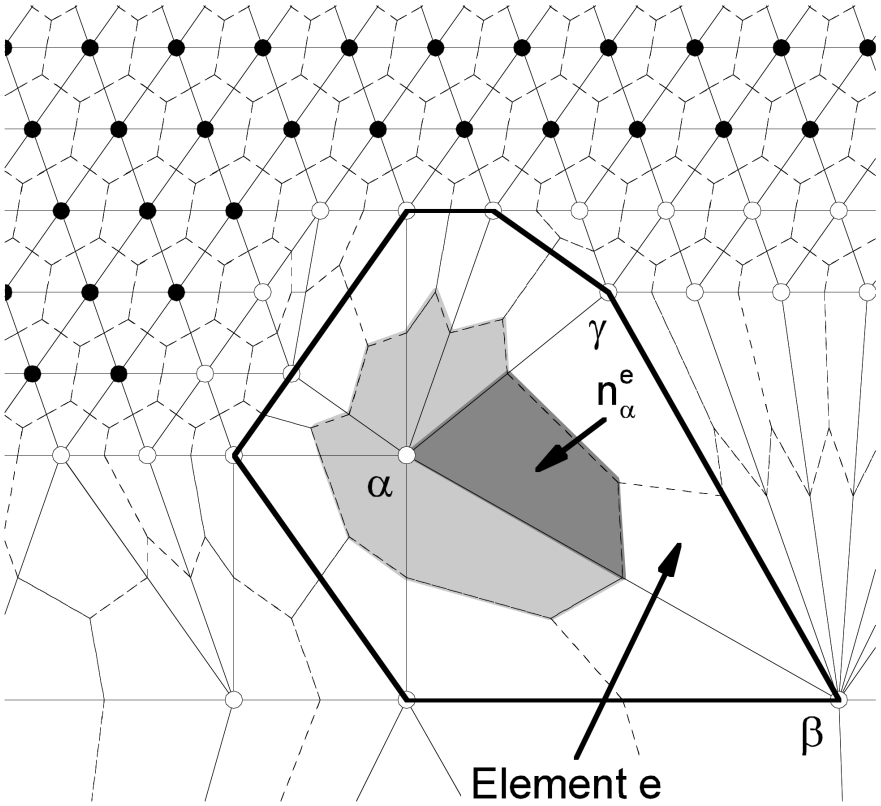
$$\mathbf{u}_h(\mathbf{X}) = \sum_j \mathbf{u}_j N_j(\mathbf{X})$$

- Deformation gradients within each element are computed from FEM shape functions:

$$\mathbf{F}_h(\mathbf{X}) = \mathbf{I} + \sum_j \mathbf{u}_j \nabla_0 N_j(\mathbf{X})$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

QC Potential Energy



$$\Pi_h(\{\mathbf{u}\}) = \sum_{\alpha=1}^{N_{NL}} E_\alpha^{NL}(\mathbf{u}_1,\ldots,\mathbf{u}_{N_R}) + \sum_{\beta=1}^{N_L} n_\beta E_\beta^L(\mathbf{F}_1,\ldots,\mathbf{F}_M) - \sum_{\gamma=1}^{N_R} \bar{\mathbf{f}}_\gamma \cdot \mathbf{u}_\gamma$$

where

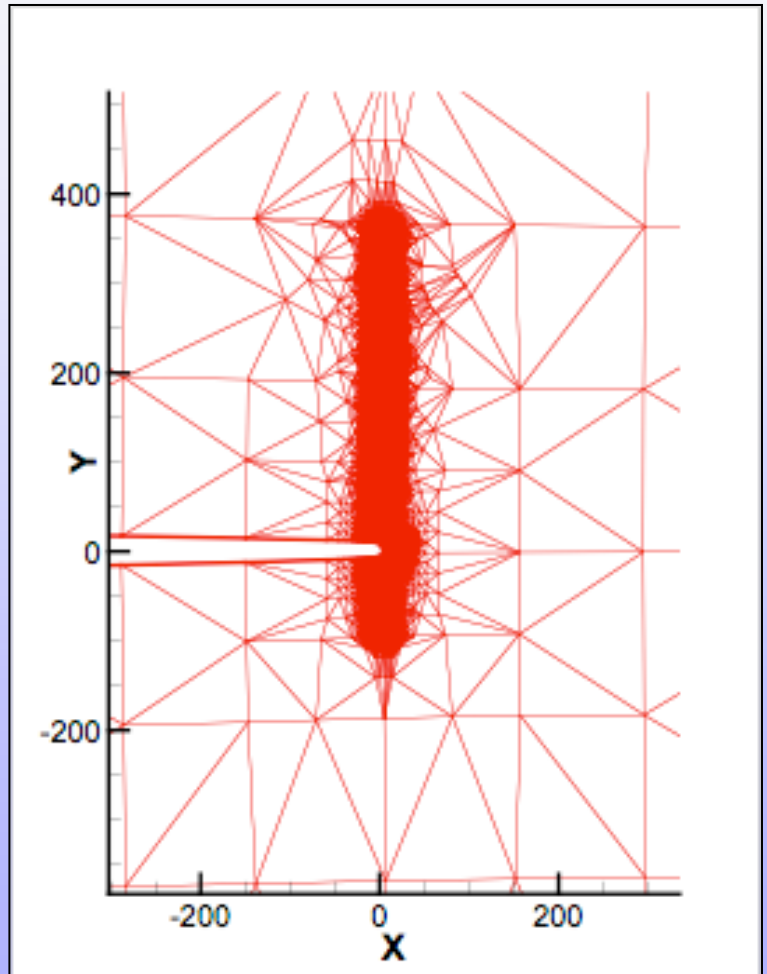
number of atoms in element e represented by atom β

$$E_\beta^L = \Omega_0 \sum_{e=1}^{M} \frac{n_\beta^e}{n_\beta} W(\mathbf{F}_e)$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

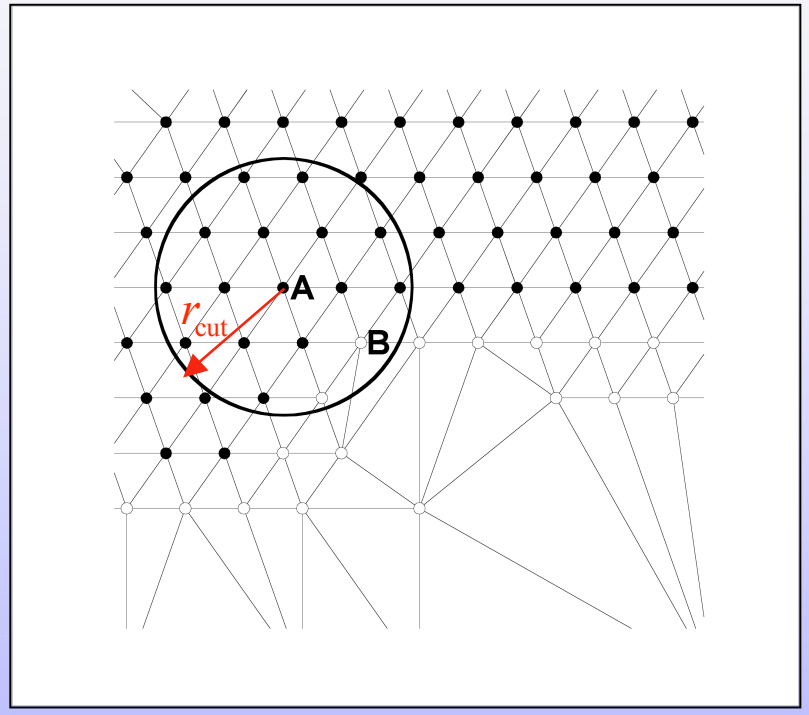
Issue 1: Ghost Forces

- Typical deformations lead to QC models that consist of well-defined nonlocal regions surrounded by local regions.
- Thus, there is typically an "interface" between atomistic and continuum regions.
- The hybrid energy functional used in the QC leads to spurious effects in the interface region.



Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Ghost Forces



$$\frac{\partial E_A^{NL}}{\partial \mathbf{u}_B} \neq 0$$

Motion of B affects energy of A

$$\frac{\partial E_B^{L}}{\partial \mathbf{u}_A} = 0$$

Motion of A does not affect energy of B

Force imbalance

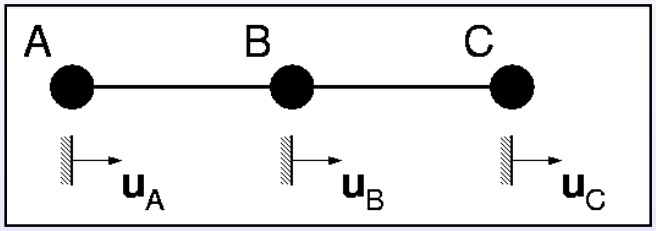
Ghost forces ~ 0.1 eV/Å
0.05 eV/atom energy noise

In finite element language this is equivalent to stating that the method does not satisfy the patch test.

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Ghost Forces: 2nd Neighbor Chain

Fully Nonlocal



$$\Pi = E_A^{NL}(u_A, u_B, u_C) + E_B^{NL}(u_A, u_B, u_C) + E_C^{NL}(u_A, u_B, u_C)$$

$$-f_A = \frac{\partial \Pi}{\partial u_A} = \frac{\partial E_A^{NL}}{\partial u_A} + \frac{\partial E_B^{NL}}{\partial u_A} + \frac{\partial E_C^{NL}}{\partial u_A}$$

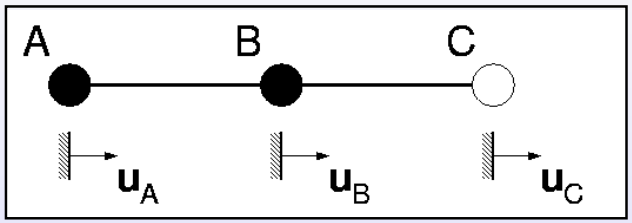
$$-f_B = \frac{\partial \Pi}{\partial u_B} = \frac{\partial E_A^{NL}}{\partial u_B} + \frac{\partial E_B^{NL}}{\partial u_B} + \frac{\partial E_C^{NL}}{\partial u_B}$$

$$-f_C = \frac{\partial \Pi}{\partial u_C} = \frac{\partial E_A^{NL}}{\partial u_C} + \frac{\partial E_B^{NL}}{\partial u_C} + \frac{\partial E_C^{NL}}{\partial u_C}$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Ghost Forces: 2nd Neighbor Chain

Local/Nonlocal



$$F_{BC} = 1 + \frac{u_C - u_B}{L_{BC}}$$

$$\Pi = E_A^{NL}(u_A, u_B, u_C) + E_B^{NL}(u_A, u_B, u_C) + E_C^{L}(F_{BC})$$

$$-f_A = \frac{\partial \Pi}{\partial u_A} = \frac{\partial E_A^{NL}}{\partial u_A} + \frac{\partial E_B^{NL}}{\partial u_A} + \frac{\partial E_C^{NL}}{\partial u_A}$$

$$-f_B = \frac{\partial \Pi}{\partial u_B} = \frac{\partial E_A^{NL}}{\partial u_B} + \frac{\partial E_B^{NL}}{\partial u_B} + \frac{\partial E_C^{L}}{\partial F_{BC}} \frac{\partial F_{BC}}{\partial u_B} + \frac{\partial E_C^{NL}}{\partial u_B}$$

$$-f_C = \frac{\partial \Pi}{\partial u_C} = \frac{\partial E_A^{NL}}{\partial u_C} + \frac{\partial E_B^{NL}}{\partial u_C} + \frac{\partial E_C^{L}}{\partial F_{BC}} \frac{\partial F_{BC}}{\partial u_C}$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Eliminating Ghost Forces

SOLUTION: Correct forces so that force acting on any atom is computed using only the formulation that corresponds to its status.

This can be done in two ways:

- *"Force-based" QC Formulation (force mixing)*
  - Force on a local atom is computed as if all of its neighbors are local
  - Force on a nonlocal atom computed as if all of its neighbors are nonlocal.
  - Problem: there is no longer an energy functional to minimize. Must resort to methods to drive forces to zero.

- Keep "Energy-based" Formulation with "Ghost force Correction"
  - Add on external deadloads that cancel the ghost forces
  - A well-defined energy is retained for the purpose of finding equilibrium.
  - Other methods involving special interface atoms (e.g. quasinonlocal) have been developed.

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Ghost Force Correction

- To maintain a well-defined energy functional:
  - compute the initial ghost forces and assume that they remain constant.
  - apply the negative of these forces as "dead loads" so that the energy functional becomes:

$$\tilde{\Pi}_h(\{\mathbf{u}\}) = \Pi_h(\{\mathbf{u}\}) - \sum_{\gamma} \mathbf{f}_{\gamma}^{G} \cdot \mathbf{u}_{\gamma}$$

- Can periodically update ghost forces as minimization proceeds.
- Somewhat *ad hoc*, but yields an acceptable compromise between accuracy and efficiency.

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Ghost Forces: 2nd Neighbor Chain

$$
\begin{aligned}
-f_A &= \frac{\partial \Pi}{\partial u_A} = \frac{\partial E_A^{NL}}{\partial u_A} + \frac{\partial E_B^{NL}}{\partial u_A} + \frac{\partial E_C^{NL}}{\partial u_A} \\
-f_B &= \frac{\partial \Pi}{\partial u_B} = \frac{\partial E_A^{NL}}{\partial u_B} + \frac{\partial E_B^{NL}}{\partial u_B} + \frac{\partial E_C^{L}}{\partial F_{BC}}\frac{\partial F_{BC}}{\partial u_B} + \frac{\partial E_C^{NL}}{\partial u_B} \\
-f_C &= \frac{\partial \Pi}{\partial u_C} = \frac{\partial E_A^{NL}}{\partial u_C} + \frac{\partial E_B^{NL}}{\partial u_C} + \frac{\partial E_C^{L}}{\partial F_{BC}}\frac{\partial F_{BC}}{\partial u_C}
\end{aligned}
$$

$$
\tilde{\Pi} = \Pi + \left(\frac{\partial E_C^{NL}}{\partial u_A}\right) u_A + \left(-\frac{\partial E_C^{L}}{\partial u_B} + \frac{\partial E_C^{NL}}{\partial u_B}\right) u_B + \left(-\frac{\partial E_A^{NL}}{\partial u_C} - \frac{\partial E_B^{NL}}{\partial u_C}\right) u_C
$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Quasicontinuum Formulation

The modified QC potential energy is:

$$\tilde{\Pi}_h(\{\mathbf{u}\}) = \sum_{\alpha=1}^{N_{NL}} E_\alpha^{NL}(\{\mathbf{u}_i\}) + \sum_{\beta=1}^{N_L} n_\beta E_\beta^{L}(\{\mathbf{F}_e\}) - \sum_{\gamma=1}^{N_R} (\bar{\mathbf{f}}_\gamma + \mathbf{f}_\gamma^G)\cdot\mathbf{u}_\gamma$$

Substituting in the local atom energy and rearranging:

$$\tilde{\Pi}_h(\{\mathbf{u}\}) = \sum_{\alpha=1}^{N_{NL}} E_\alpha^{NL}(\{\mathbf{u}_i\}) + \Omega_0 \sum_{e=1}^{M} \nu_e W(\mathbf{F}_e) - \sum_{\gamma=1}^{N_R} (\bar{\mathbf{f}}_\gamma + \mathbf{f}_\gamma^G)\cdot\mathbf{u}_\gamma$$

Total number of rep atoms falling inside element e

$$\nu_e = \sum_{\beta=1}^{N_L} n_\beta^e$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Energy Minimization

➔ Equilibrium configurations are associated with minimizers of the potential energy subject to kinematic constraints:

$$\min_{\mathbf{u}_i} \tilde{\Pi}_h(\mathbf{u}_1, \ldots, \mathbf{u}_{N_R}) \quad \Rightarrow \quad \text{EQUILIBRIUM}$$

➔ The energy is minimized using one of two methods:

- Conjugate Gradients (CG)
- Newton Raphson (NR)

➔ Minimization requires gradients of the potential energy

- CG : First gradient
- NR : First and second gradients

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

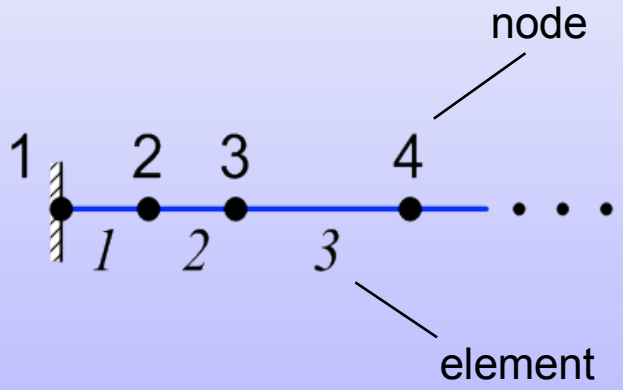
Example: 1D Lennard-Jones Chain

➔The QC potential energy for the 1D chain is

$$\tilde{\Pi}_h(\{\mathbf{u}\}) = \sum_{i=1}^{N_R} E_i \; - \; \sum_{\gamma=1}^{N_R} (\bar{f}_\gamma + f_\gamma^G) u_\gamma$$

where

$$\begin{cases} \dfrac{1}{2}\displaystyle\sum_{j \neq i} \phi(r_{ij}) & \text{if } i \text{ is nonlocal} \\ \dfrac{h_{i-1}}{2} W(F_{i-1}) + \dfrac{h_i}{2} W(F_i) & \text{if } i \text{ is local} \end{cases}$$



$$r_{ij} = |X_j + u_j - X_i - u_i| \qquad h_i = X_{i+1} - X_i \qquad F_i = 1 + \frac{u_{i+1} - u_i}{h_i}$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Example: 1D Lennard-Jones Chain

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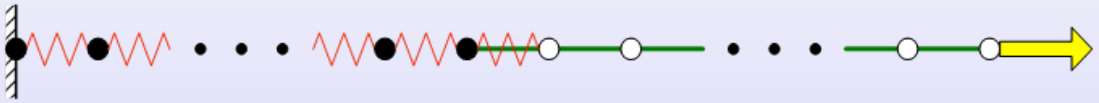
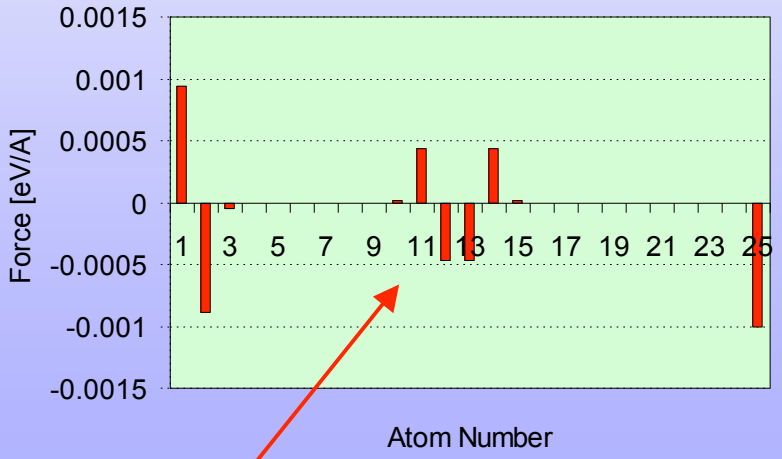
➔Half nonlocal – Half local chain (no ghost-force correction)

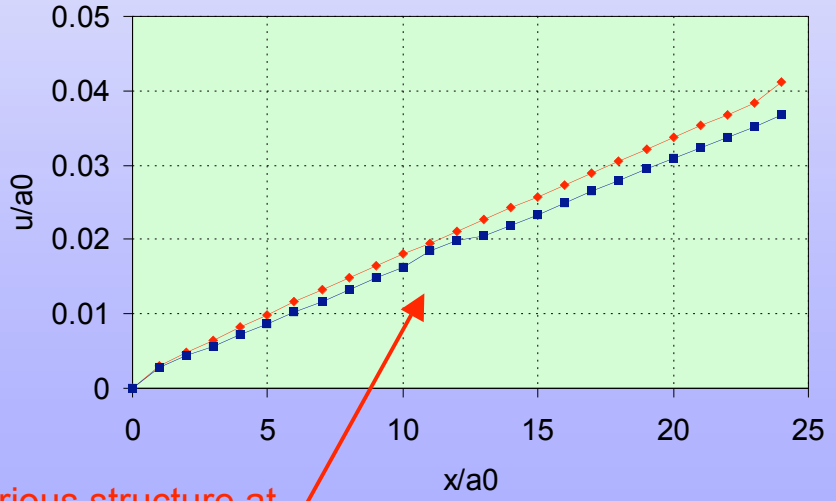


Initial out-of-balance force



ghost forces

Final Axial Displacement



spurious structure at local-nonlocal interface

$err = 4.29 \times 10^{-4}$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

Example: 1D Lennard-Jones Chain

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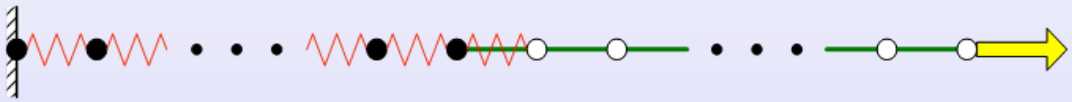
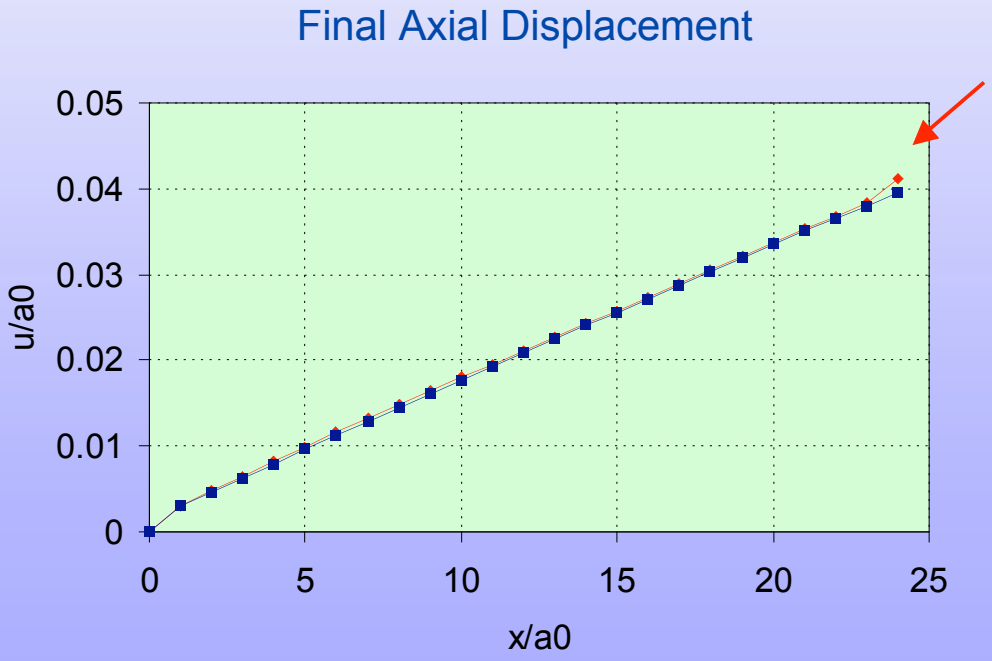
➔Half nonlocal – Half local chain (with ghost-force correction)





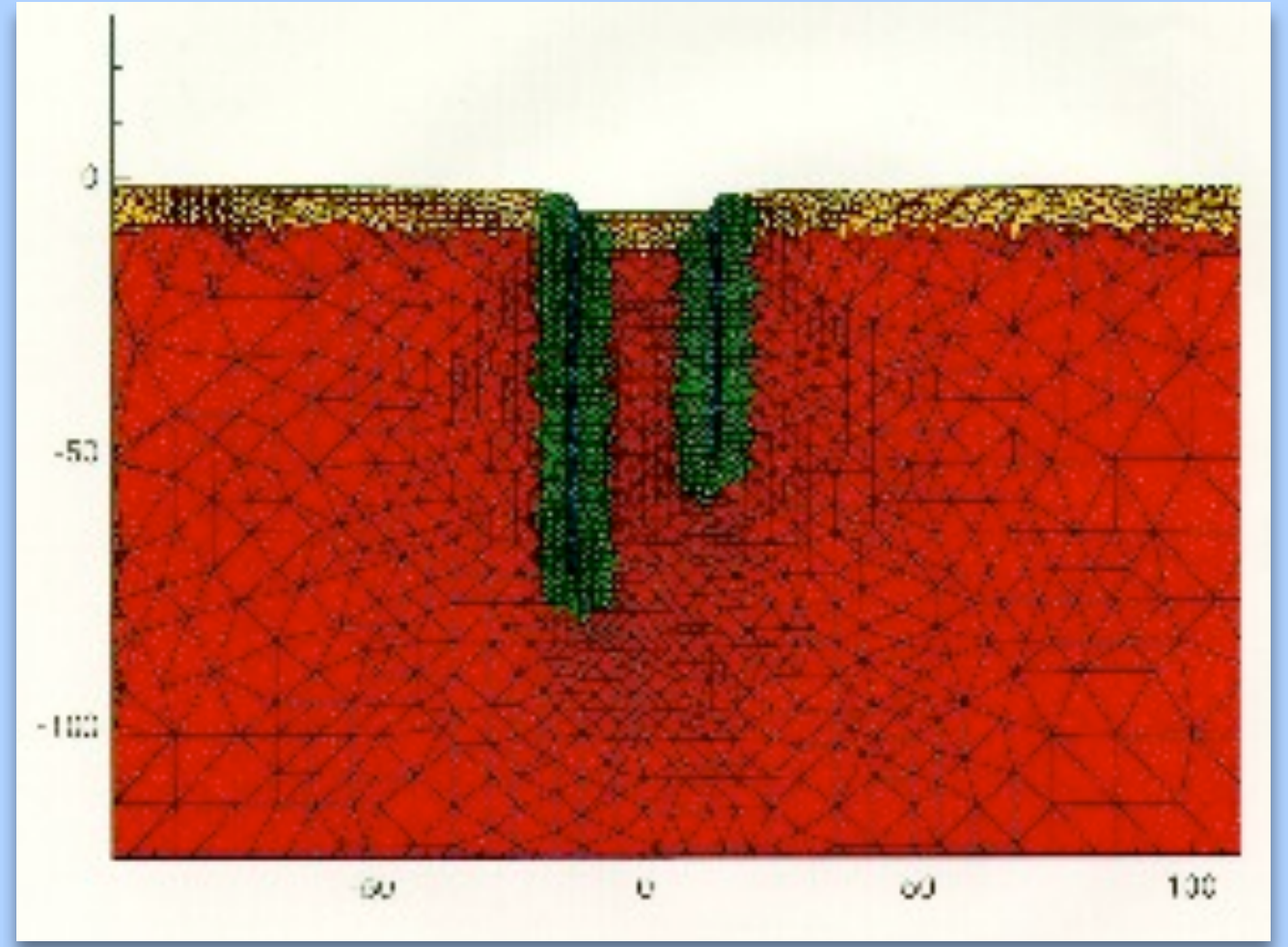
at local end model cannot resolve surface structure

- With ghost-force correction excellent agreement is obtained with exact results.
- error:

$$\text{err} = \frac{1}{N}\left[\sum_{i=1}^{N}(u_i^{\text{aprx}} - u_i^{\text{exact}})^2\right]^{1/2} = 8.48 \times 10^{-5}$$

Adapted from E. Tadmor Multiscale Methods for Materials Science, Paris, June 25 – July 5, 2007.

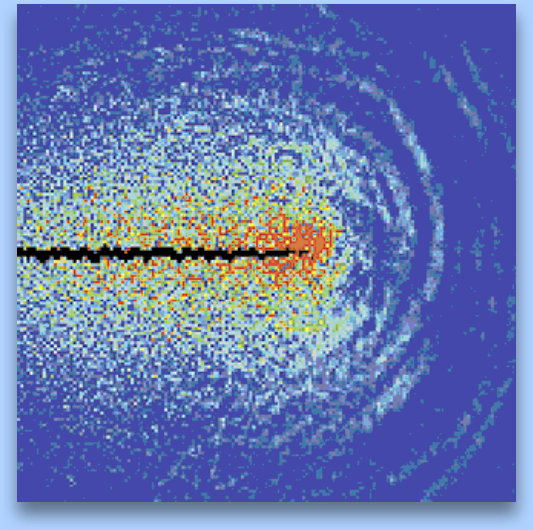
Application of Quasicontinuum



Nanoindentation of an aluminum thin film by
Tadmor, Miller, Phillips and Ortiz

Issue 2: Dynamics

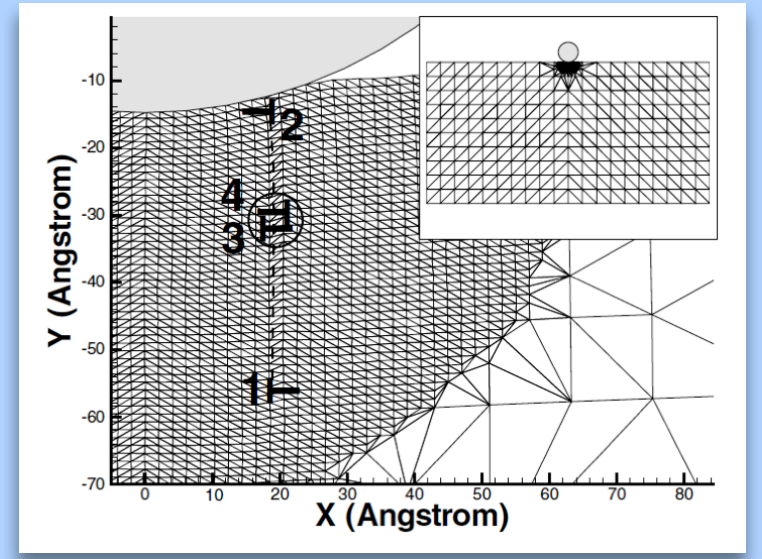
- The Quasicontinuum method, like much of continuum mechanics, works on a fundamental assumption that energy is minimized and changes to the system occur only due to changes in external loads, typically applied at the boundary.
- If we include inertia, sound waves arise.
- Elastic waves mediate communication between regions of the material+boundaries.
- The sound speed is a material parameter, but waves come in a range of wavelengths.
- Large elements cannot resolve short wavelength modes, and so reflect them.

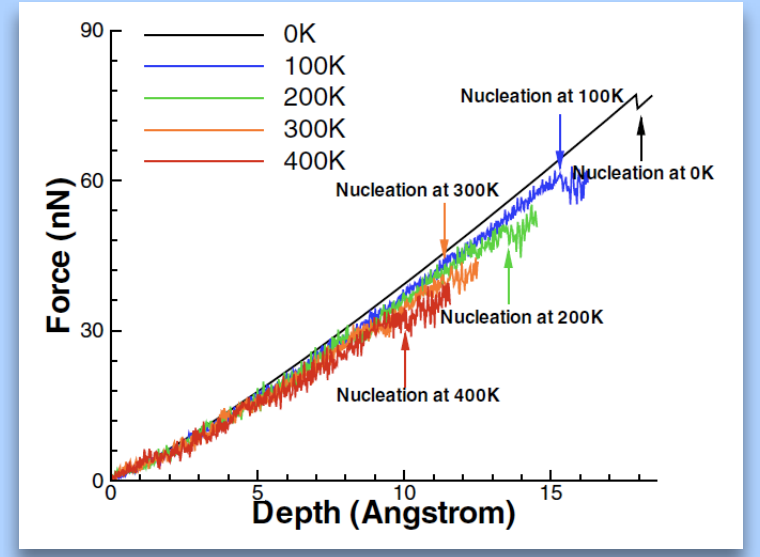


Sound waves in front of a crack simulated by MD in a quasicrystal, Hans-Rainer Trebin

Issue 3: Temperature

- In addition, but considering potential energy, but ignoring thermal fluctuations we are making a local equilibrium assumption and ignoring the effects of entropy/temperature, i.e. free energy.
- Methods have been developed to incorporate equilibrium thermal effects into quasicontinuum, but not heat transport.

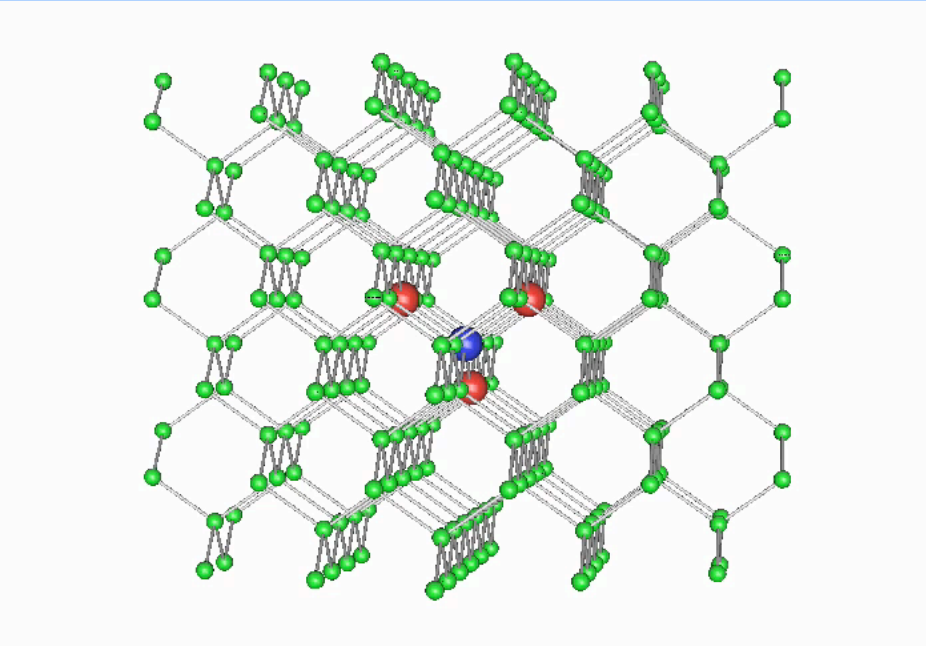




Dupuy, Tadmor, Miller, Phillips,
Phys. Rev. Lett., 95, 060202 (2005)

Issue 4: Activated Processes

- Finally, the equilibrium assumption precludes long time scale processes such as viscous relaxation and thermally induced mass transport.
- These processes occur because thermal fluctuations permit the system to explore a range of configurations, particularly in systems with defects or disorder.



Diffusion of arsenic (red) due to a vacancy (blue) in silicon by Puchala, Garikipati and Falk.

Problem of Time Scales

- This quite general problem that physical processes are often going on at several different time scales is perhaps the most daunting.
- This will be the subject of the next lecture.

Stay Tuned!