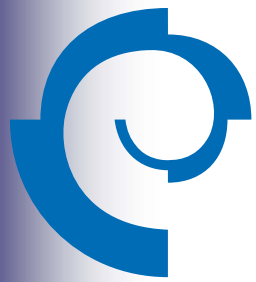
Concurrent scale coupling techniques: From nano to macro

Lecture 3



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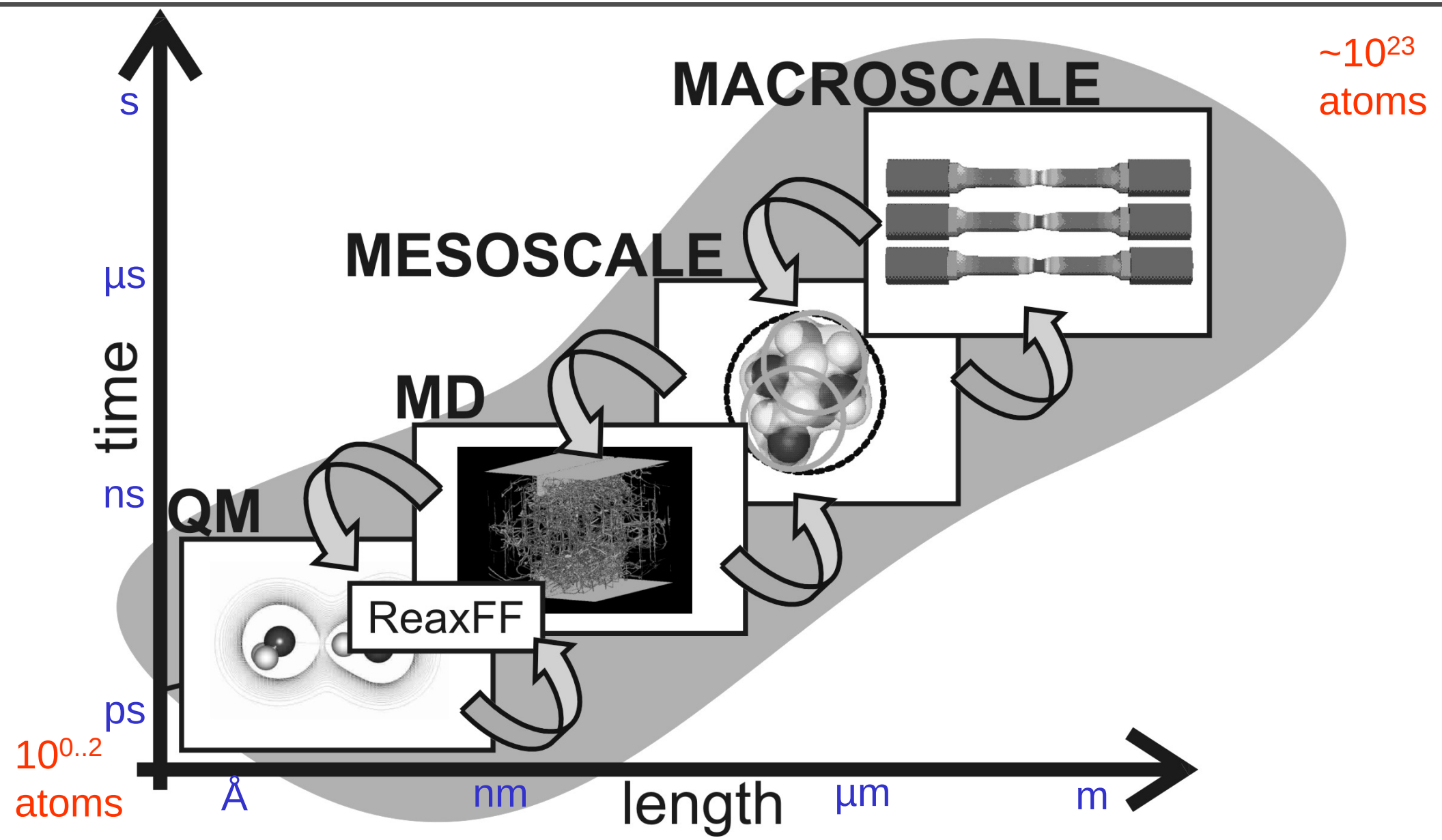
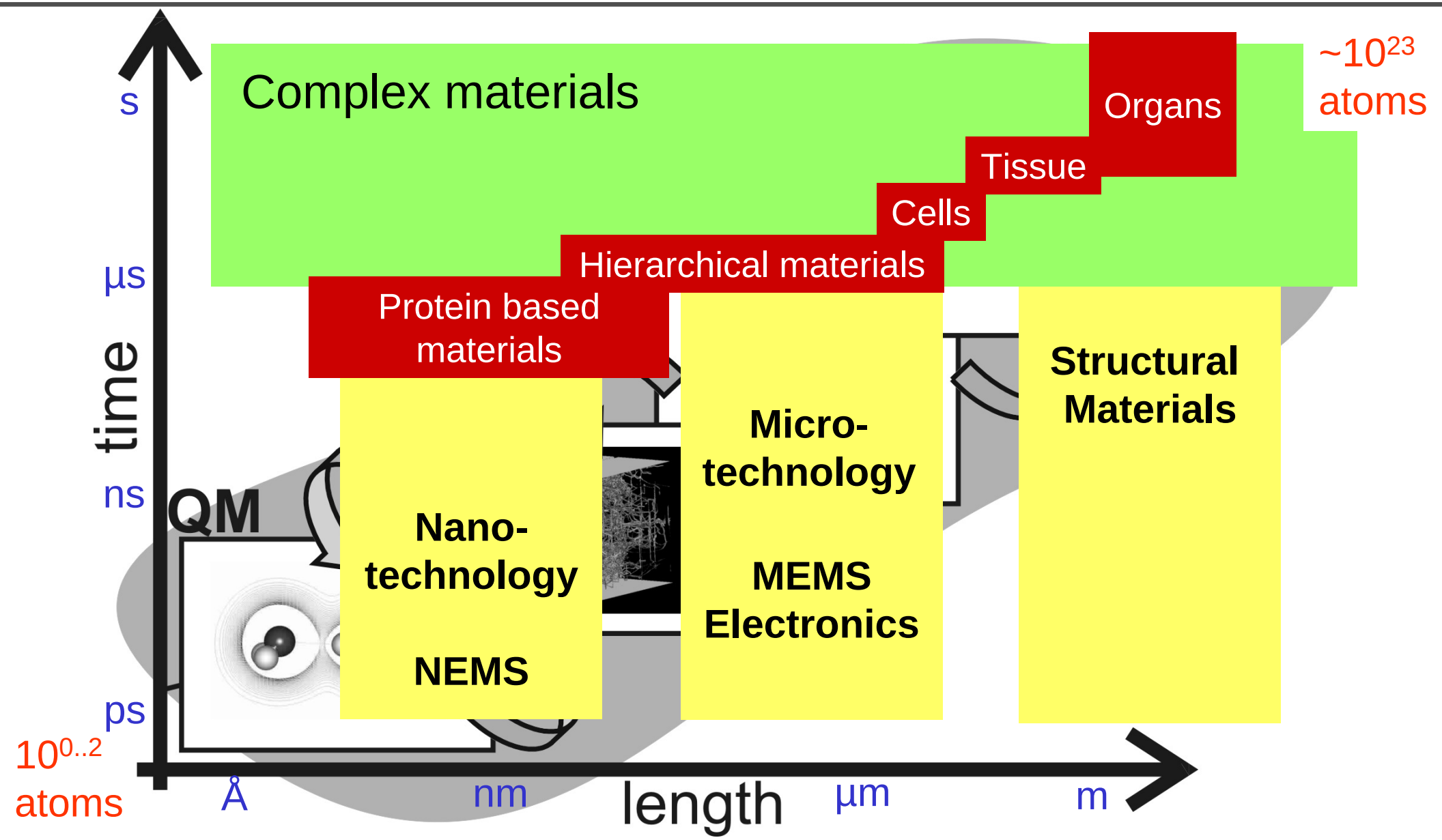
Markus J. Buehler

Challenges: Modeling engineering materials



Modeling complex materials is challenging: Need new modeling techniques

Challenges: Modeling engineering materials



Modeling complex materials is challenging: Need new modeling techniques

The vision for multi-scale modeling

- **Long-standing dream**
  Calculate macroscopic properties of materials by theoretical modeling or computer simulation from a very fundamental, *ab initio* perspective

- Strategy to solve this problem is to use methods based on distinct paradigms, operating at different scales

- This progress is possible with
  - The advent of efficient and accurate quantum mechanical methods (e.g. DFT),
  - Development of new empirical and semi-empirical potentials (EAM, ReaxFF…),
  - Enormous growth of computing power enabling studies with billions of particles.

- **Critical**: Breakthroughs in scale coupling techniques (e.g. QC method) and analysis methods for complex systems (centrosymmetry technique)

Vision: Atomistic simulations of engineering properties at macroscopic scales to 1) understand fundamental mechanisms in materials (e.g. deformation, assembly), and to 2) predict properties of new materials to design new materials

Definition of multi-scale modeling

- Multi-scale computational modeling aims at developing systematic techniques for bridging scales, for example between atomistic models and continuum models, in order to increase the speed of, or enable dynamical calculations

- Payoff:
  - Continuum level models can simulate large volumes of material, typically at the expense of accuracy
  - Conversely, nanoscale models can accurately capture small-scale features, but are computationally too slow to simulate large (useful) volumes of material

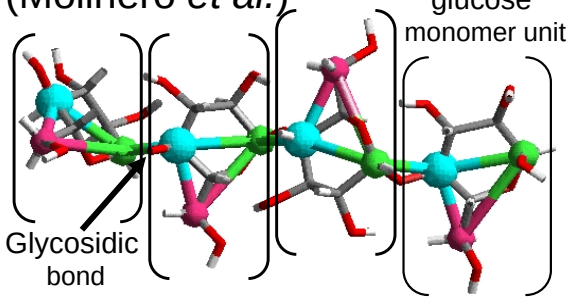
- The goal of multi-scale modeling is to take advantage of the fact that in many systems, only a small percentage of the total region is of interest.

- Main challenges in multi-scale modeling:
  - Determining which regions are simulated with a continuum model or a nanoscale model,
  - Adequately model the transition region.

S. Prudhomme, JP. Bauman and T. Oden

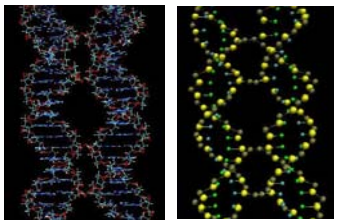
Concurrent versus hierarchical multi-scale simulations

(Molinero *et al.*)

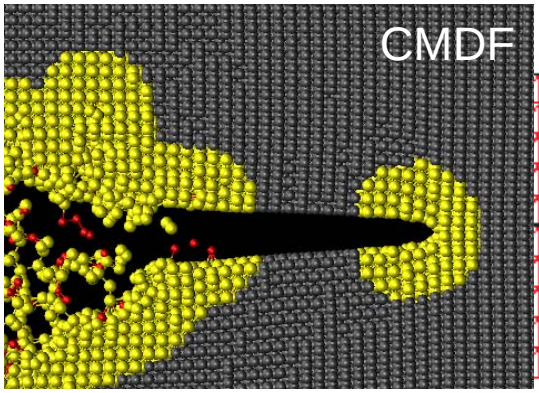


atomistic and M3B meso model of oligomer

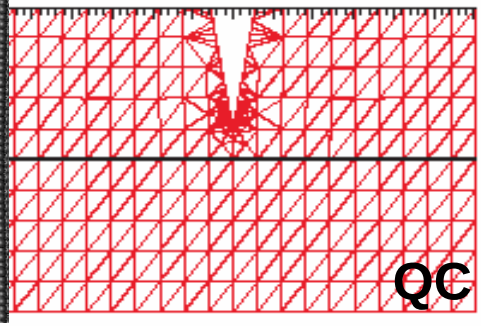
DNA

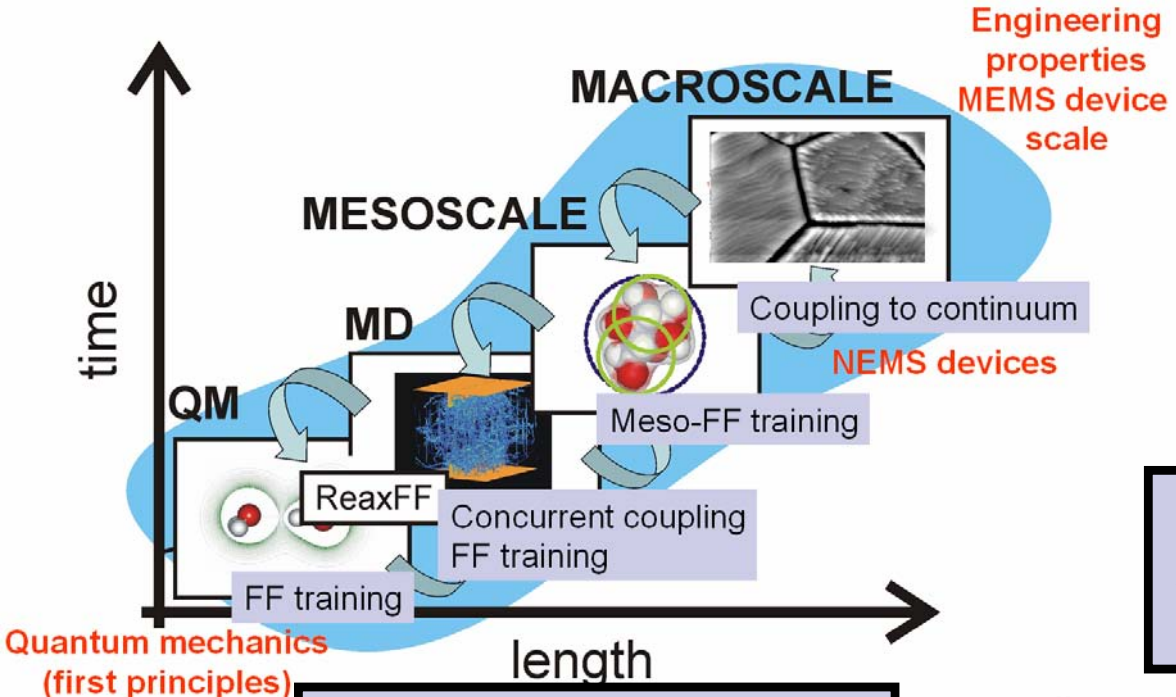


(Pascal *et al.*)



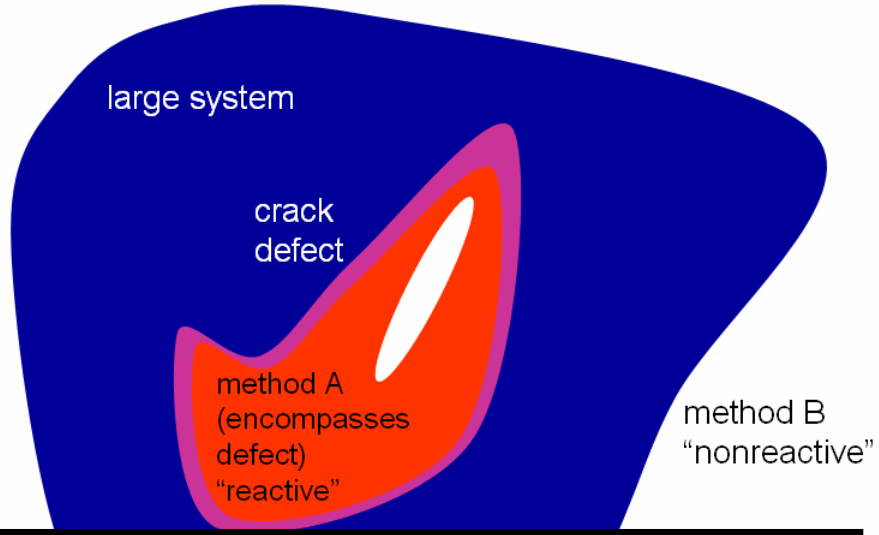
(Buehler *et al.*)





Hierarchical coupling

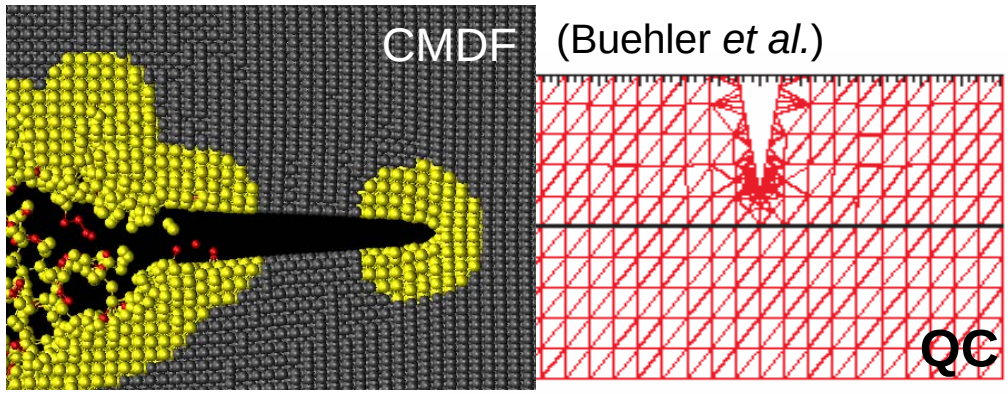
"finer scales train coarser scales"



Concurrent coupling
(QC-Tadmor, Ortiz, Phillips,…
MAAD-Abraham *et al.*, Liu & Wagner, Park *et al.*)

"Spatial variation of resolution and accuracy"

Concurrent versus hierarchical multi-scale simulations



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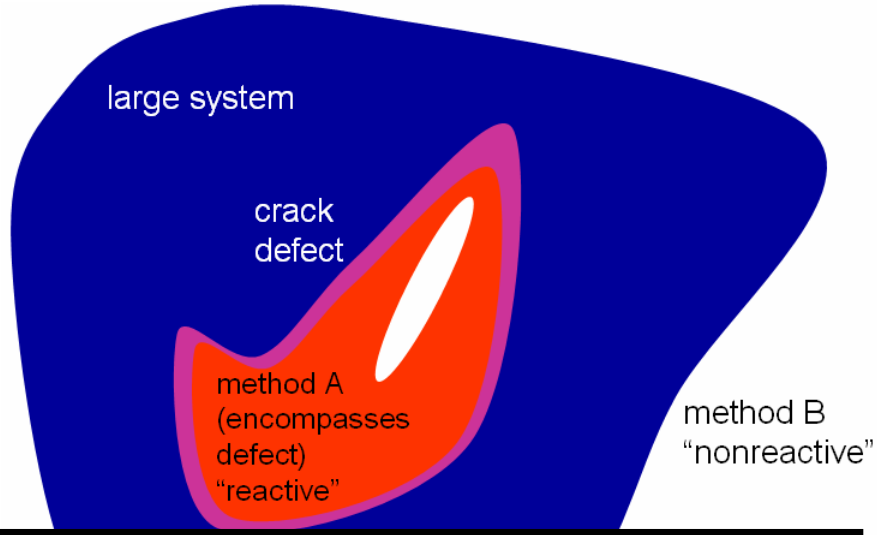


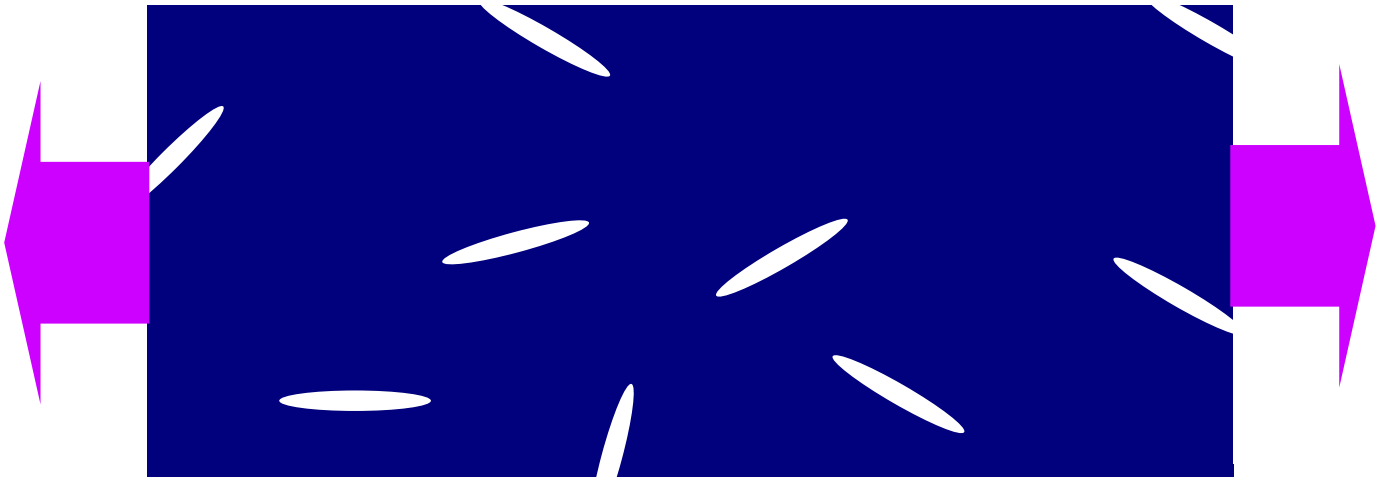
Concurrent coupling
(QC-Tadmor, Ortiz, Phillips,…
MAAD-Abraham *et al*., Liu & Wagner, Park *et al*.)

"Spatial variation of resolution and accuracy"

The concept of concurrent multi-scale modeling

- The strength of materials is dominated by the existence of cracks or other defects (“flaws”)
- Cracks and similar defects lead to stress concentrations, which in turn lead to nucleation of dislocations or generation of new material surfaces

- Defects lead to highly localized regions in materials at which material undergoes strong deformation; therefore, division of computational domain into regions of different accuracy is possible (e.g. dependent on strain gradient)



T.H. Courtney, Mechanical Behavior of Materials, T, Timoshenko, History of strength of materials. New York: McGraw Hill

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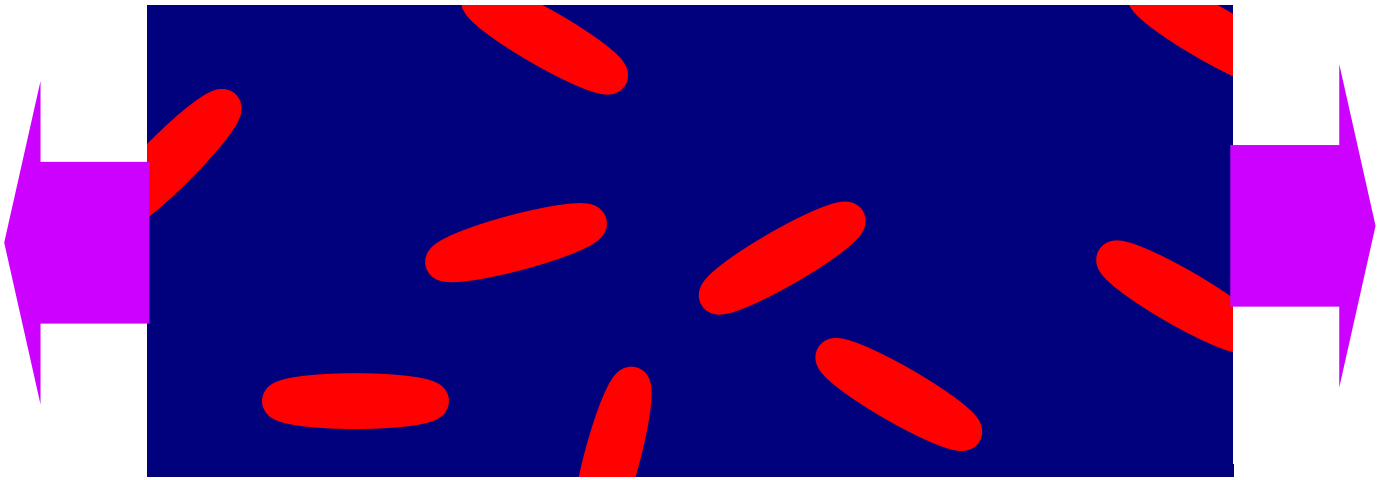

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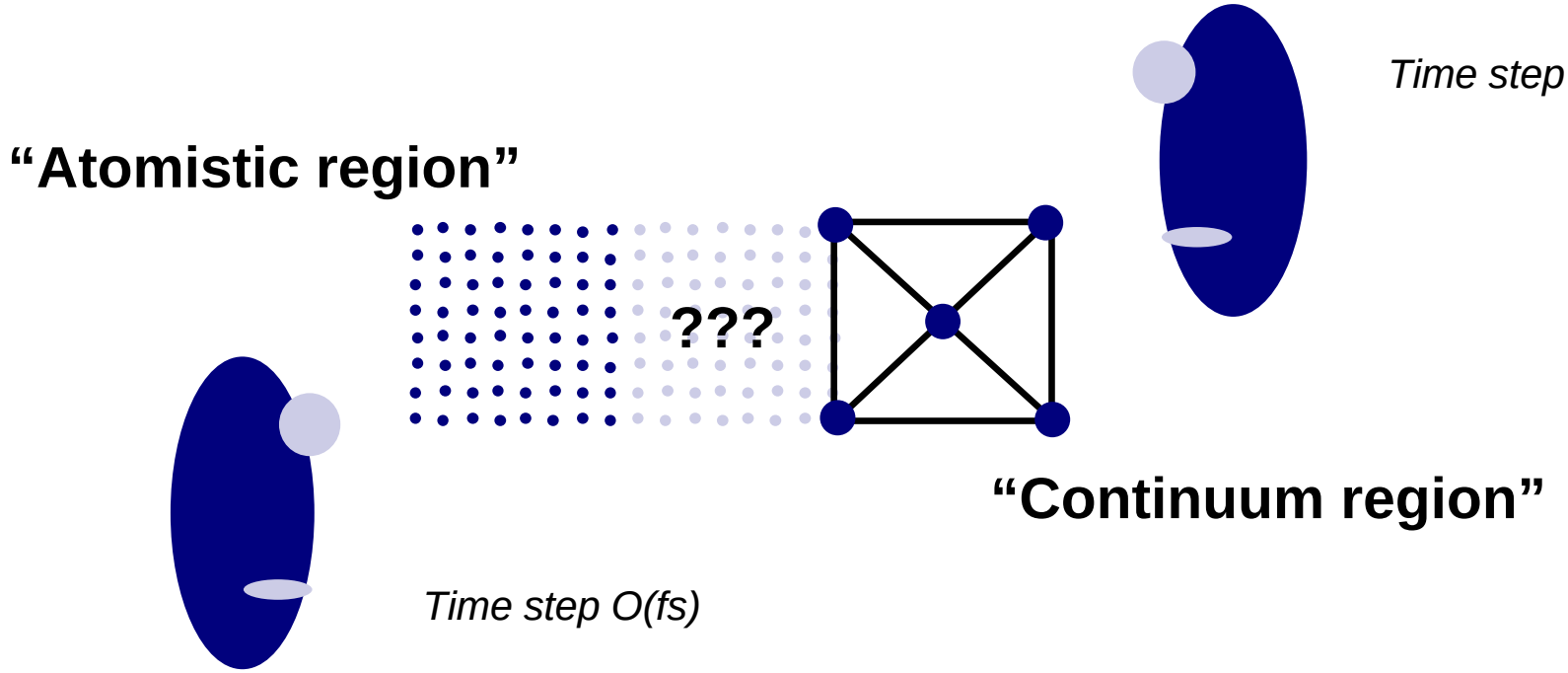
Outline and content (Lecture 3)

- Introduction
- Historical perspective on multi-scale modeling and multi-paradigm modeling
- Modeling codes and established methods:
  - MAAD method: Direct handshaking DFT-empirical MD-continuum (displacement)
  - QC method (Cauchy-Born rule, local and newer nonlocal formulation)
  - QC-DFT method (extension of QC method to couple in DFT via handshake region)
  - Bridging scale method (no handshake region, FE and MD exist simultaneously in computational domain)
  - CADD method (handshake FE/mesoscale DD with atomistic)
- Discussion and conclusion

Challenges in coupling atomistic-continuum scales

Sees: Continuum displacement field, slow oscillations…



Sees: Atomic displacement field, fast oscillations of atoms…

- Goal: Avoid wave reflection at MD/FE interface: Make seamless interface (wave reflection may have dramatic impact on results, leads to melting)
- Earliest attempts by Sinclair (1975), Fischmeister/Gumbsch-FEAt (1991)

Generally: Handshaking requires physical insight

The concept of handshake regions

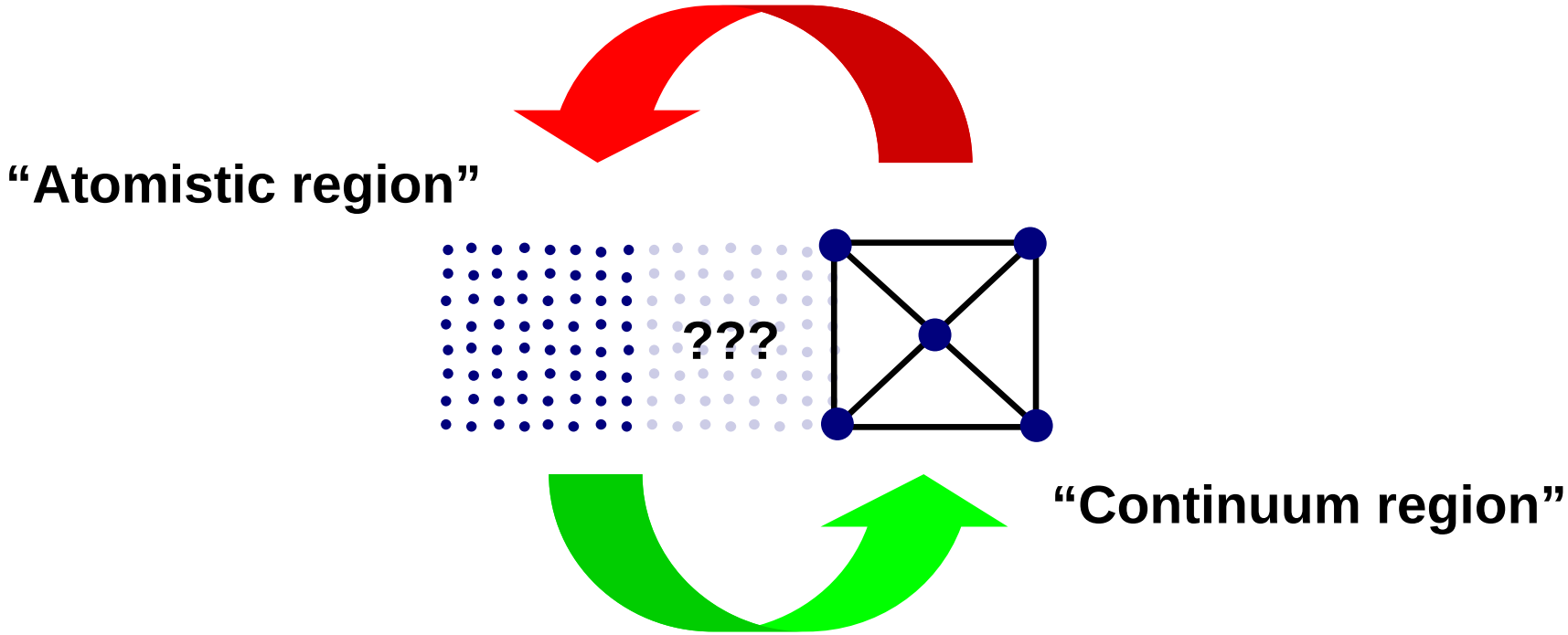
- Coupling between regions of different level of scale/accuracy can be achieved using handshake regions
- Exchange information associated with each modeling paradigm (translation rules or algorithms)

Property	Atomistic scale	Continuum scale
Temperature	Random velocities	Thermodynamic energy
Displacements	Atomic displacements “fine”	Continuum displacements “coarse” (atoms are subset)
Particle velocity	Includes high frequency vibrations	Only low frequency vibrations
Particle forces	Atomic forces (point-wise “discrete”)	Continuum forces (distributed)

Development of filter algorithms to handshake regions is essential
Energy conserving formulations for both MD and FEM

From atoms to continuum and back…

Continuum-Atomistic: Difficult, since atomistic contains information that continuum does not provide (or only indirectly, e.g. temperature)



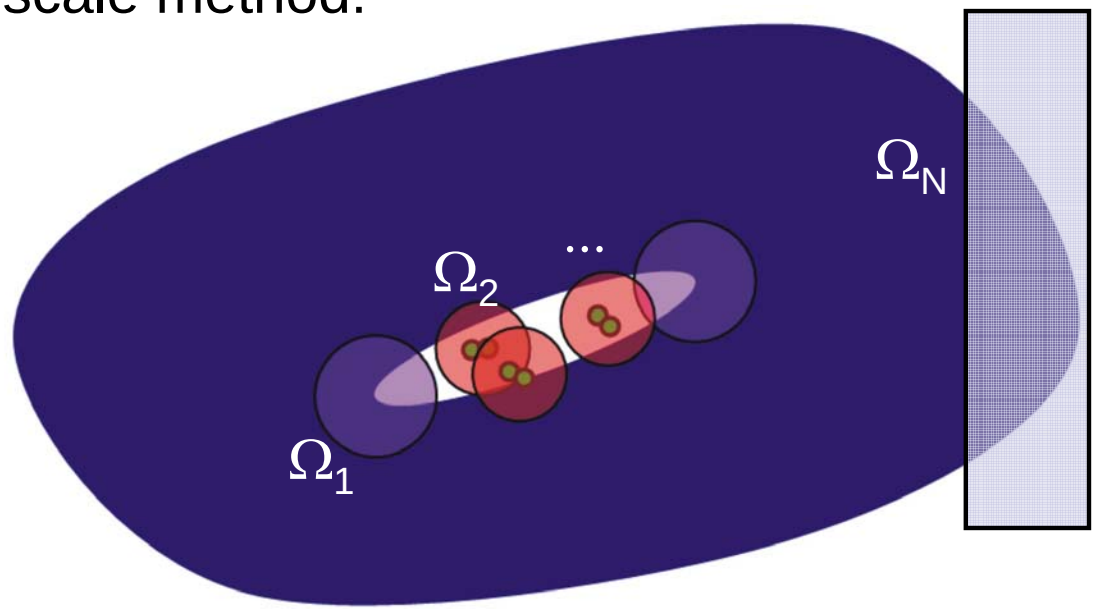
Atomistic-Continuum: Averaging (e.g. stress, displacement etc.), statistical mechanics, once "real" dynamical trajectory is known; "filter" useful information

Still: Boundary effects critical!

Domain decomposition algorithms

- First step in a concurrent multi-scale model is typically decomposition of the computational domain, according to criteria such as
  - Foreign atom types (e.g. only method A treats atom type Y and X-Y interactions)
  - Strain (atomic) or stress (localization)
  - Large forces (between atoms, suggests bond breaking/formation)
  - Large strain/cohesive energy
  - Or, simply geometric criteria and information (e.g. interfaces, boundaries or others)
- The union of many domains associated with fine scale represents the area treated by the fine scale method:

$$\Omega = \cup \Omega_i$$



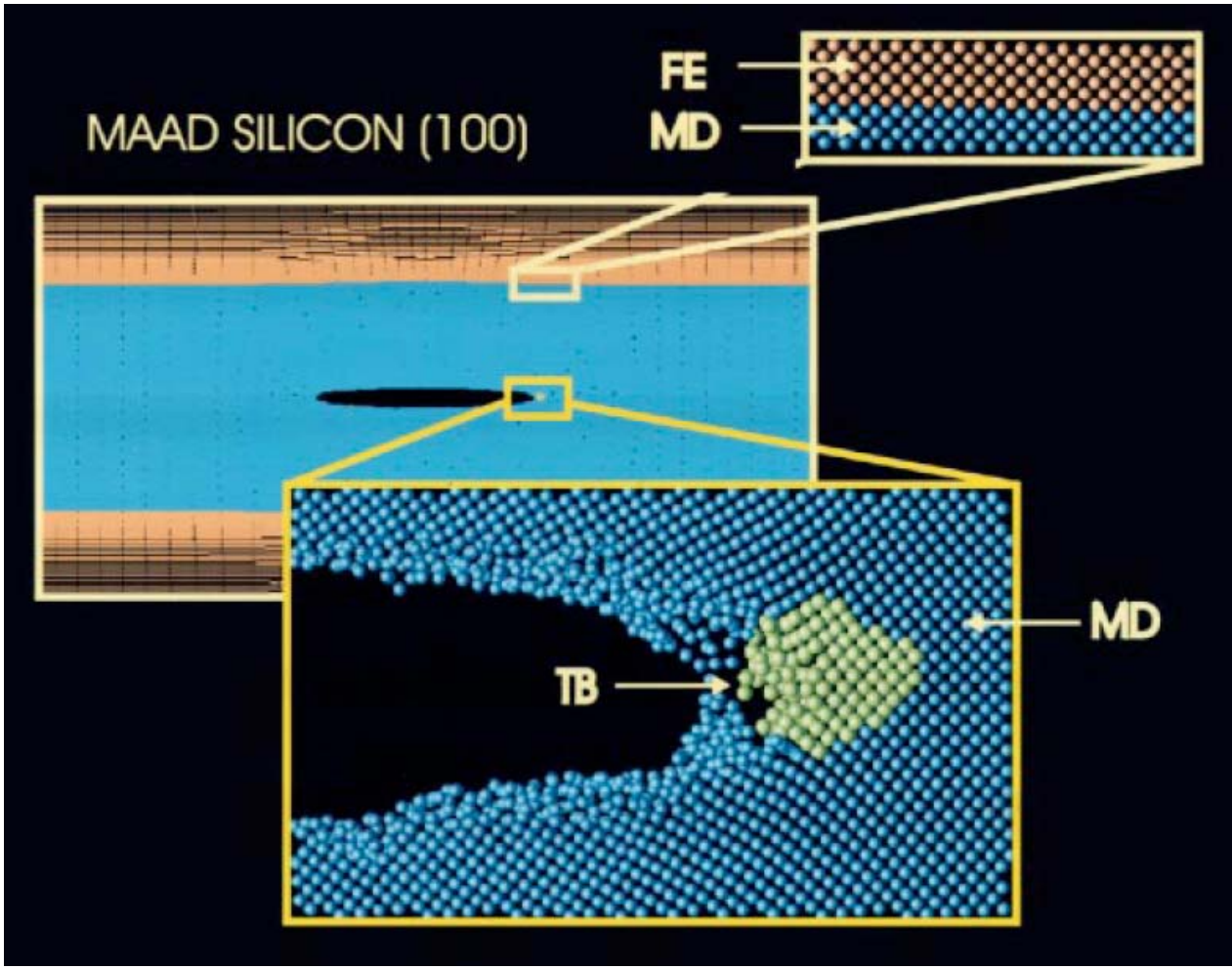
MAAD Method

Coupling DFT to Continuum

Abraham, Kaxiras, Broughton and coworkers, 1998-2000

Concurrent Multiscale/Coupling of Length Scales: The MAAD method

- Finite elements (FE), molecular dynamics (MD), and tight binding (TB) all used in a single calculation (MAAD)
- MAAD = macroscopic, atomistic, *ab initio* dynamics
- Atomistics used to resolve features of interest (crack)
- Continuum used to extend size of domain
- Developed by Abraham, Broughton, Kaxiras and co-workers



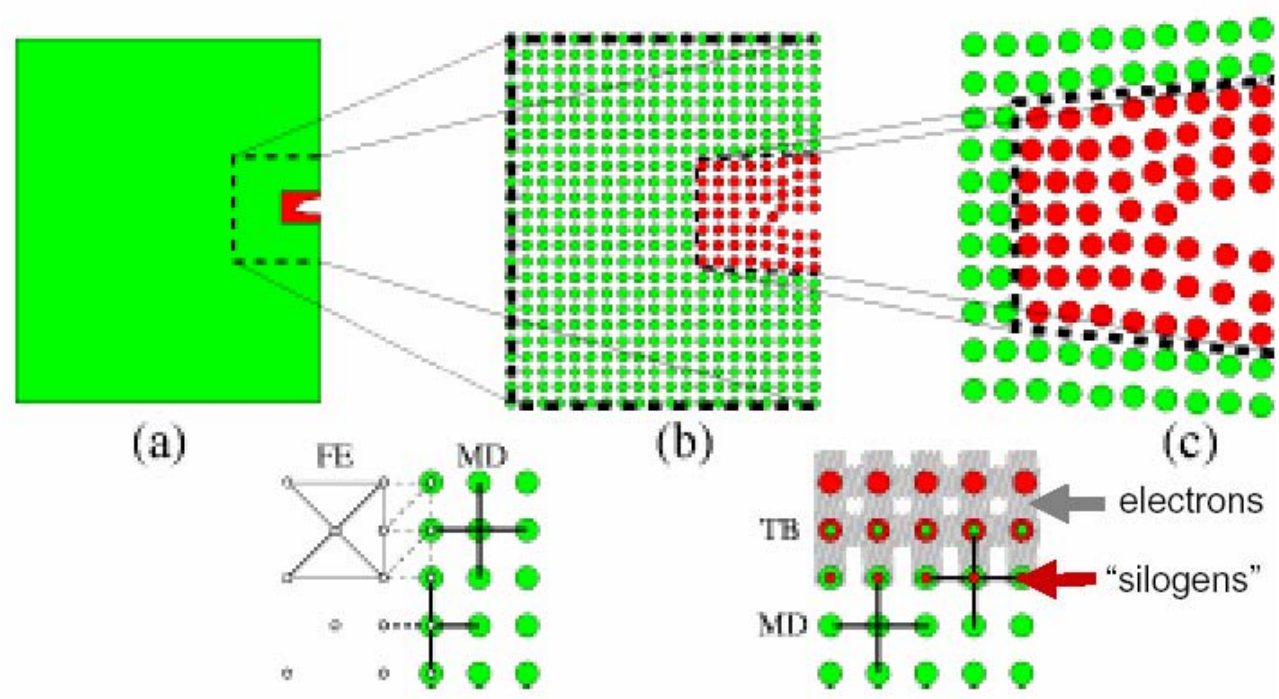
MAAD was one of the first methods of its kind
Received lots of attention

http://www.nnin.org/doc/kaxiras.pdf Abraham, Kaxiras, Broughton and coworkers, 1998-2000

Schematic of the MAAD Method

- Provides coupling of TB-MD-FEM
- Transition regions are very thin (desired due to computational expenses)
- Displacement and velocity link between scales (“kinematic”)
- Time step governed by atomistic scale/TB-MD (O(fs)): Limit to ns

Expect wave reflection from the FE-MD interface



Abraham, Kaxiras, Broughton and coworkers, 1998-2000
http://www.nnin.org/doc/kaxiras.pdf

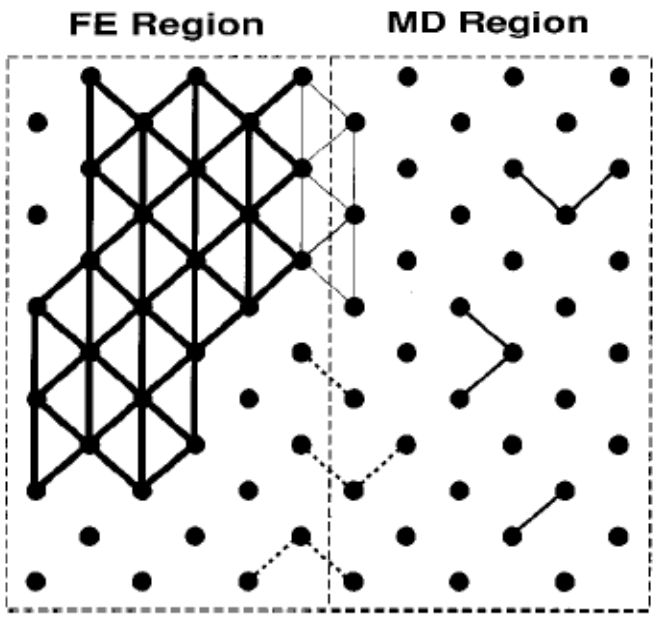
Fundamentals of the MAAD Method

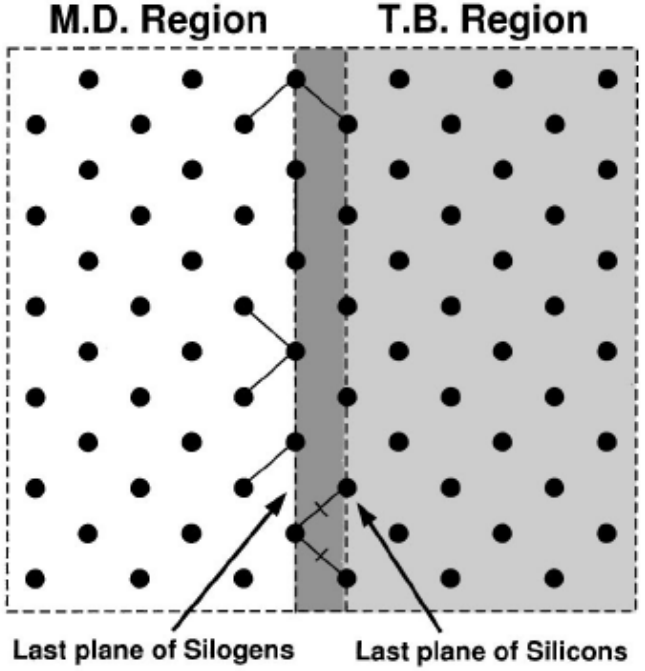
Abraham *et al.*, Europh. Lett., 1998

$$H_{\mathrm{Tot}} = H_{\mathrm{FE}}(\{\mathbf{u},\dot{\mathbf{u}}\} \in \mathrm{FE}) + H_{\mathrm{FE/MD}}(\{\mathbf{u},\dot{\mathbf{u}},\mathbf{r},\dot{\mathbf{r}}\} \in \mathrm{FE/MD}) + H_{\mathrm{MD}}(\{\mathbf{r},\dot{\mathbf{r}}\} \in \mathrm{MD}) + H_{\mathrm{MD/TB}}(\{\mathbf{r},\dot{\mathbf{r}}\} \in \mathrm{MD/TB}) + H_{\mathrm{TB}}(\{\mathbf{r},\dot{\mathbf{r}}\} \in \mathrm{TB}).$$

Mixed Hamiltonian
Conserves energy

FE/MD and MD/TB: "Handshake" regions



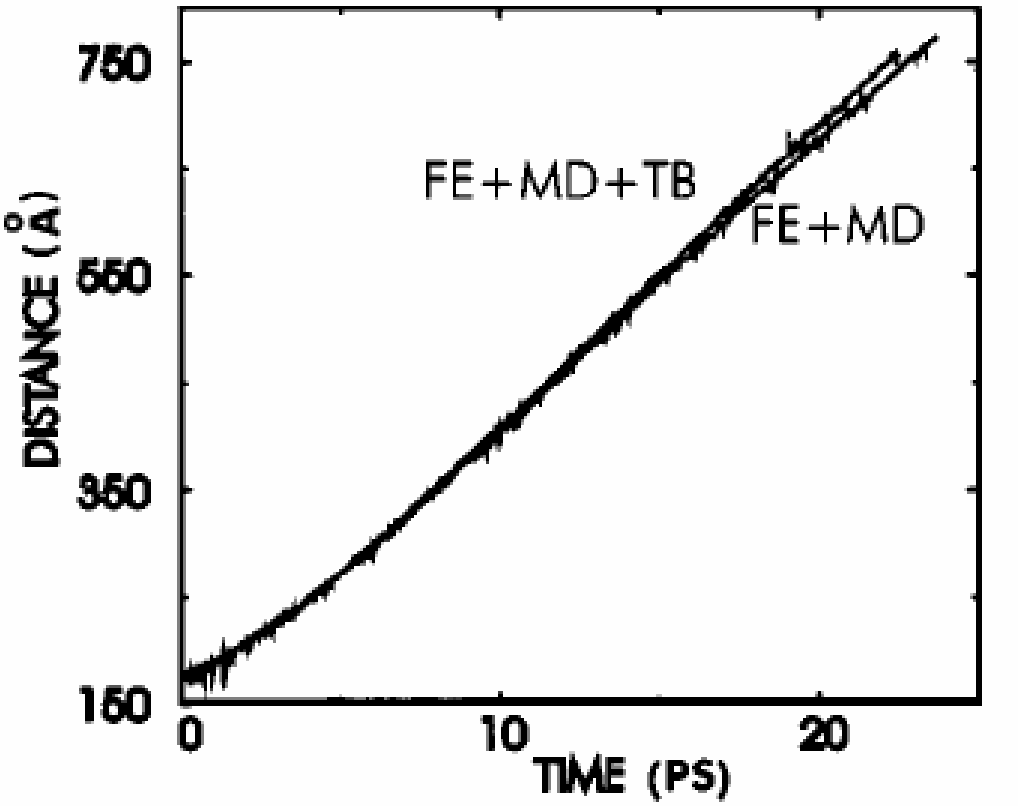


FE mesh down to atomic scale
Problem: Short-wave length oscillations "see" the interface

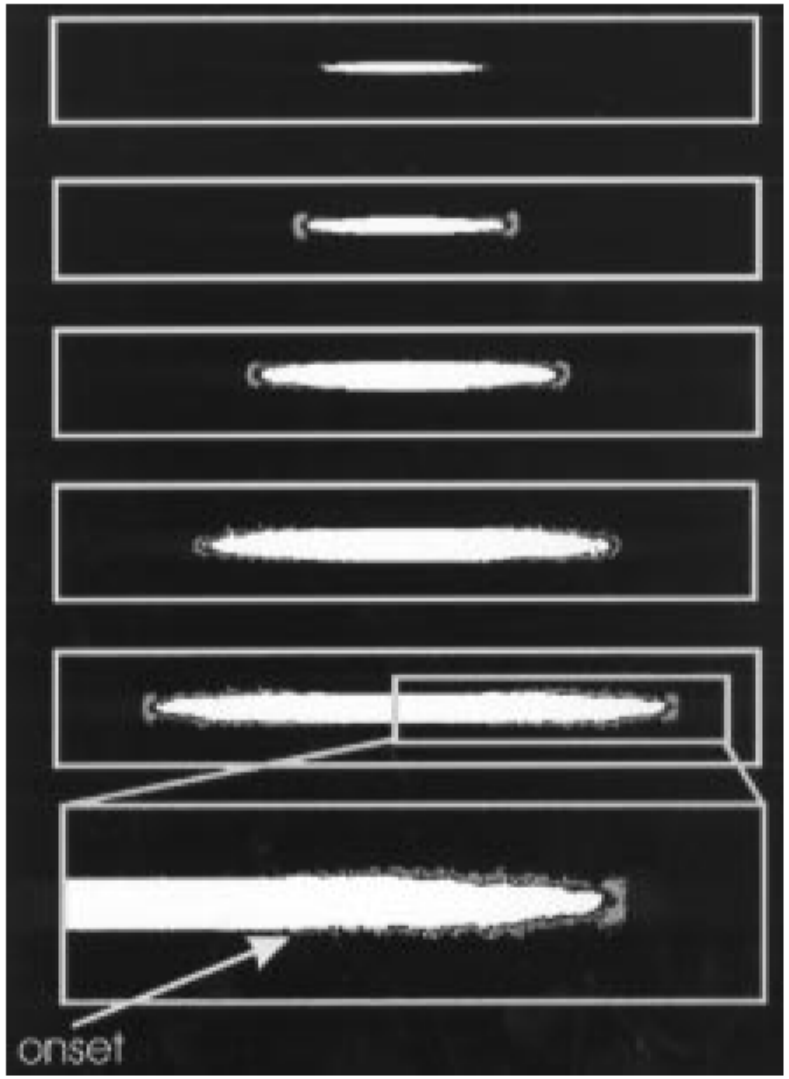
Silogens=H terminated Si atoms (behave monovalent, hydrogenic Si atoms)

TB determines elasticity, then hierarchically transported upwards in scale

Example results: MAAD method



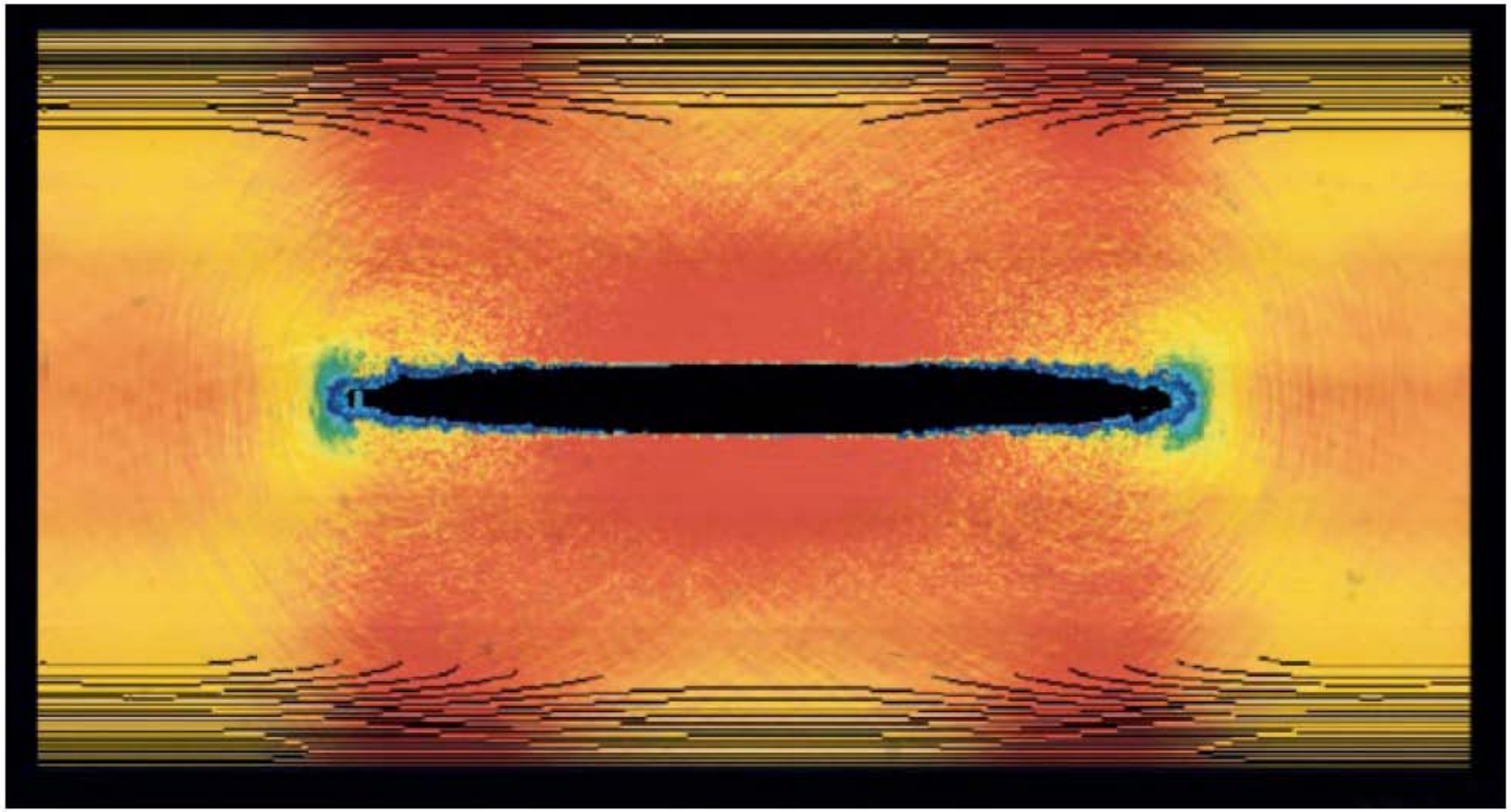
Distance versus time history of crack tips



Increased roughness with increased crack speed ([100] Si)

Abraham *et al.,* Europh. Lett., 1998

Example results: MAAD method



Stress waves propagating through the slab

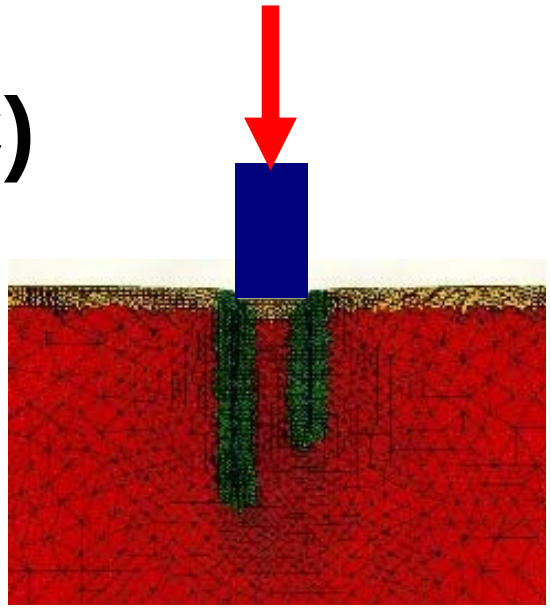
Blue=high stress, red= low stress

Abraham *et al.,* Europh. Lett., 1998

The quasicontinuum method (QC)

Coupling empirical potentials (EAM) to continuum (FE)

http://www.qcmethod.com/qcreview.pdf
http://www.qcmethod.com/



Historical perspective: Development of QC

- Key idea: Selective representation of atomic degrees of freedom
- Instead of treating all atoms making up the system, a small relevant subset of atoms is selected to represent, by appropriate weighting, the energetics of the system as a whole.
- Based on their kinematic environment, the energies of individual "representative atoms" are computed either in nonlocal fashion in correspondence with straightforward atomistic methodology or within a local approximation as befitting a continuum model.
- The representation is of varying density with more atoms sampled in highly deformed regions (such as near defect cores) and correspondingly fewer in the less deformed regions further away, and is adaptively updated as the deformation evolves.

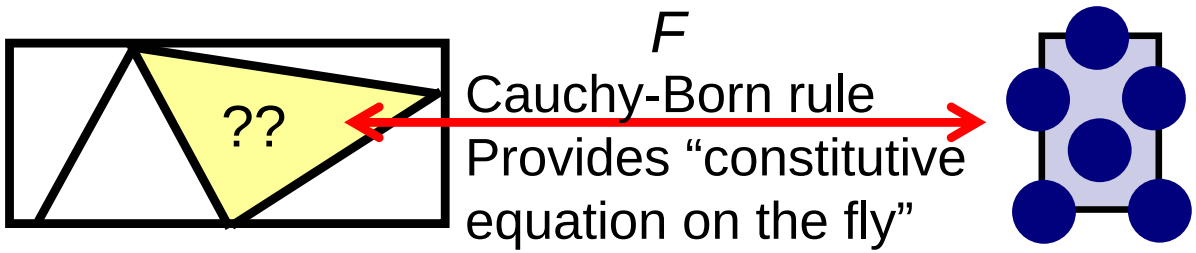
Development history: Early stages

- The QC method was originally developed by Dr. Ellad B. Tadmor as part of his Ph.D. research at the department of Mechanics of Solids and Structures at Brown University between 1992 and 1996 under the advisement of Prof. Michael Ortiz and Prof. Rob Phillips.
- The method was applied to single crystal fcc metals and shown to reproduce Lattice Statics results for a variety of line and surface defects and used to study nanoindentation in thin films.

Taken from: www.qcmethod.org

QC method: Fundamentals

- QC provides alternative to handshaking
- Basic idea: Obtain FE stiffness matrix on the fly based on atomic lattice/potential (no *a priori* assumptions)
- Zero temperature relaxation technique
- Elastic energy used in FEM region is computed by applying the FEM interpolated displacement field (via Cauchy-Born rule) to a reference system of atoms interacting by MD forces, e.g. based on EAM potential
- Difficulties:
  - No thermal fluctuations, since atoms are at reference positions (displaced)
  - "Ghost forces" due to discreteness in FE setup, and the problem that the MD probing is based on discrete displacement fields



Cauchy-Born rule: Hypothesizes that the infinite crystal underlying each continuum particle deforms according to a locally uniform, continuum deformation gradient *F*; used to extract constitutive law

QC method: Fundamentals

In Bravais lattice, lattice vectors deform by deformation gradient **F**

$$\mathbf{r} = \mathbf{F}\mathbf{r}^0$$

Due to periodicity of Bravais lattice, this leads to strain energy per atom is

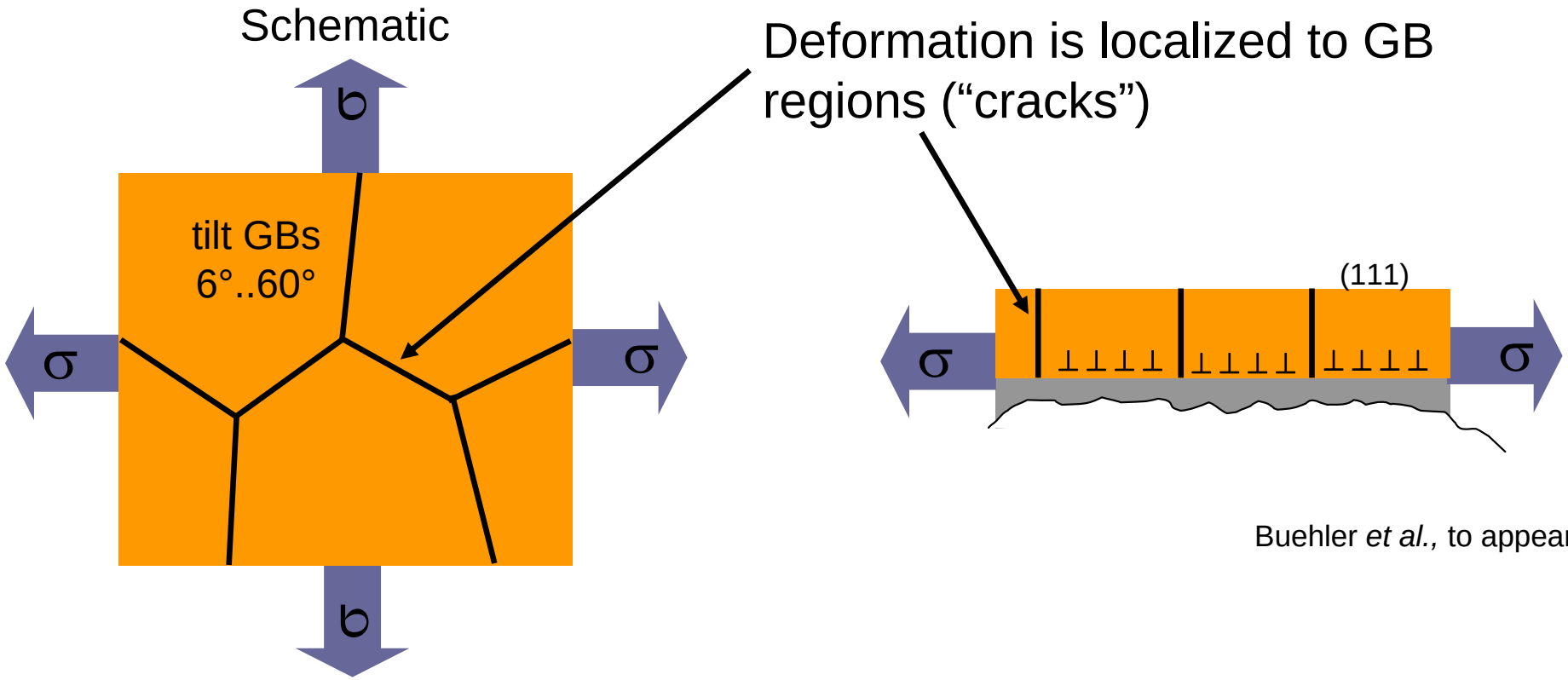
$$\Lambda = \frac{1}{2}\sum_j V(r^j)$$

May calculate continuum Cauchy stress at the deformed configuration

$$\boldsymbol{\sigma} = \frac{1}{2\Omega}\sum_j \frac{\partial V}{\partial r^j}\frac{\mathbf{r}^j \otimes \mathbf{r}^j}{r^j}$$

This represents the “local” QC formulation

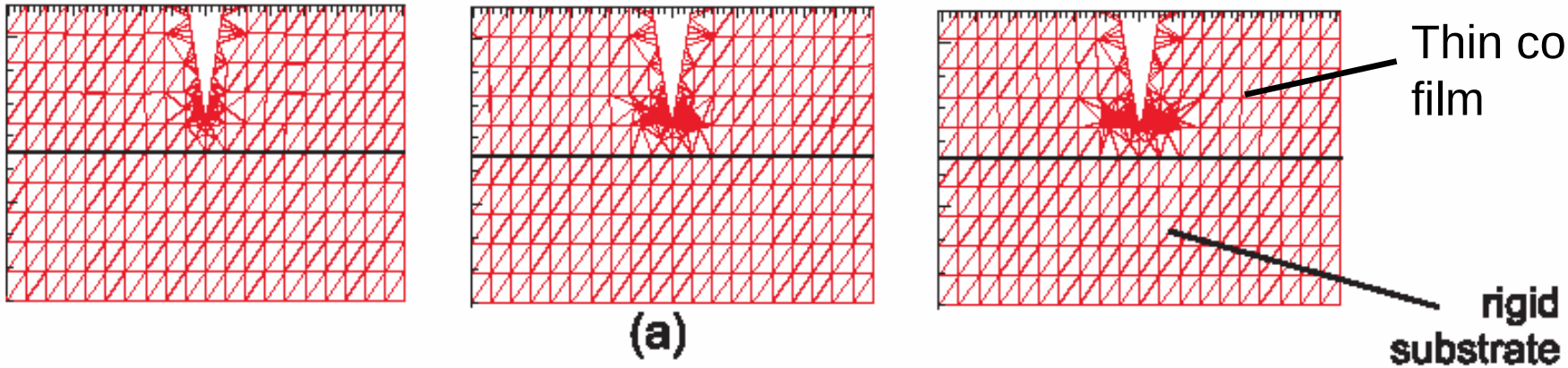
Example application: Deformation of thin films (geometry)

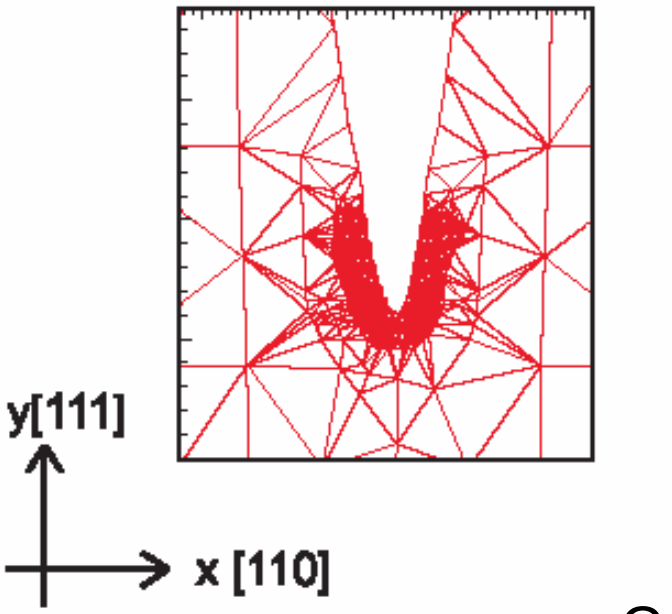


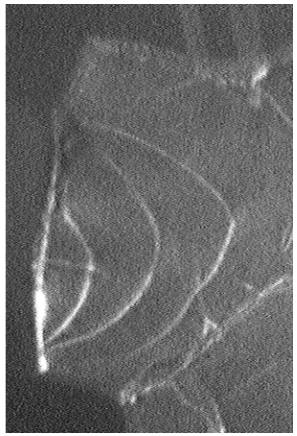
Buehler *et al.,* to appear 2006

- Biaxial loading by thermal mismatch of film and substrate material: High stresses cause severe problems during operation of the device
- Ultra thin, submicron copper films become critically important in next generation integrated circuits (see, e.g. *Scientific American*, April 2004), MEMS/NEMS

The Quasicontinuum (QC) Method





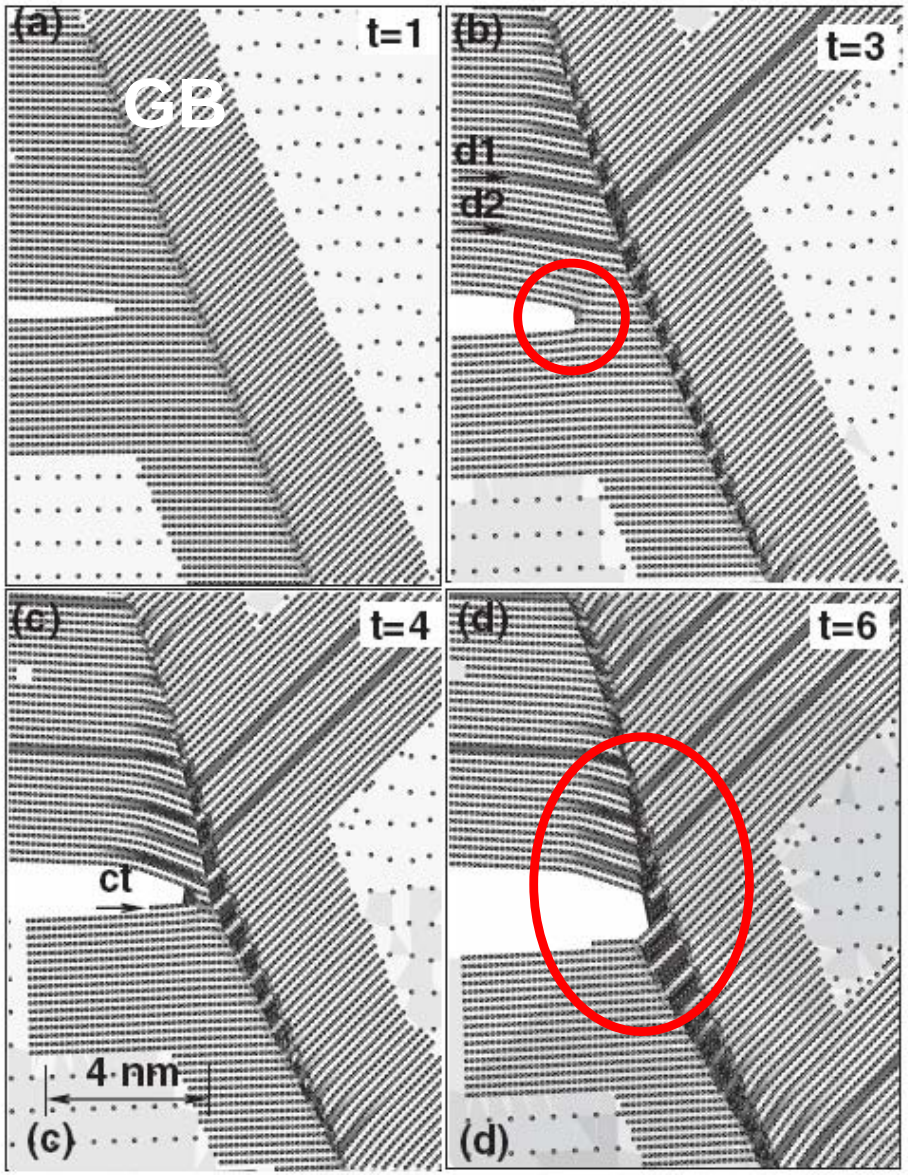


(Balk et al., MPI-MF)

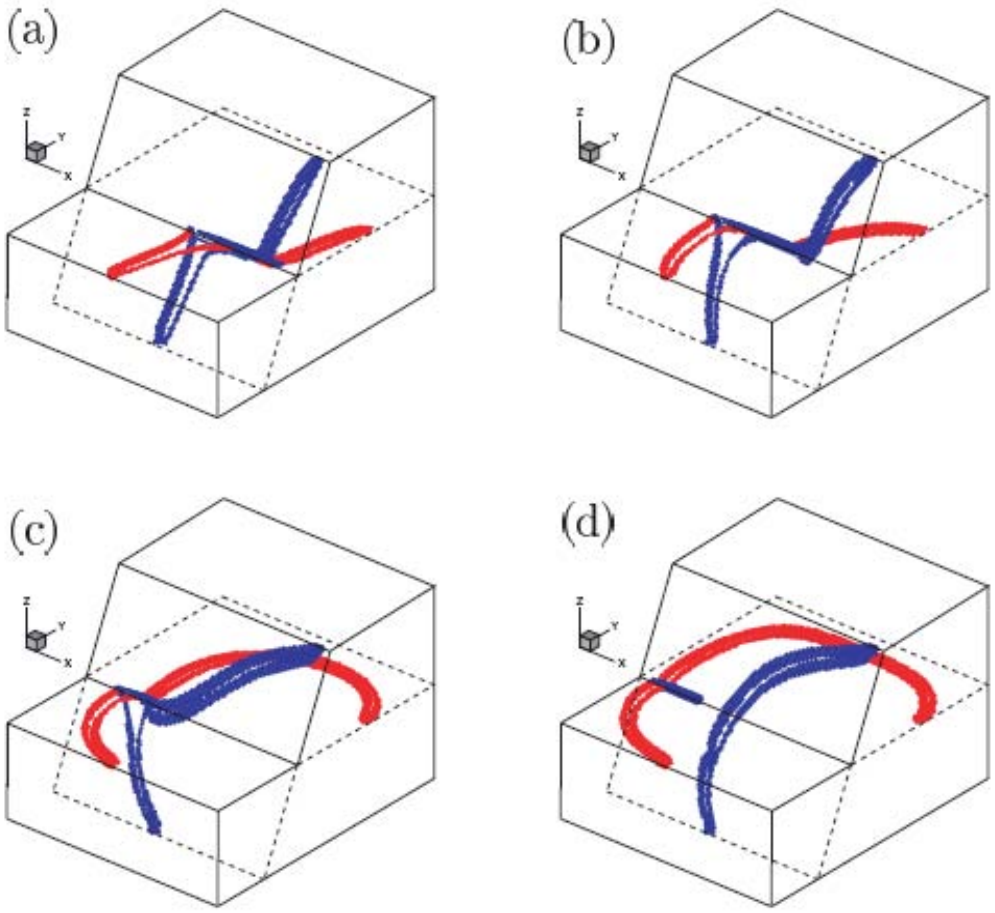
Combine atomistic regions embedded in continuum region

(Buehler *et al*., 2006)

The Quasicontinuum (QC) Method



Dislocation-GB interaction



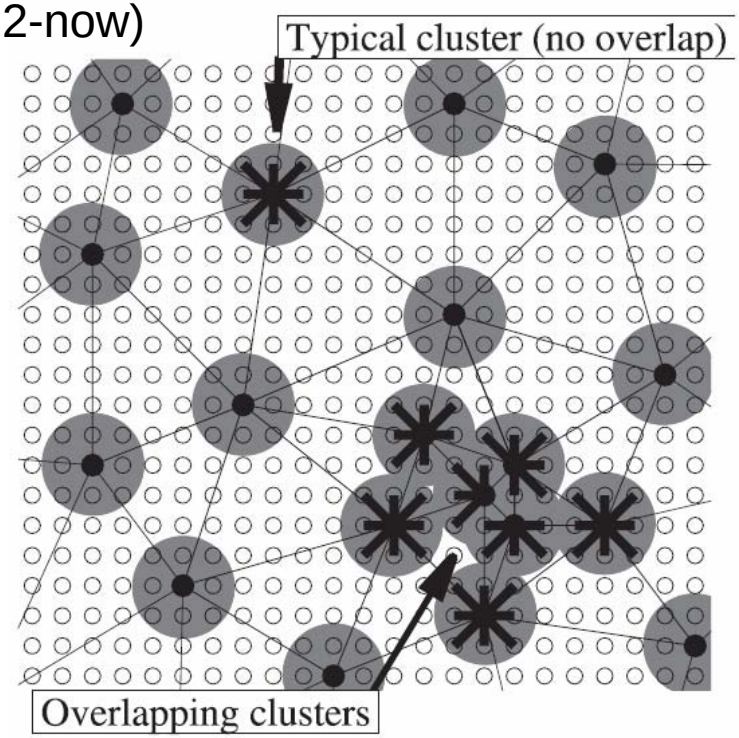
3D dislocation junction
(long-range field critical)

Non-local QC method

- Does not use Cauchy-Born rule as does the local QC method
- Instead: Use full non-local (atomistic) representation to determine forces
- Developed by Knap and Ortiz at Caltech (2002-now)

Features:

- Truly seamless!
- There is no boundary present between atomistic and continuum region
- Smart scheme to avoid double counting of bonds (demarcation)



$$f_j \equiv -\frac{\partial E^a}{\partial U_i} = -\sum^{N} \frac{\partial E_i(\boldsymbol{u})}{\partial \boldsymbol{u}} \frac{\partial \boldsymbol{u}}{\partial U_j}$$

$$f_j = -\sum_{i=1}^{N} \frac{\partial E_i(\boldsymbol{u})}{\partial \boldsymbol{u}} S_j$$

$$f_j \approx -\sum_i n_i \left[\sum_{c \in \mathcal{C}_i} g_c S_j(X_c) \right]$$

Use explicit expression for forces on the nodes
(atomic limit: each node=one atom)

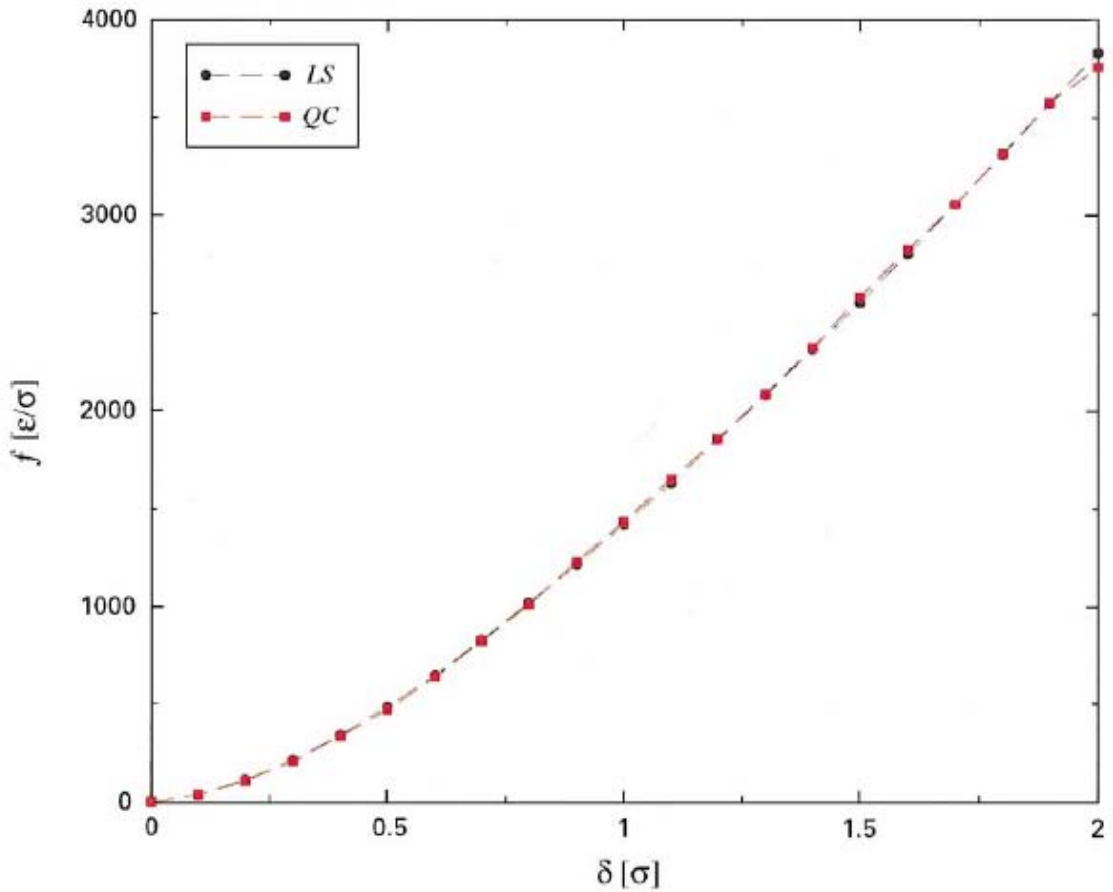
Evaluate in small cluster around node *j*

Knap and Ortiz, 2001, JMPS

Example results: Non-local QC method

Example: Nanoindentation

3D dislocation structure below an indenter



Load-displacement curve comparing full atomistic with NL-QC formulation

Knap and Ortiz, 2001, JMPS

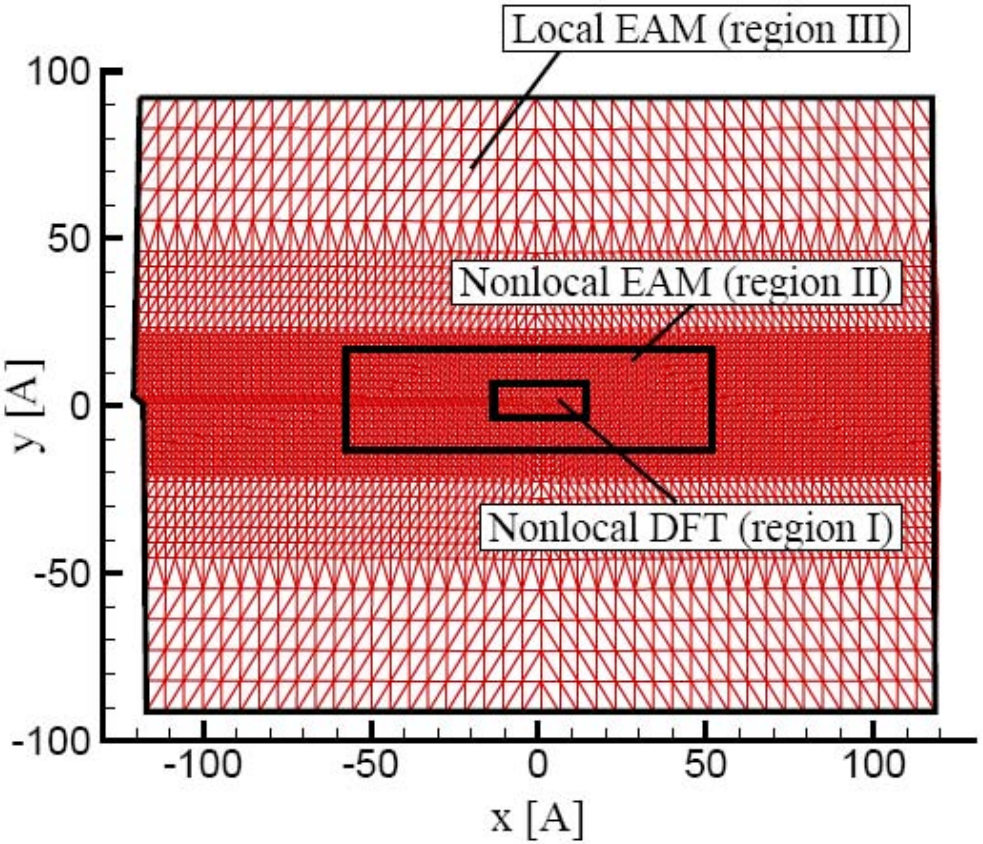
QC-DFT method

- Multiscale modeling approach that concurrently couples quantum mechanical, classical atomistic and continuum mechanics simulations in a unified fashion for metals.
- This approach is particular useful for systems where chemical interactions in a small region can affect the macroscopic properties of a material.
- Quasi-static conditions: 0K

"local EAM"=FE

"nonlocal EAM"=atomistic

"nonlocal DFT"=QM regime

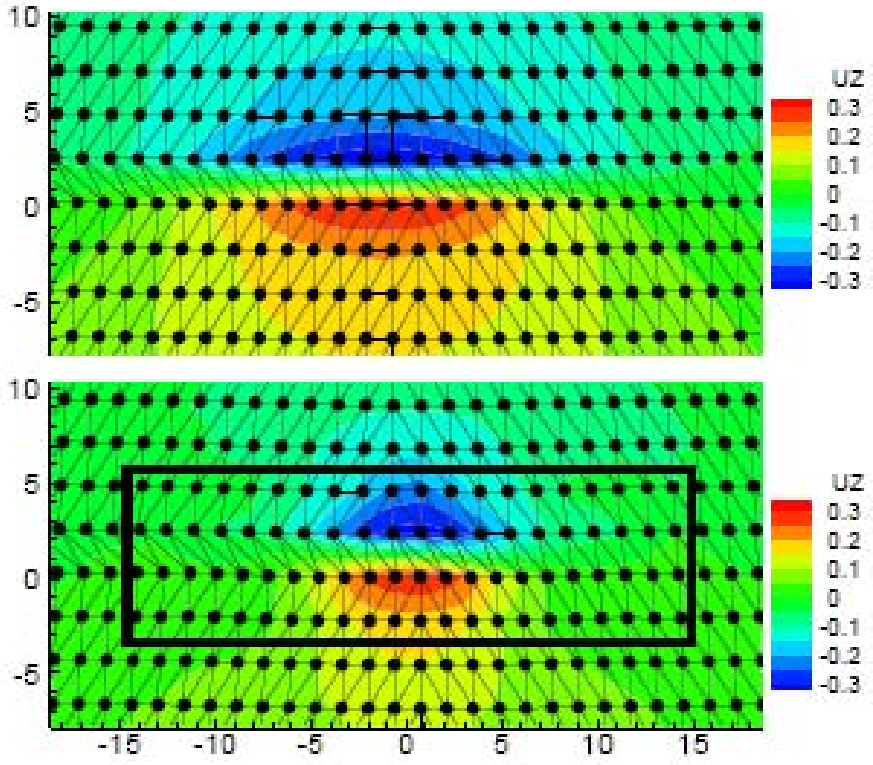


Gang Lu, Ellad Tadmor, Tim Kaxiras

QC-DFT method: Example results

EAM-QC

DFT-QC



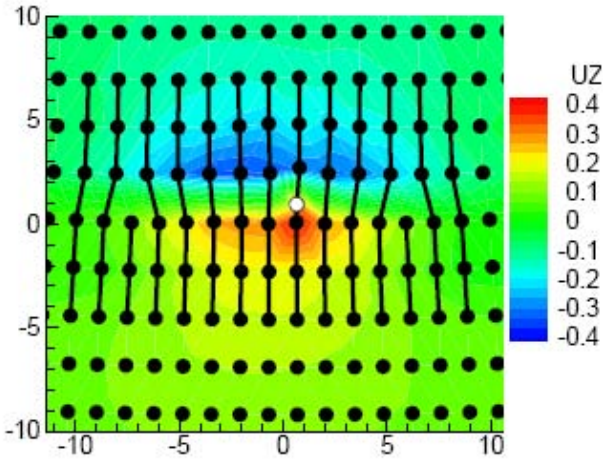
- Dislocation core structures obtained from the EAM-based QC (top) and the present QCDFT method (bottom)
- The black circles are atoms

- Contours correspond to out-of-plane (z) displacement (in Å).
- Contours clearly indicate the splitting of the dislocation.
- Atoms within the black box in the bottom panel are DFT atoms.

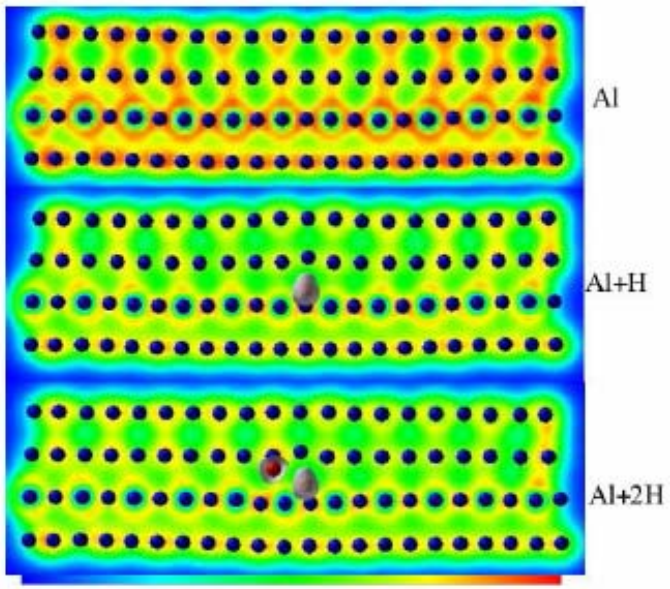
- Note: The finite element mesh serves no other purpose in this nonlocal atomistic region other than as a guide to the eye to help visualize deformation.

Gang Lu et al., 2005

QC-DFT method: Example results



- QC-DFT dislocation core structure in the presence of a column of H impurities.
- The circles are Al atoms (black) and H atom (white).
- The black lines are a guide to the eye, indicating atomic planes.



- Charge density distribution in region I in the absence (top) and in the presence of one (middle) and two H impurity atoms (bottom).
- The blue spheres are Al atoms and the red spheres are H atoms.
- Gray iso-surfaces illustrate the charge density distribution at 0.28 electrons/Å^3.
- Electron density values range from 0 to 0.30 electrons/Å^3.

Gang Lu et al., 2005

Various Cauchy-Born based techniques

Atomistically informed FE model

VIB technique

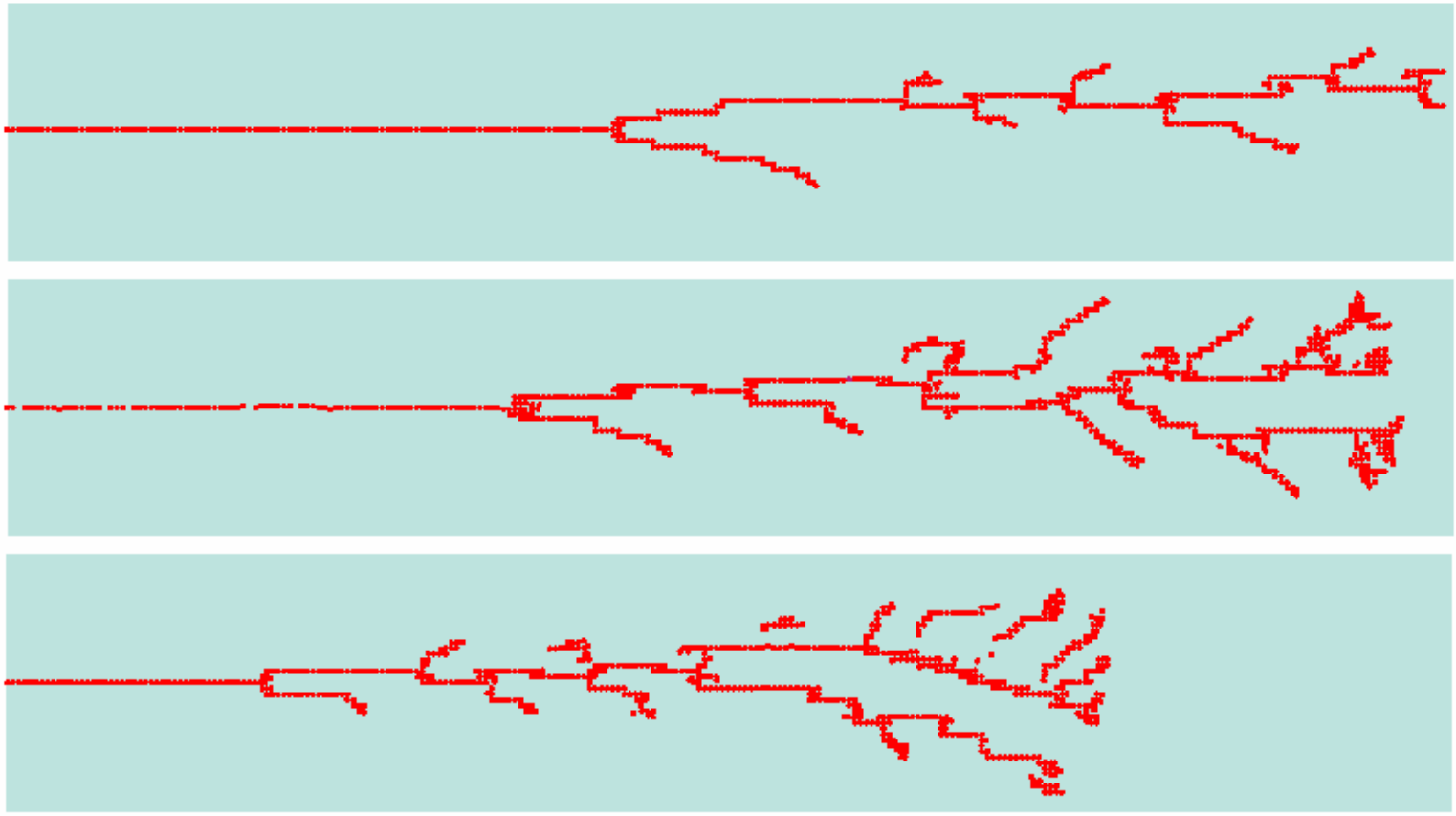
- Developed by Gao and Klein (JMPS, 1998)
- Virtual internal bond method enables immediate link of interatomic potential with constitutive FE equation via Cauchy-Born rule, accounting for hyperelastic (nonlinear) effects
- Unlike QC, no atomic resolution present
- Represents an attempt to avoid difficulties of FE formulations to model fracture (e.g. imposed cohesive surfaces etc.); and make those formulations physically sound
- **Example**: Used to model fracture since the failure of each FE can be determined on the fly by instability criterion; no *a priori* determination of fracture surface is required
- Localization (fracture) estimated by determinant of the acoustic tensor approaches zero (element itself "breaks"):

$$C_{IJKL} = D_0 l_0^{*4}\left(\frac{U''}{l^2} - \frac{U'(l)}{\beta}\right)\int_{-\pi}^{\pi} \xi_I \xi_J \xi_K \xi_L d\phi = \mu(\delta_{IJ}\delta_{KL} + \delta_{IK}\delta_{JL} + \delta_{IL}\delta_{KJ})$$

$$(\sigma + \mu\lambda^2)(\sigma + 3\mu\lambda^2) = 0$$

$$(C_{1111}\lambda_1^2 + S_{11})(C_{1212}\lambda_2^2 + S_{11}) - 4(C_{1212}\lambda_1\lambda_2)^2\psi^2 = 0$$

VIB applications



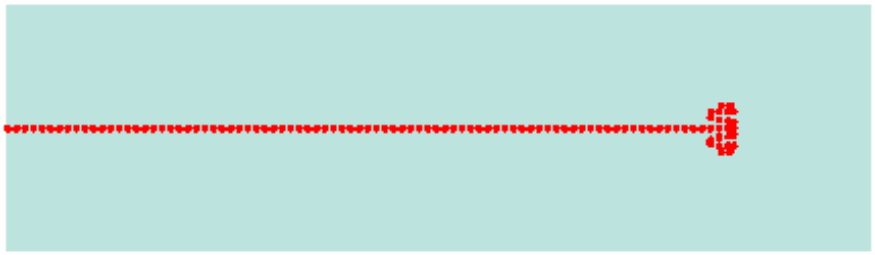
Fracture patterns for different impact velocities

Klein, Gao, 2001

VIB applications: Onset of instability

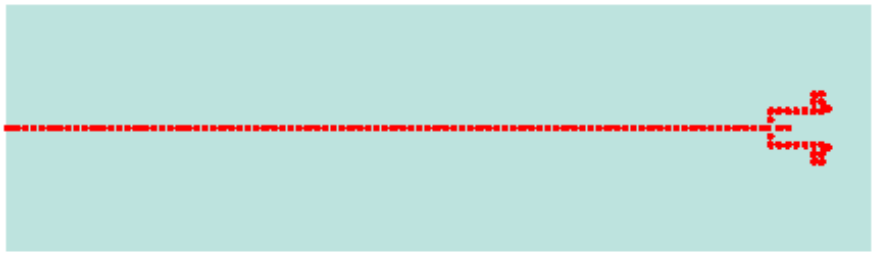
(a) $t = 4.6\mu s$

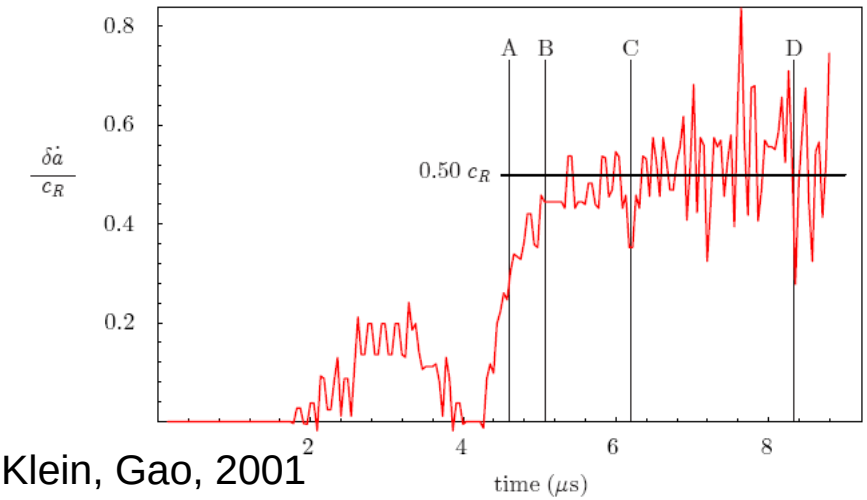
(c) $t = 5.9\mu s$



(b) $t = 5.1\mu s$

(d) $t = 6.1\mu s$

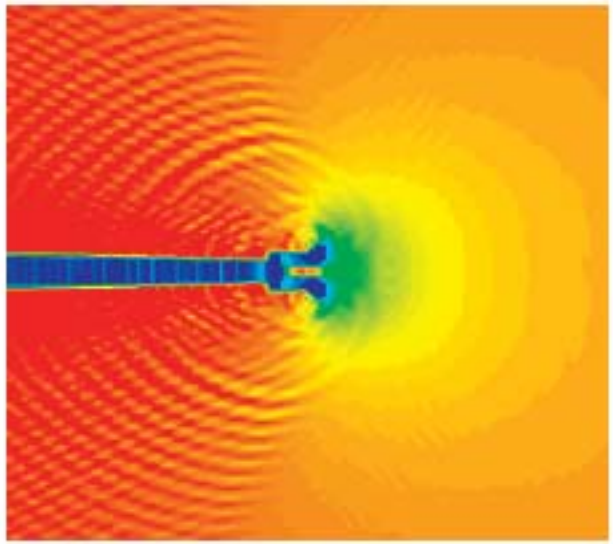




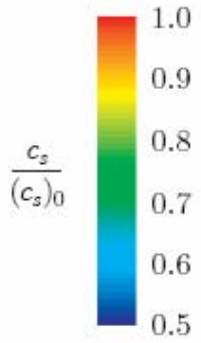
Klein, Gao, 2001

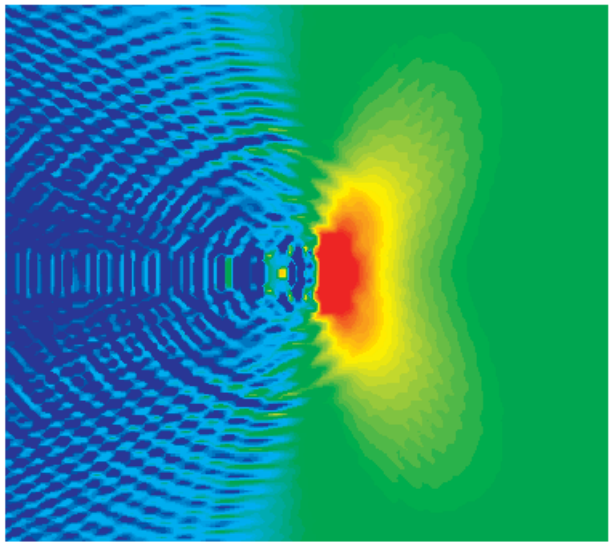
VIB predicts many of the experimental observations, including reduced instability speed and branching patterns

VIB applications: Local elasticity

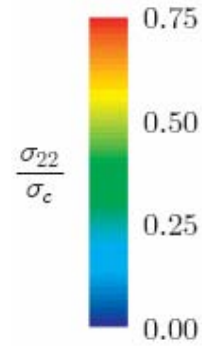


Acoustical shear wave speed
Indicates softening at crack tip





Distribution of opening stress



Klein, Gao, 2001

Atomistically informed finite temperature FE method (Huang *et al*.)

Use concept of local harmonic approximation to impose thermal fluctuations (only valid for small homologous temperatures)

$$S = -k_B \sum_{n=1}^{3N} \ln\left[2\sinh\left(\frac{h\omega_n}{4\pi k_B T}\right)\right]$$

"account for atomic vibration"

$$\left|\omega_n^2 I_{3N\times 3N} - \frac{1}{m}\frac{\partial^2 U_{\text{tot}}}{\partial x\,\partial x}\right| = 0$$

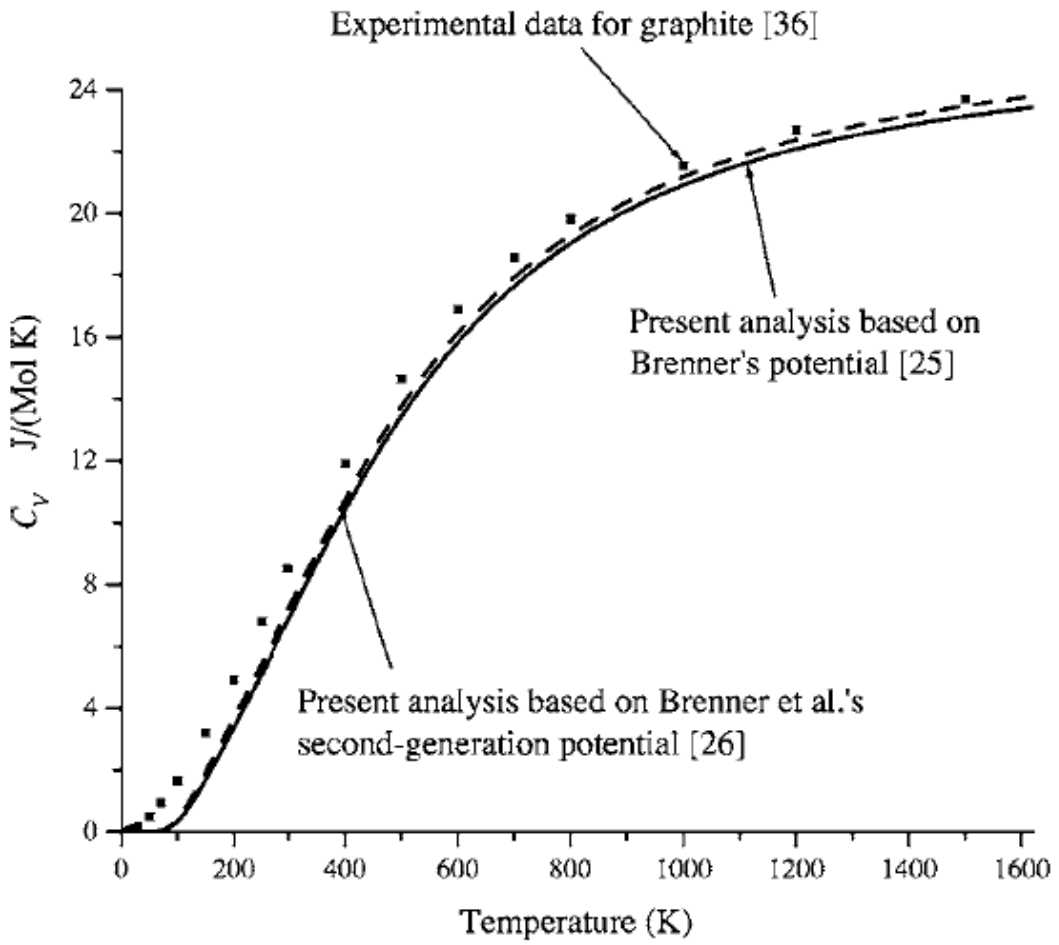
Helmholtz free energy

$$A(r,T) = U_{\text{tot}}(r) + k_B T \sum_{i=1}^{N}\sum_{\kappa=1}^{3} \ln\left[2\sinh\left(\frac{h\omega_{i\kappa}}{4\pi k_B T}\right)\right]$$

Key:
Use Helmholtz free energy in Cauchy-Born rule instead of potential energy

Young Huang et al., JEMT, 2005

Atomistically informed finite temperature FE method (Huang *et al*.)



Example:

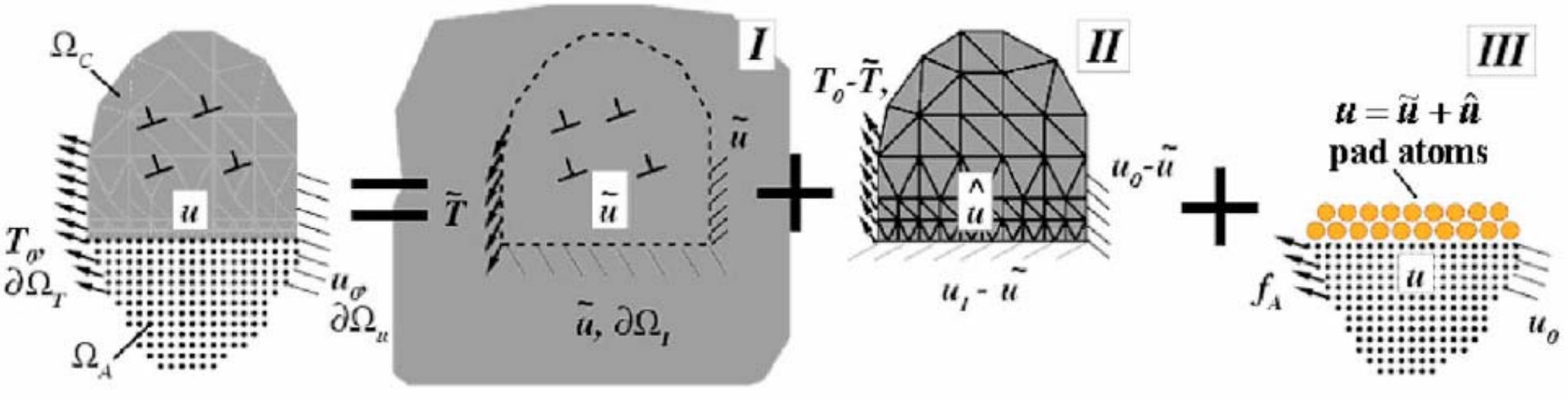
- Temperature dependence of specific heat c_v
- Compare pure MD, experiment and new multi-scale method

Huang et al., JEMT, 2005

The CADD approach

Coupling Discrete Dislocation Dynamics with atomistic simulation

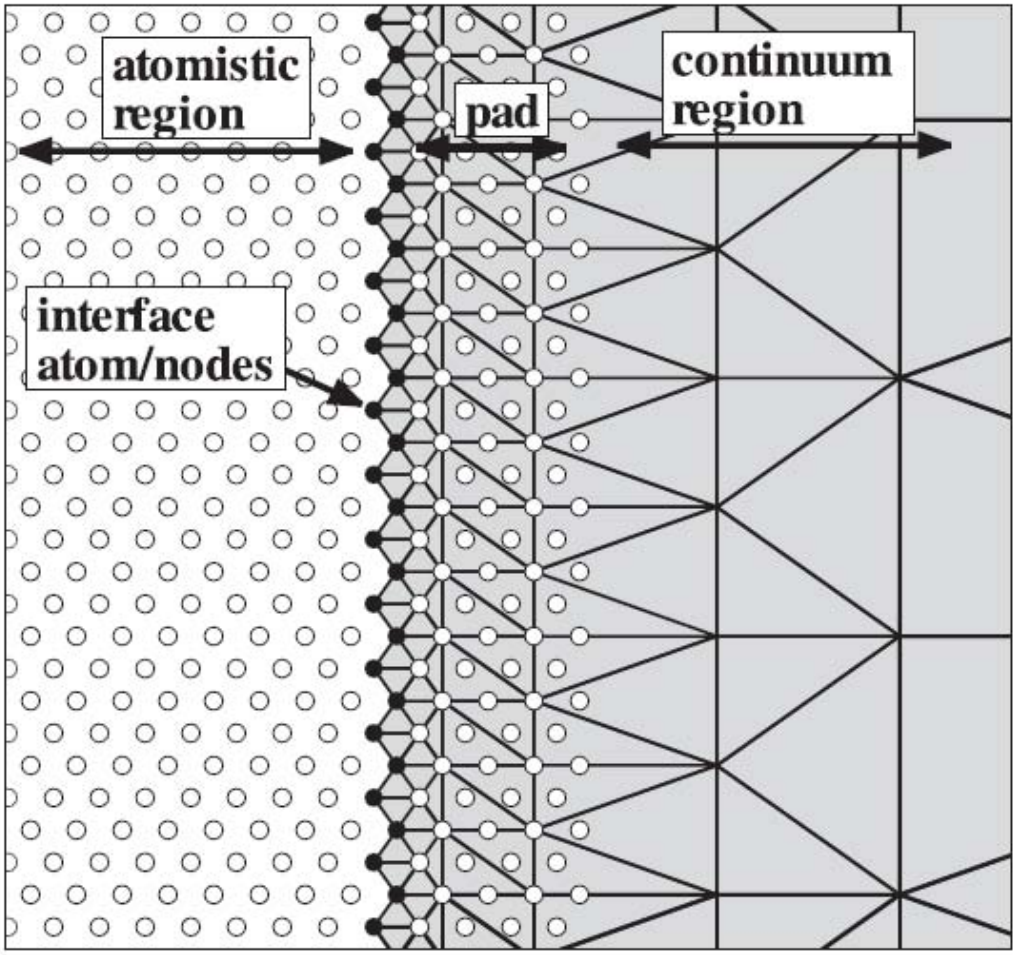
Coupling atomistics-DD/mesoscale CADD method: Fundamentals



- Method provides interface of DD region with atomistic region
- Coupling achieved by nodal displacement in handshake region (atomic displacement forced to agree with FE displacement, and pad atoms to agree with FE displacement)

Gurtin and Miller, 2004-2005

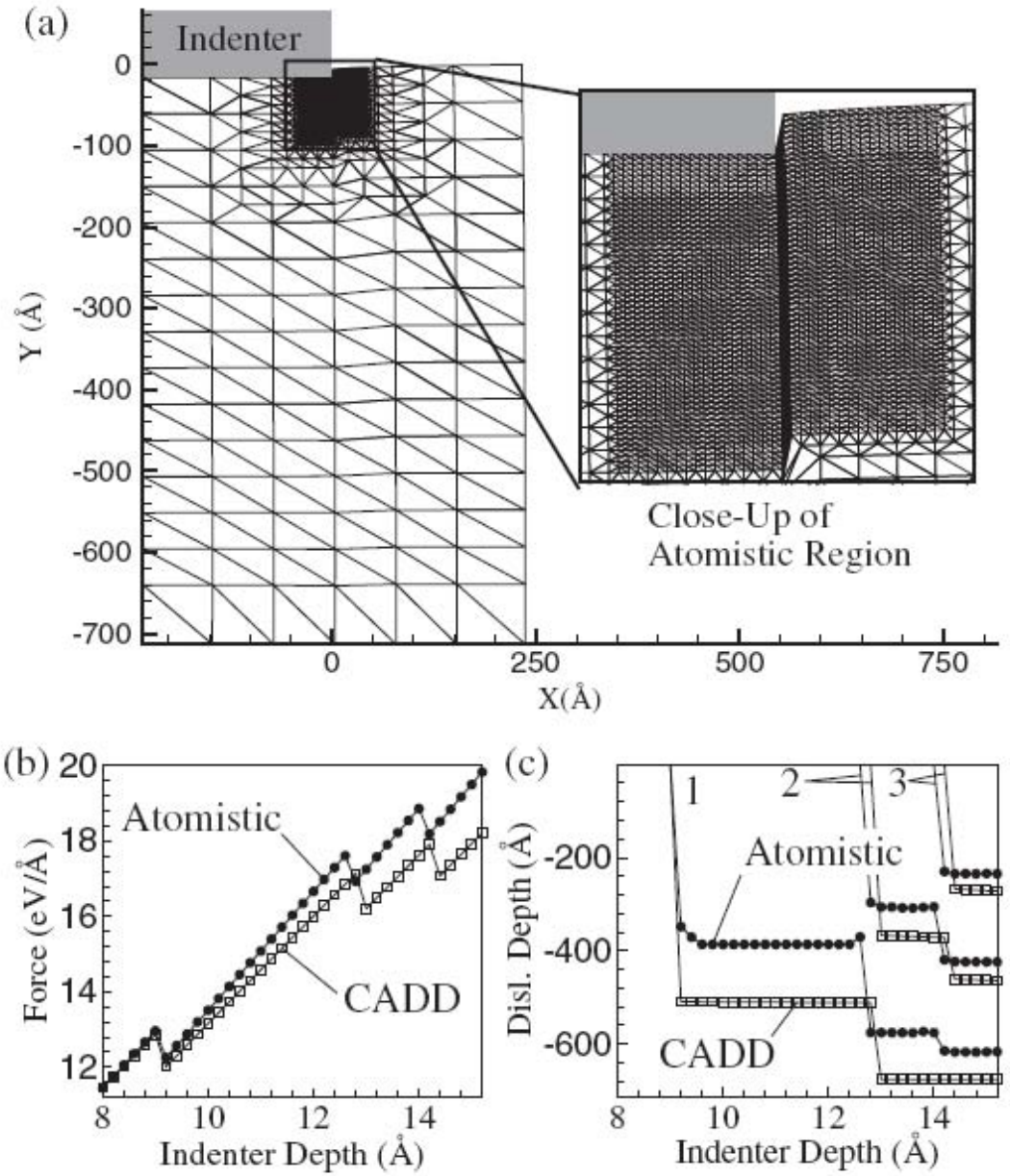
CADD method: Schematic



Coupling similar to MAAD approach; quasi-static conditions

Gurtin and coworkers, Brown, 2005

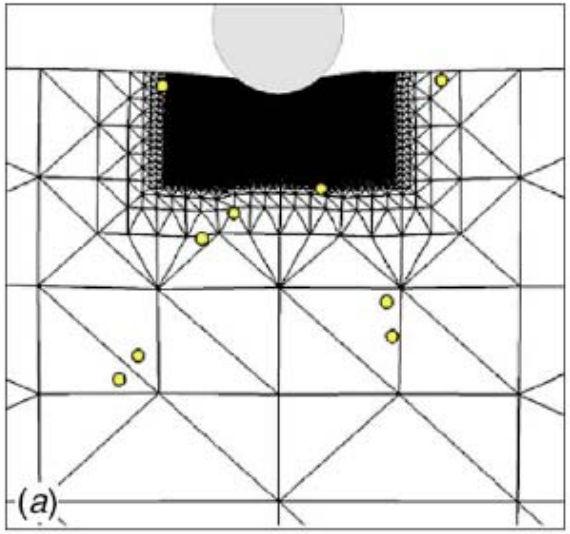
CADD method: Example results

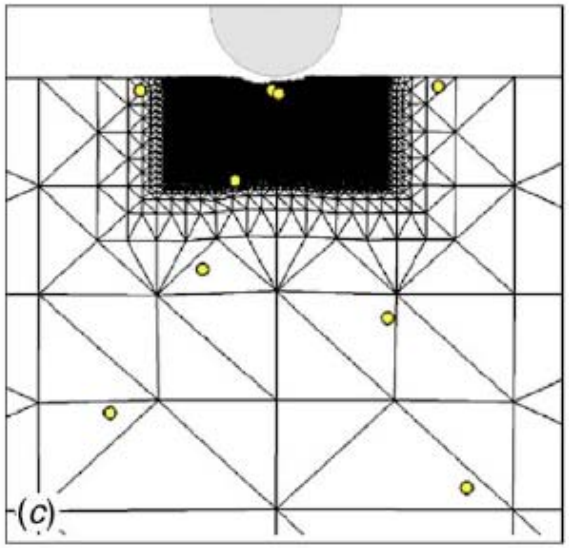


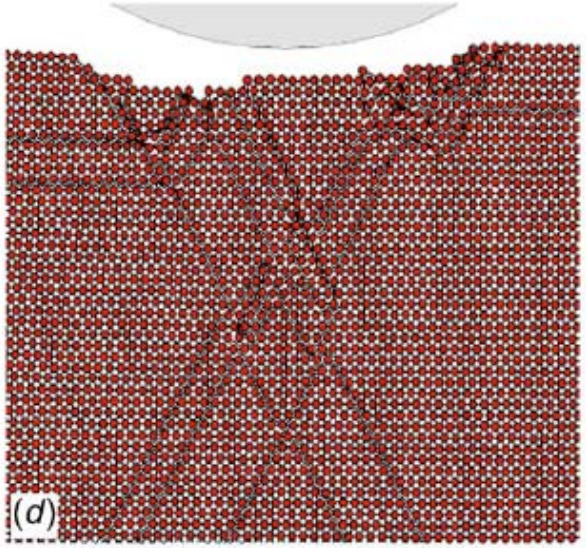
Gurtin and coworkers, Brown, 2005

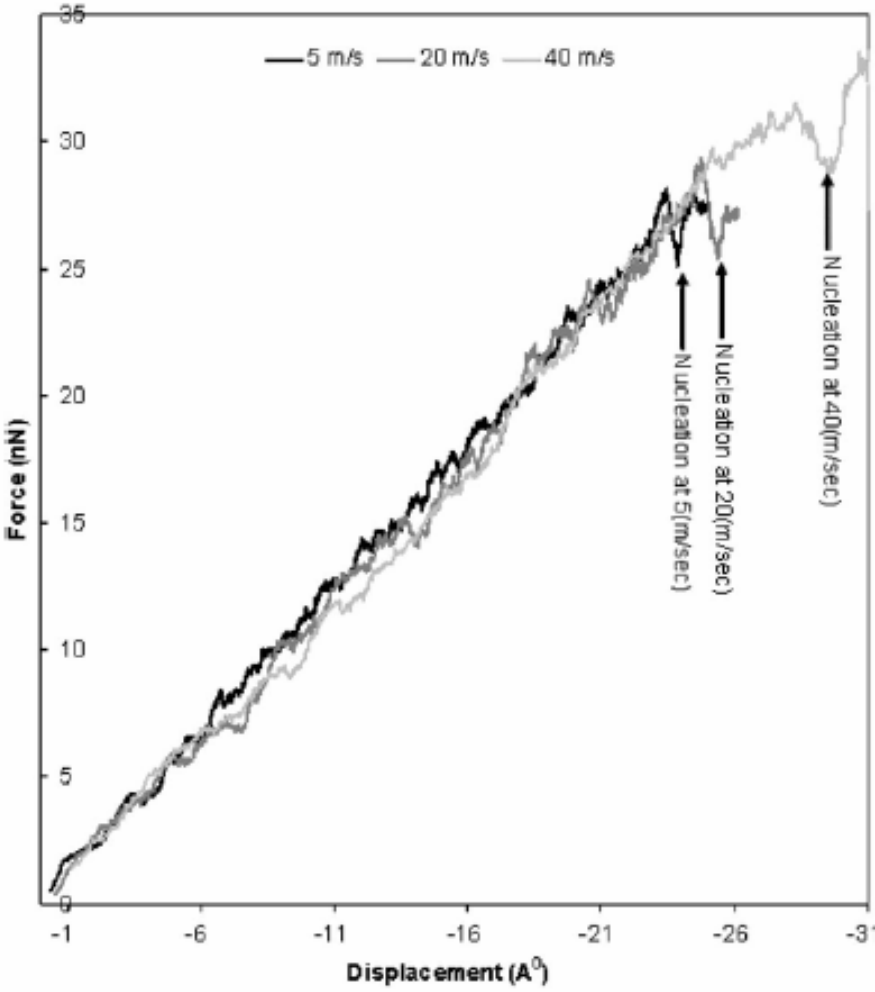
CADD method: Example results

Gurtin and coworkers, Brown, 2005









Dislocations nucleated in atomistic region move into FE domain

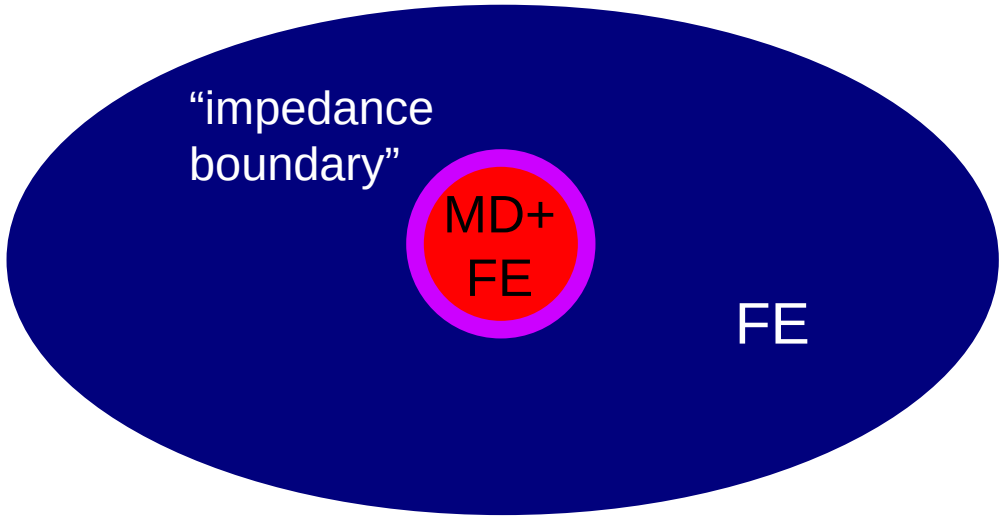
Coupling atomistic scale to continuum scale at finite temperature

The Bridging Scale Method (BSM)

Park, Wagner, Liu

Features of the bridging scale method

- FE representation exists everywhere in domain, also where MD is present
- Use projector operator to represent the displacement field as a orthogonal combination at
  - (i) small and
  - (ii) coarse scale
- Advantage: Atomistic and continuum scale do not have to be integrated using same time step (as e.g. in MAAD)
- High frequency oscillations naturally disappear when leaving the atomistic core region (via impedance force)
- Atomistic region senses finite temperature in FE region via stochastic force

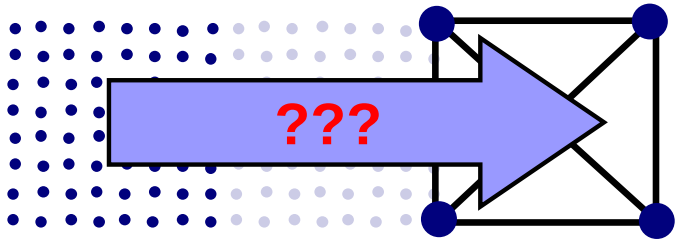


Park, Wagner, Liu

Eliminating atomistic degrees of freedom

- E.g. Adelman and Doll, 1976, use kernel function resulting in time-history dependent force added to boundary atoms (applied to 1D chain); physical meaning of the force: Dissipate energy into the eliminated degrees of freedom (avoid wave reflection)
- Kernel function difficult to obtain analytically (in particular in higher dimensions); therefore use numerical approaches (Cai *et al*., 2000, E and Huang, 2002)
- Kernel function for non-nearest neighbor interactions obtained by Park *et al*., 2005 (example: use EAM method for gold), computationally very efficient

FE BCs: Atomistic displacements



MD boundary condition: FE displacements
Plus kernel function forces,
plus stochastic force for EQ

Park, Wagner, Liu

The Bridging scale method: Concept

- Based on coarse/fine decomposition of displacement field $u(x)$:

$$u(x) = \bar{u}(x) + u'(x)$$

coarse **fine**

- Coarse scale defined to be projection of MD displacements $q(x)$ onto FEM shape functions N_I:

$$\bar{u}(x) = Pq(x) = \sum_I N_I(x) d_I$$

- P minimizes least square error between MD displacements $q(x)$ and FEM displacements d_I

G.J. Wagner and W.K. Liu, "Coupling of atomistic and continuum simulations using a bridging scale decomposition", *Journal of Computational Physics* 190 (2003), 249-274

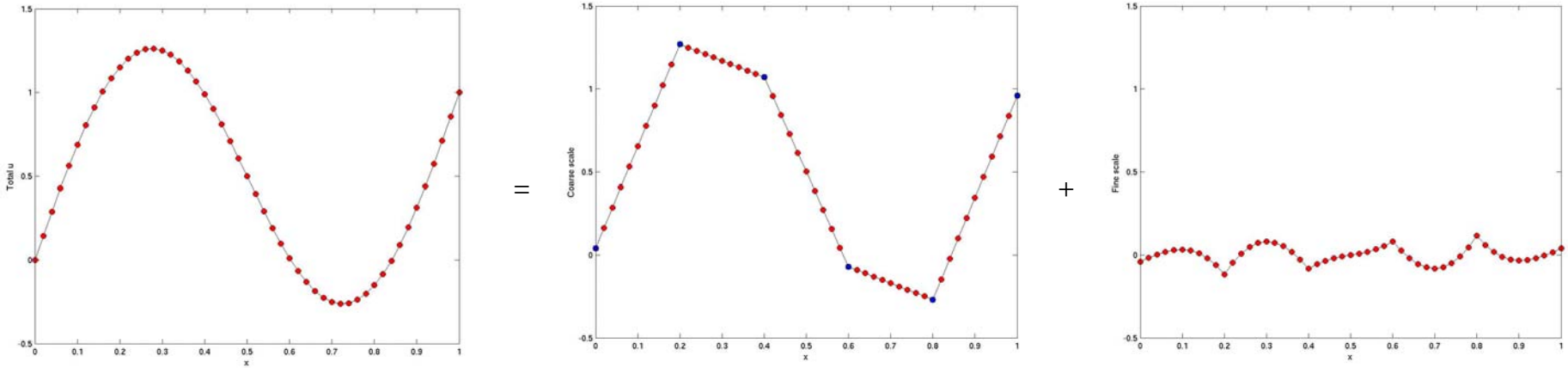
The Bridging scale method: Concept

- Fine scale defined to be that part of MD displacements *q(x)* that FEM shape functions cannot capture:

$$u'(x) = q(x) - Pq(x)$$

- Example of coarse/fine decomposition of displacement field (linearly independent of each other)

$u(x)$ = $\bar{u}(x)$ + $u'(x)$



(by G. Wagner, Park)

Important: Not necessary to refine FEM mesh to atomic scale

Multiscale Lagrangian

- Total displacement written as sum of coarse and fine scales:

$$u = Nd + q - Pq$$

- Write multiscale Lagrangian as difference between system kinetic and potential energies:

$$L(u, \dot{u}) = K(\dot{u}) - V(u)$$

- Multiscale equations of motion obtained via:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{d}}}\right) - \frac{\partial L}{\partial \mathbf{d}} = 0 \qquad \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right) - \frac{\partial L}{\partial \mathbf{q}} = 0$$

FE displacement Atomistic displacement

Slide courtesy H. Park

Coupled Multiscale Equations of Motion

$$\mathbf{M}_A \ddot{\mathbf{q}} = \mathbf{f}^{\text{int}}$$ Regular MD

$$\mathbf{M}_A \ddot{\mathbf{d}} = \mathbf{N}^{\mathbf{T}} \mathbf{f}^{\text{int}}(u)$$

Coupling term

Interatomic potential, e.g.

$$\phi_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$f^{\text{int}} = -\frac{\partial \phi(r)}{\partial r}$$

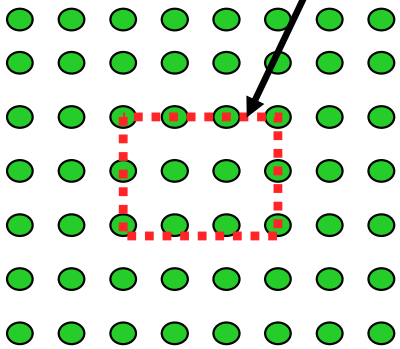
- First equation is MD equation of motion
- Second equation is FE equation of motion with internal force obtained from MD forces
- Kinetic energies (and thus mass matrices) of coarse/fine scales decoupled due to bridging scale term “Pq” (!)
- Note: FE equation of motion is *redundant* if MD and FE exist everywhere

Slide courtesy H. Park

Bridging Scale Schematic

Area of interest (e.g. crack)
Need atomistic information

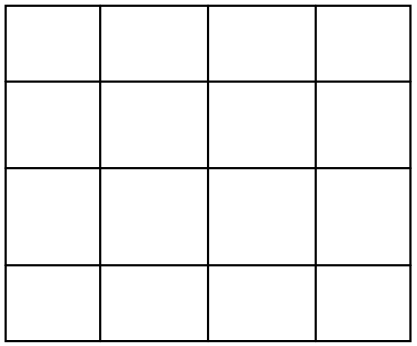
MD



$$\mathbf{M}_A\ddot{\mathbf{q}} = \mathbf{f}^{\text{int}}$$

+

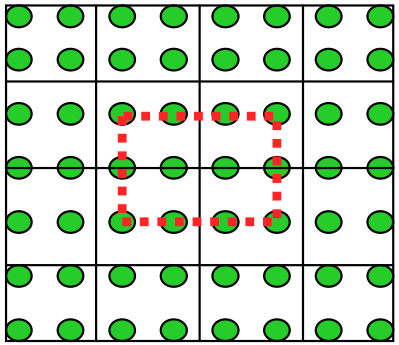
FEM



$$\mathbf{M}_A\ddot{\mathbf{d}} = \mathbf{N}^{\mathbf{T}}\mathbf{f}^{\text{int}}(u)$$

=

MD + FEM

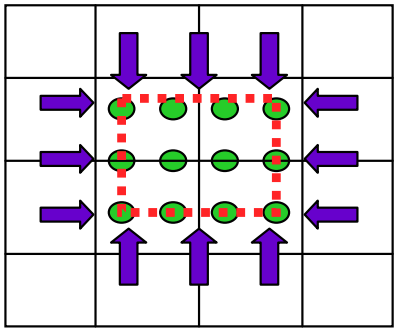


$$\mathbf{M}_A\ddot{\mathbf{q}} = \mathbf{f}^{\text{int}}$$

$$\mathbf{M}_A\ddot{\mathbf{d}} = \mathbf{N}^{\mathbf{T}}\mathbf{f}^{\text{int}}(u)$$

equivalent

Reduced MD & Impedance Force + FEM



$\mathbf{f}^{\text{imp}}$

$$\mathbf{M}_A\ddot{\mathbf{q}} = \mathbf{f}^{\text{int}} + \mathbf{f}^{\text{imp}}$$

$$\mathbf{M}_A\ddot{\mathbf{d}} = \mathbf{N}^{\mathbf{T}}\mathbf{f}^{\text{int}}(u)$$

Impedance force

$$\mathbf{f}^{\text{imp}}(t) = \int_0^t \boldsymbol{\Theta}(t-\tau)(\mathbf{q}(\tau) - \bar{\mathbf{u}}(\tau))\,\mathrm{d}\tau + \mathbf{R}(t)$$

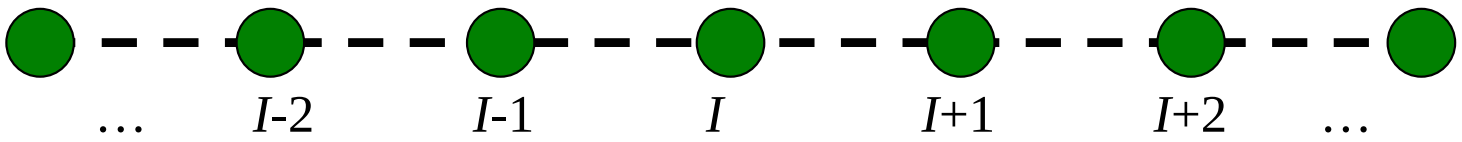
Random force (T)

Slide courtesy H. Park, Wagner *et al.*

Impedance force **f** and kernel θ

- θ is typically a mxm matrix, where m is the number of degrees of freedom in the boundary region
- To obtain θ need to calculate dynamics long enough to capture all impedance effects (involving Laplace transform): Computational challenge
- Karpov, Wagner *et al.*: For crystalline lattices the impedance force matrix is much simplified by relying on lattice response functions (also known as lattice dynamics Green's functions)
- Then: θ is m_Bxm_B (m_B number of DOF in Bravais lattice)

Example:

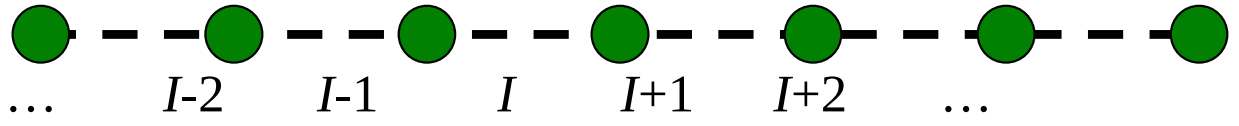


1D string of atoms

Park, Liu, Wagner *et al.*

One-dimensional example

Semi-discrete EOM:



$$\begin{pmatrix} m\ddot{u}_{I-1} \\ m\ddot{u}_I \\ m\ddot{u}_{I+1} \end{pmatrix} = \begin{pmatrix} f^{\text{ext}}_{I-1} \\ f^{\text{ext}}_I \\ f^{\text{ext}}_{I+1} \end{pmatrix} - \begin{pmatrix} 2K & -K & 0 \\ -K & 2K & -K \\ 0 & -K & 2K \end{pmatrix} \begin{pmatrix} u_{I-1} \\ u_I \\ u_{I+1} \end{pmatrix}$$

$$K = AE/l_e$$

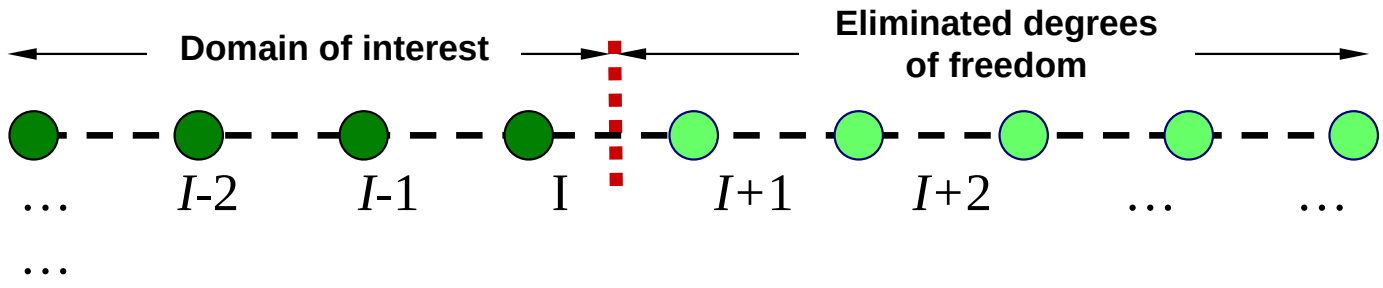
Stiffness coefficients; from potential:

$$K = \frac{\partial^2 \phi(r)}{\partial r^2} = \frac{624\varepsilon\sigma^{12}}{r^{14}} - \frac{168\varepsilon\sigma^{6}}{r^{8}}$$

$$f_I^{\text{int}} = Ku_{I-1} - 2Ku_I + Ku_{I+1}$$ Repetitive structure

$$\theta(t) = \frac{2}{t} J_2(2\omega t) \qquad \omega = (\sqrt{E/\rho})/l_e$$ (ρ density, l_e length of element)

J_2 is a second order Bessel function

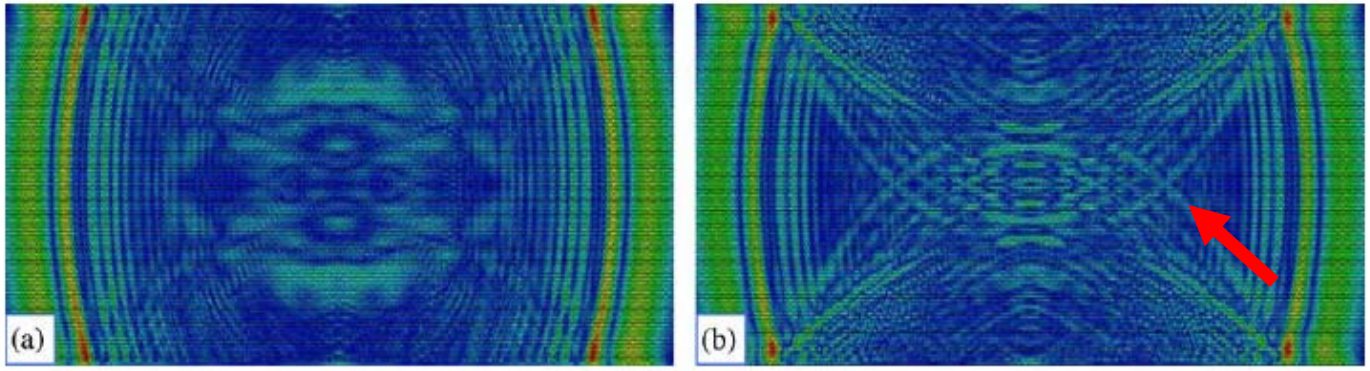


$$f_I^{\text{int}} = Ku_{I-1} - 2Ku_I + K\int_0^t \theta(t-\tau)u_I(\tau)\,\mathrm{d}\tau$$

Equation accounts for all eliminated nodes in FE region (right)

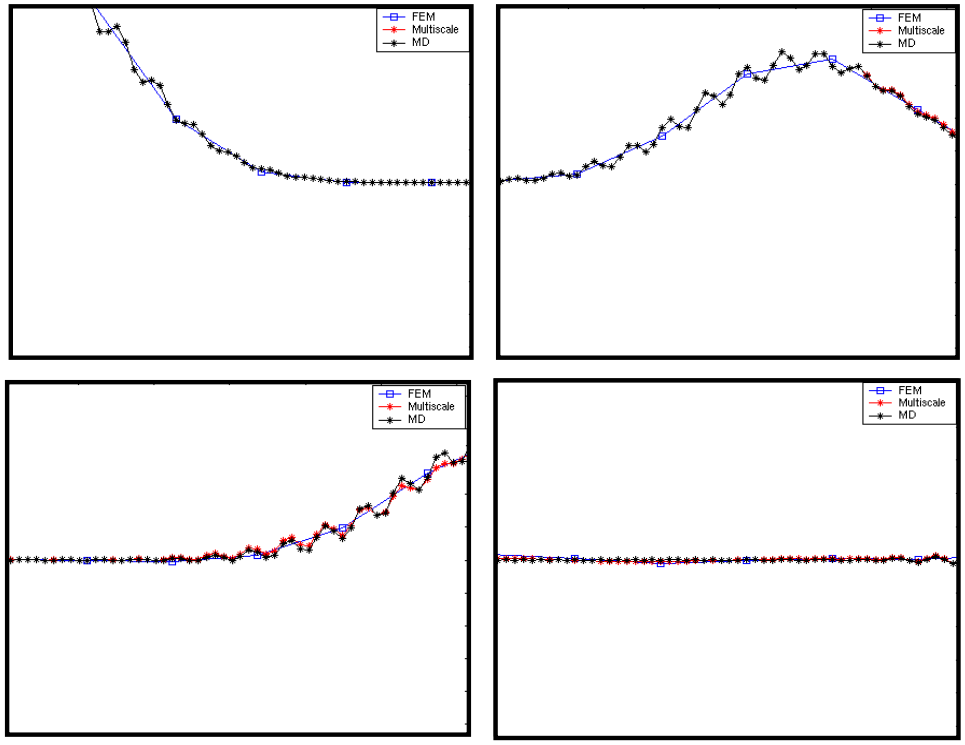
Park, Liu, Wagner *et al.*

Wave propagation across atomistic-continuum interface



With impedance force

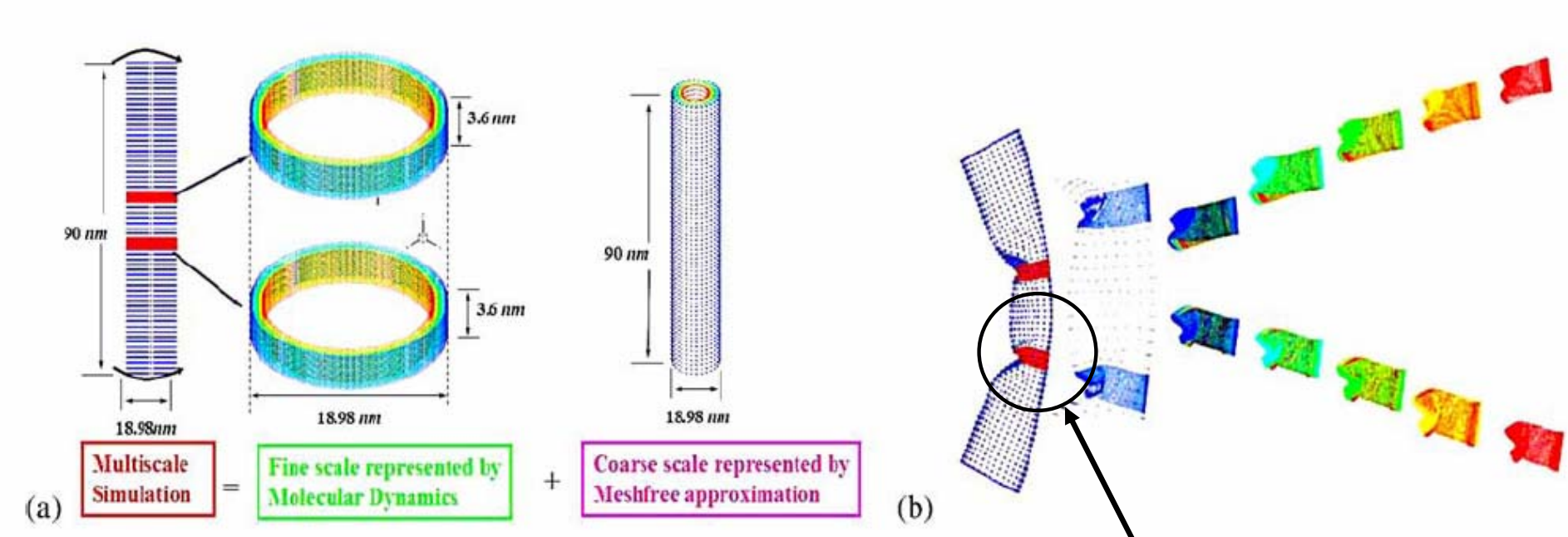
No impedance force



Example:
1D string of atoms

Park, Liu, Wagner *et al.*

BSD: Example application



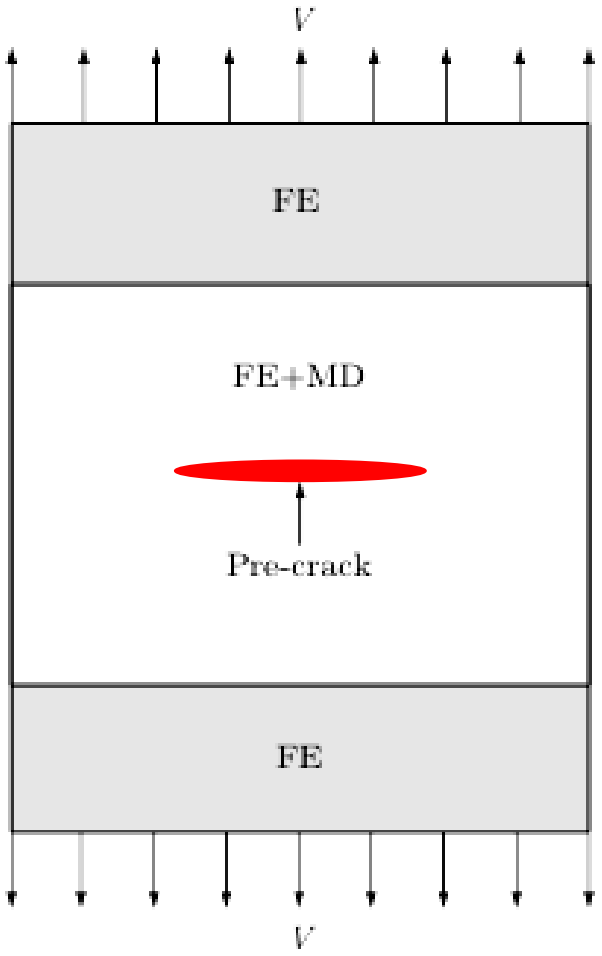
Original system: 3,000,000 atoms
Reduced to: 27,450 particles

Reveals atomistic structure at the kinks

Bending of a carbon nanotube: Model defects using molecular dynamics methods, the rest using FE description; quasi-static application (0K)

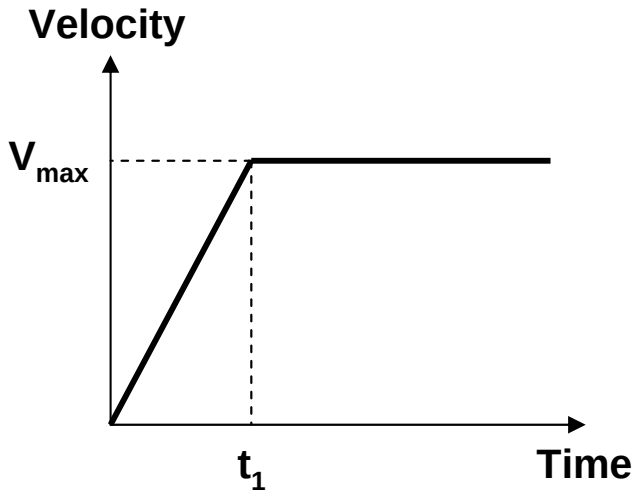
Wagner and Liu, 2004

2D Bridging Scale Dynamic Crack Propagation



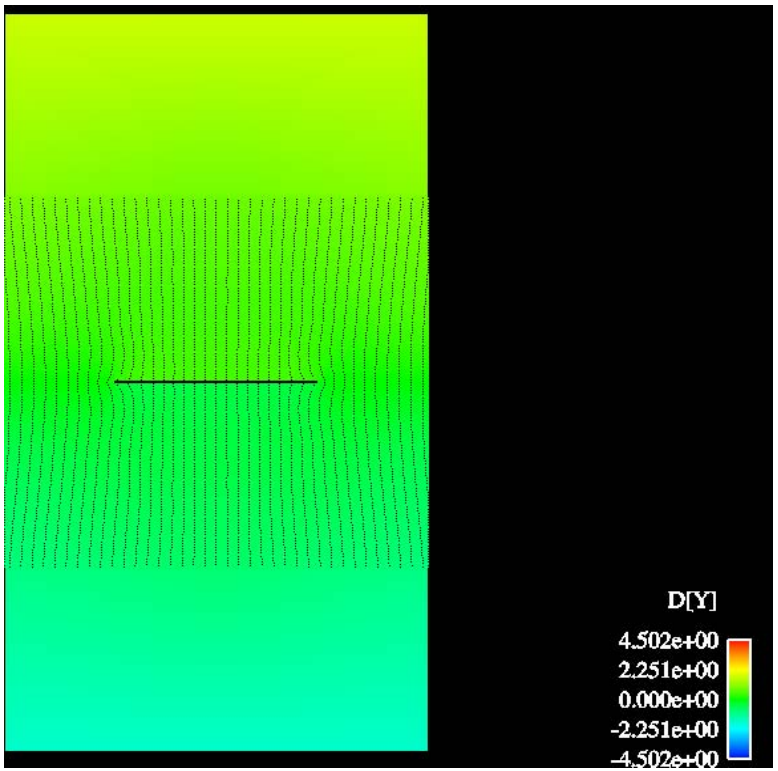
Problem Description

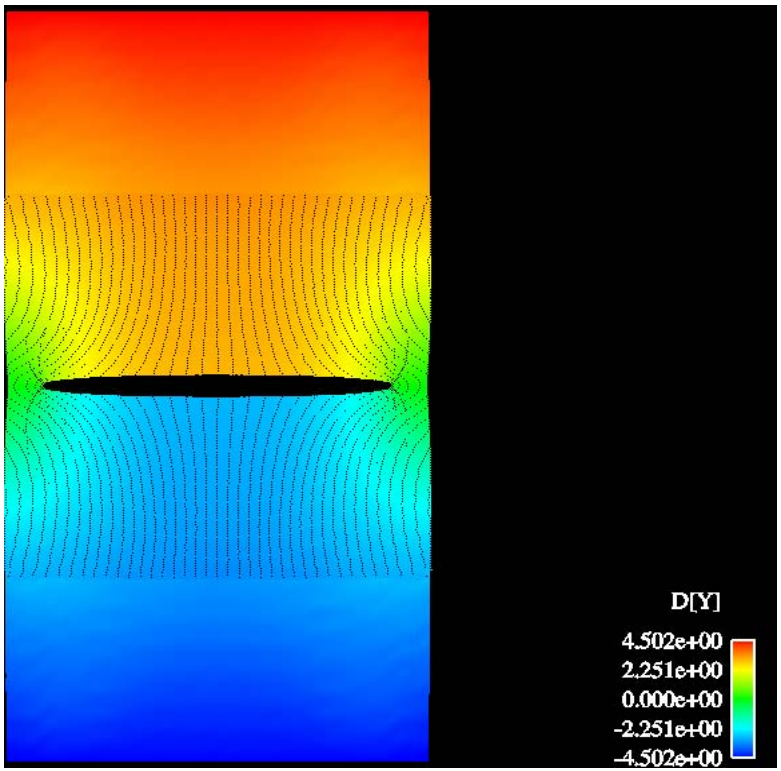
- 90,000 atoms, 1,800 finite elements (900 in coupled region)
- Full MD = 180,000 atoms
- 100 atoms per finite element
- $\Delta t_{FE}=40\Delta t_{MD}$
- Ramp velocity BC on FEM



Park et al., 2005

2D Bridging Scale Dynamic Crack Propagation





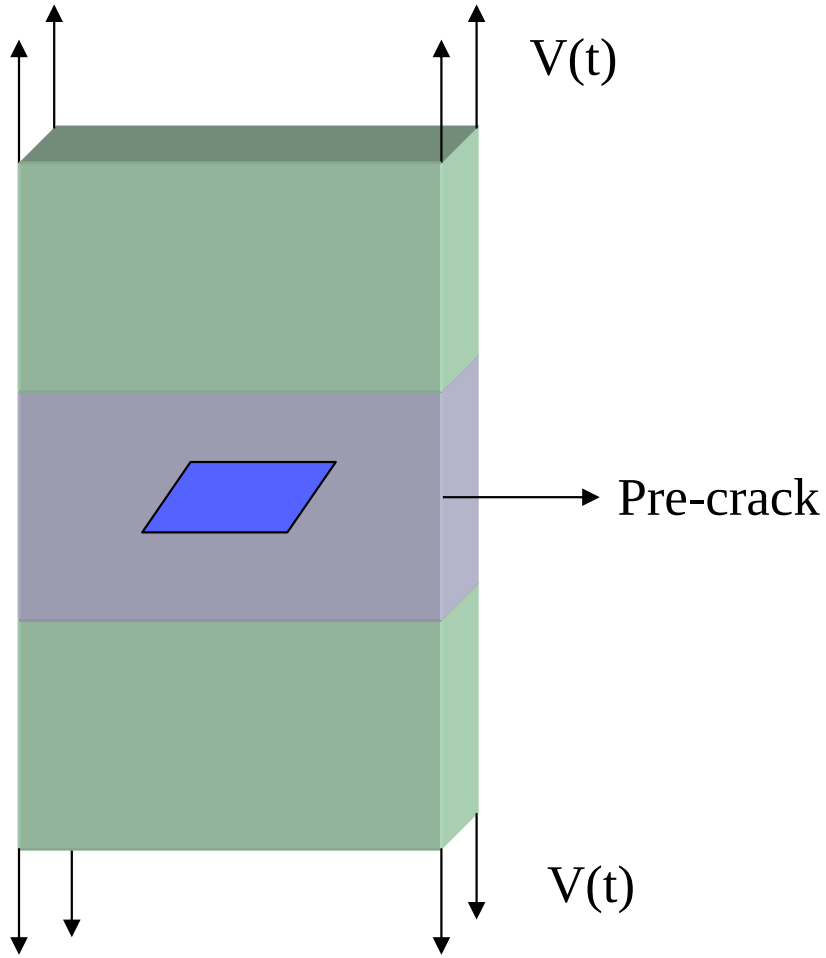
- Beginning of crack opening

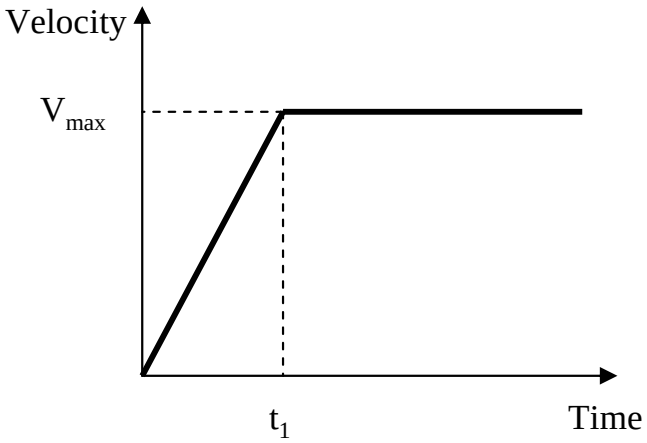
- Crack propagation just before complete rupture of specimen

Park et al., 2005

3D Bridging Scale Dynamic Crack Propagation

- 3D FCC lattice
- Lennard Jones 6-12 potential
- Each FEM = 200 atoms
- 1000 FEM, 117000 atoms
- Fracture initially along (001) plane

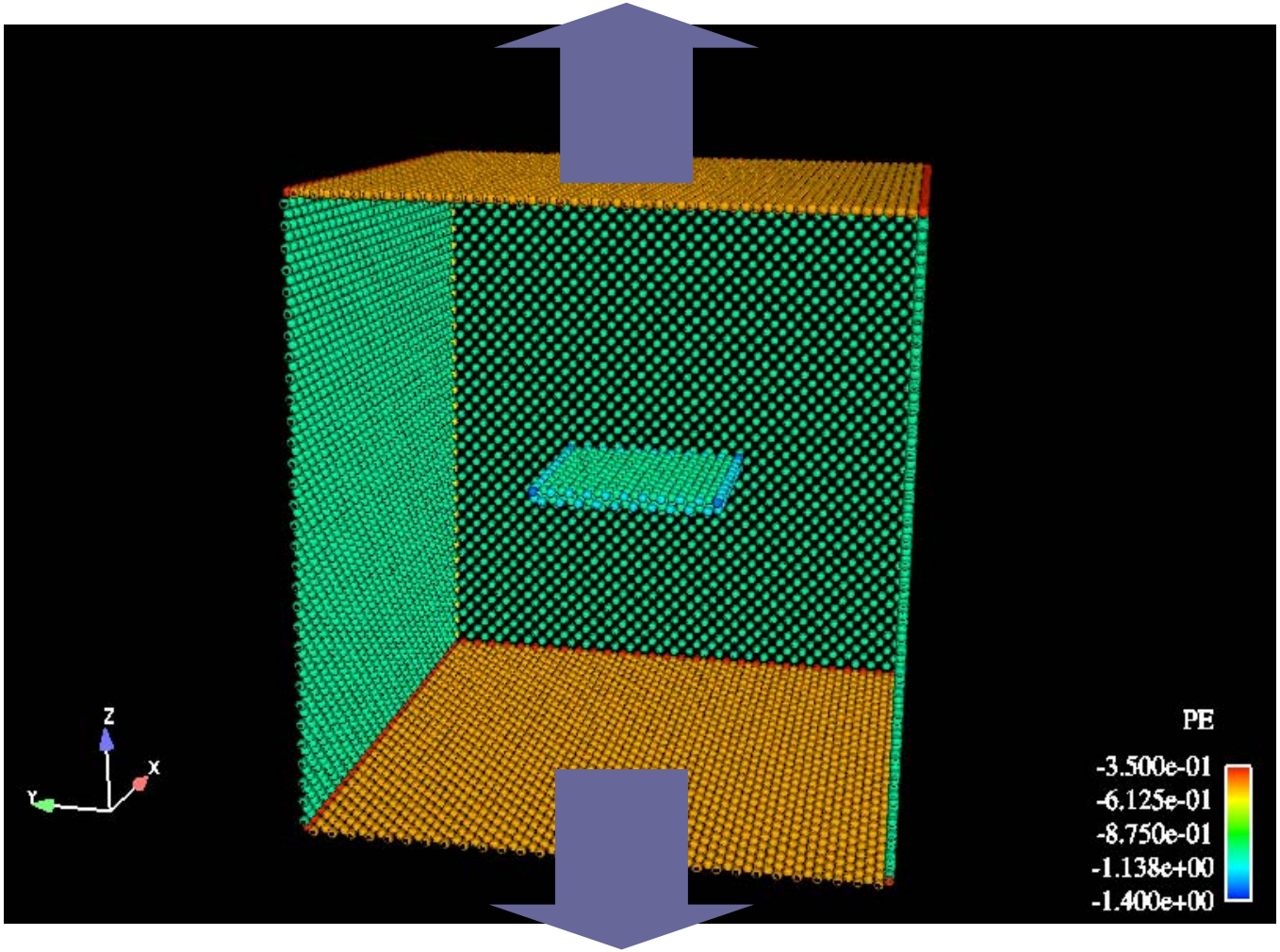




Park et al., 2005

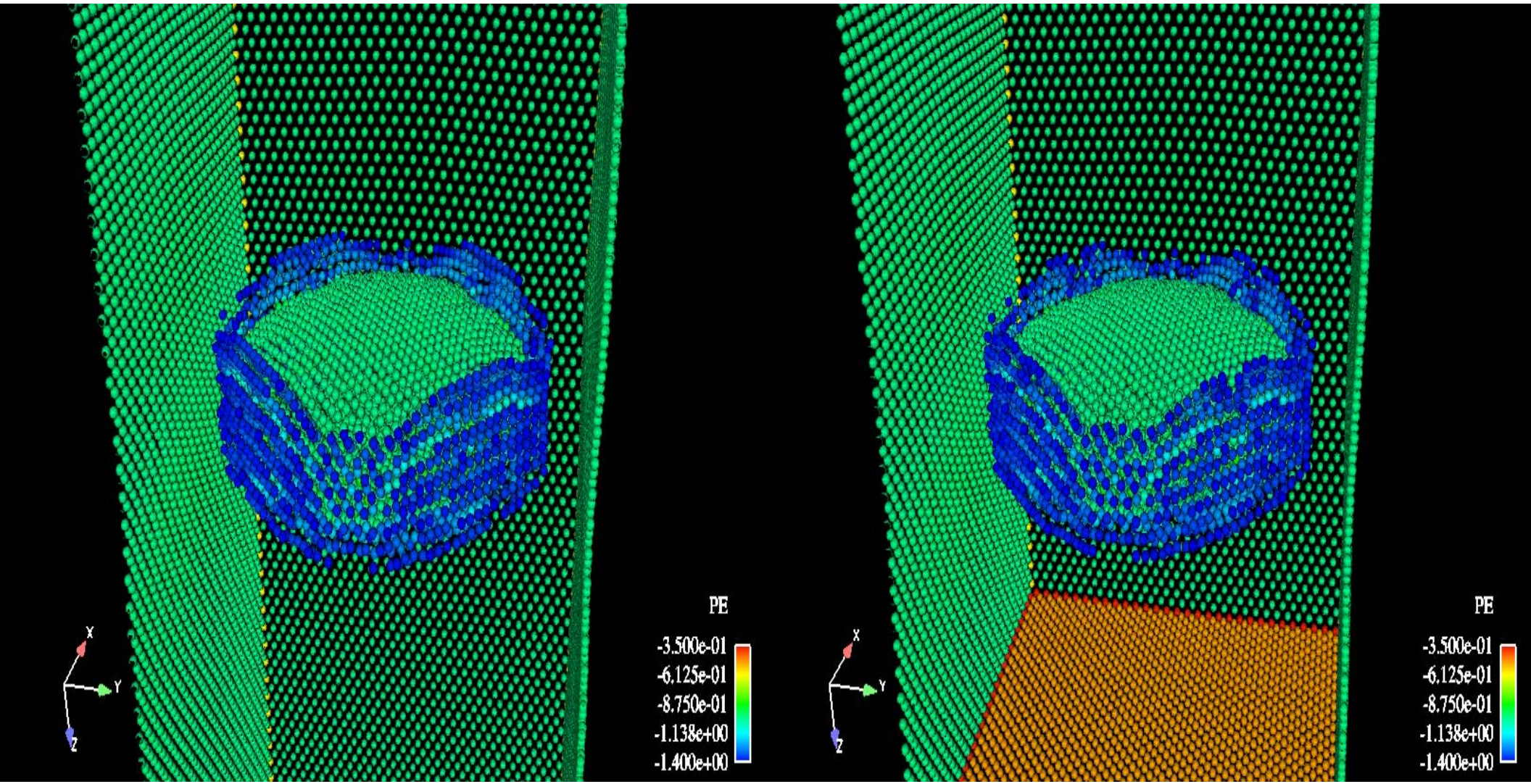
Initial Configuration and Loading

- Velocity BC applied out of plane (z-direction)
- All non-equilibrium atoms shown



Park et al., 2005

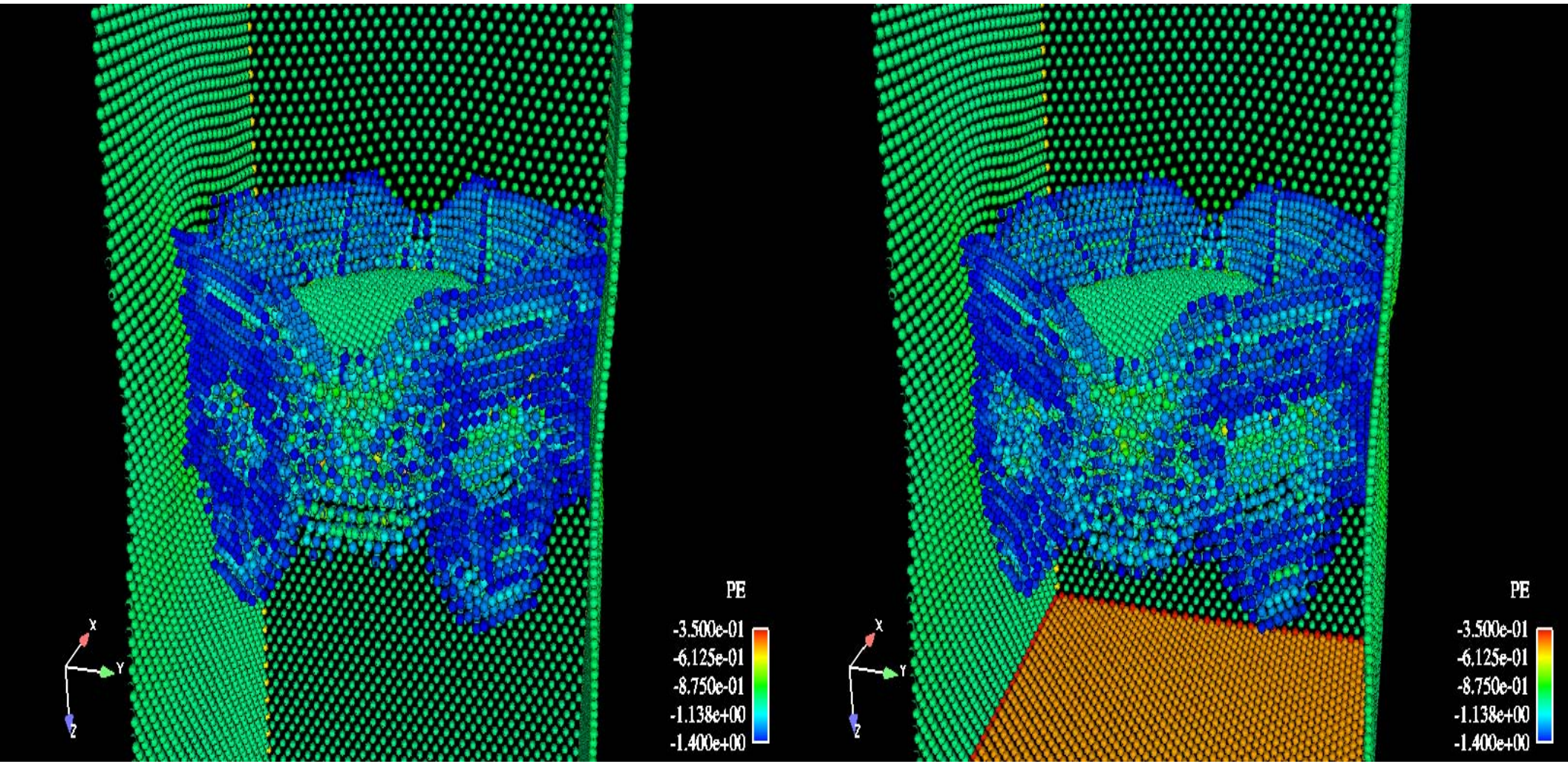
3D Bridging Scale Dynamic Crack Propagation



- Full MD
- Bridging Scale

Park et al., 2005

3D Bridging Scale Dynamic Crack Propagation



- Full MD
- Bridging Scale

Park et al., 2005

Additional references related to the Bridging Scale Method

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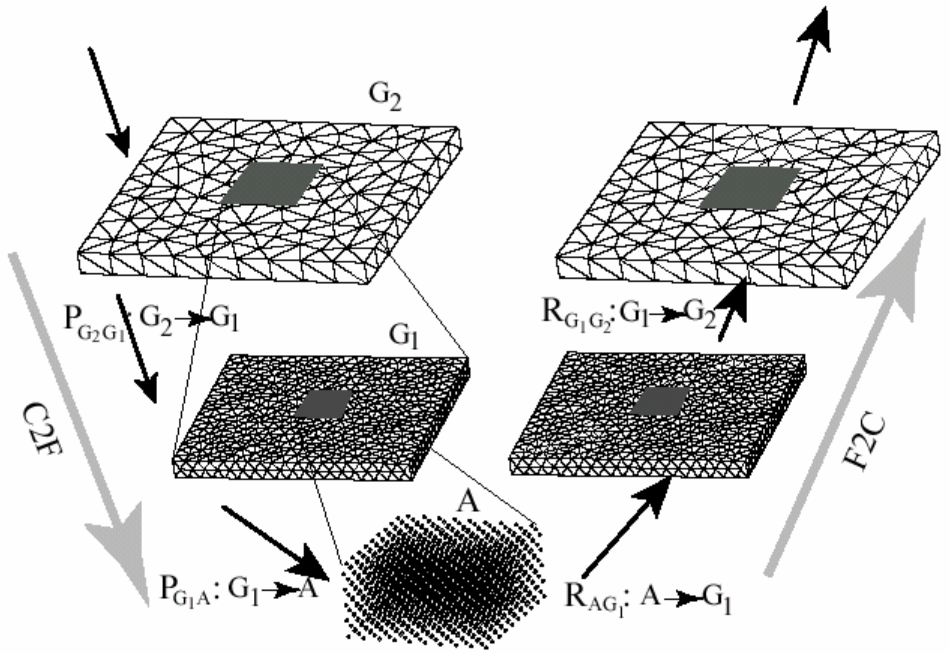
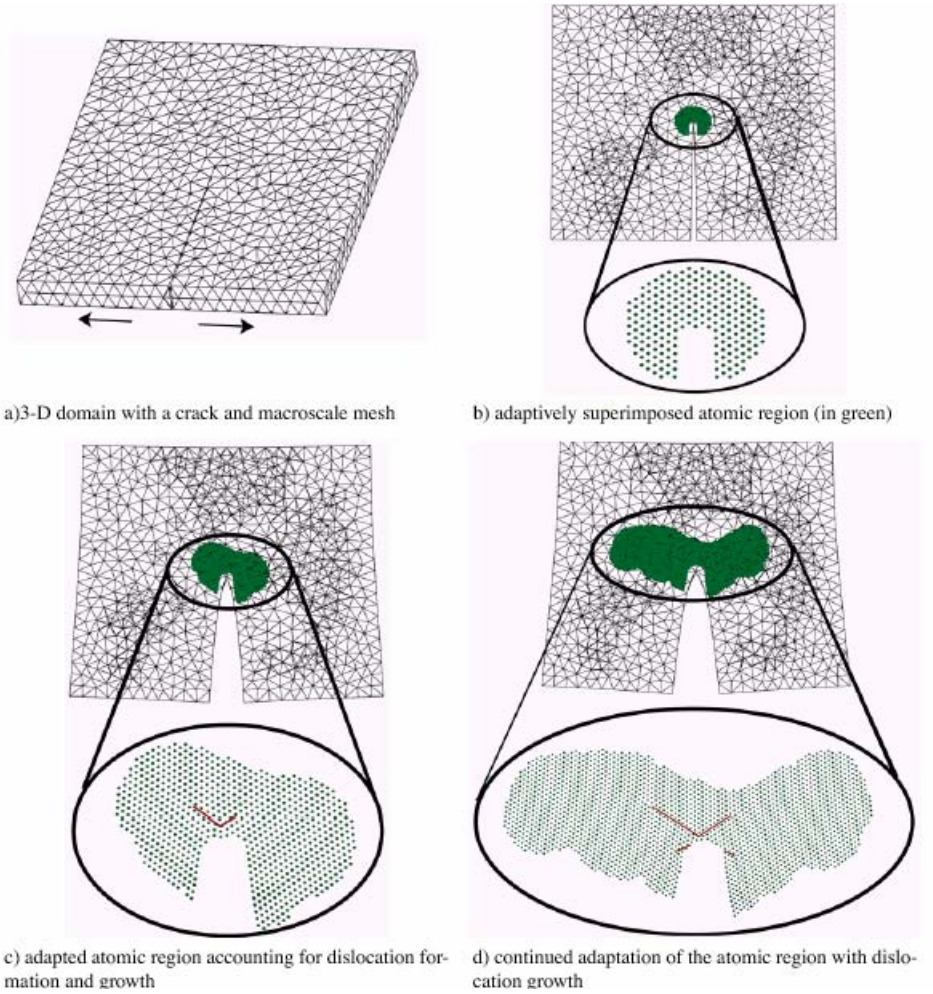
Concurrent Atomistic-Continuum Modeling
An Adaptive Multigrid Formulation

The multigrid idea applied to concurrent atomistic-continuum modeling



Results of adaptive selection of the atomistic region at the crack tip at various loads



a)3-D domain with a crack and macroscale mesh

b) adaptively superimposed atomic region (in green)

c) adapted atomic region accounting for dislocation formation and growth

d) continued adaptation of the atomic region with dislocation growth

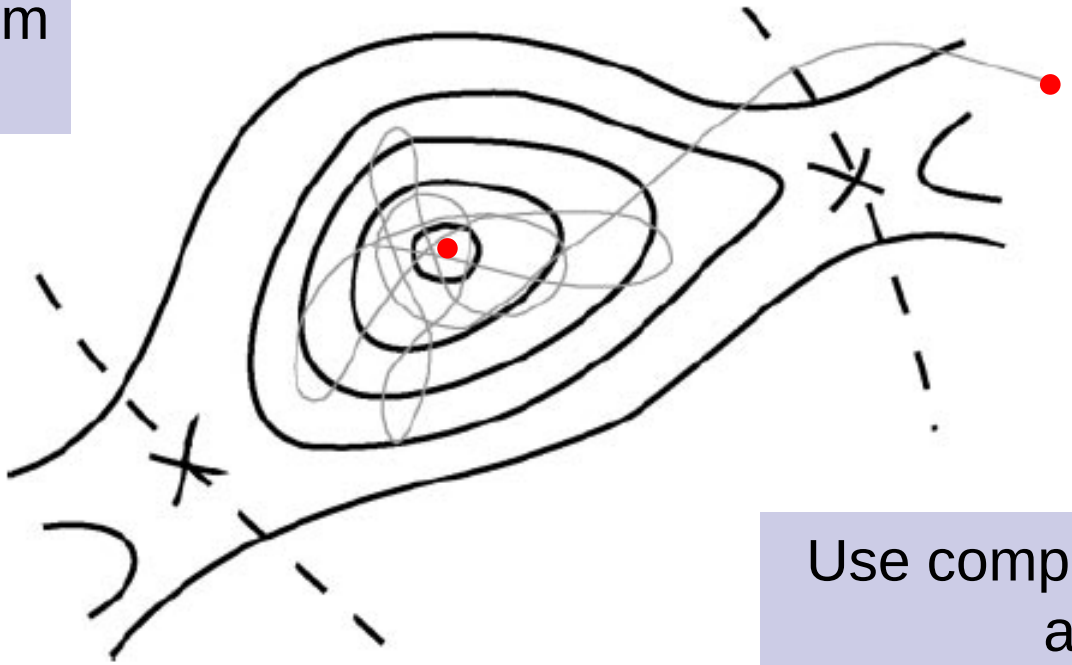
Slide courtesy R. Picu

D. Datta, R.C. Picu, M. Shephard, Int. J. Multiscale Comput. Eng., 2004

Outlook: Bridging time scales

- Similar to bridging length scales, the bridging of time scales is a similarly difficult (maybe more difficult…) matter
- In past years, many methods have been proposed; among the most prominent ones are bias potential methods, temperature accelerated dynamics, or parallel replica methods (many more)…

How to escape from local basin?

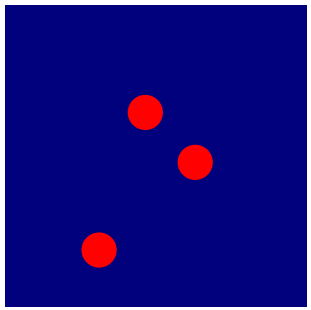


Use computational methods to achieve rapid escape

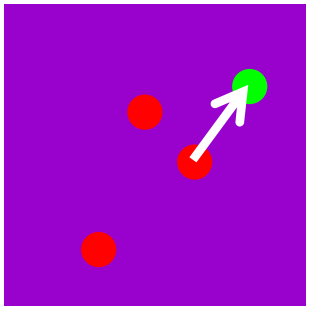
http://www.t12.lanl.gov/home/afv/publications.html;
http://www.t12.lanl.gov/home/afv/acceleratedynamics.html

Outlook: Bridging time scales

- **Example**:
  Temperature accelerated dynamics (TAD); developed by Art Voter
  Can reach up to microseconds and longer, while retaining atomistic length scale resolution



System of interest
(low temperature T_0)



Sample for state transitions at high temperature T_1)

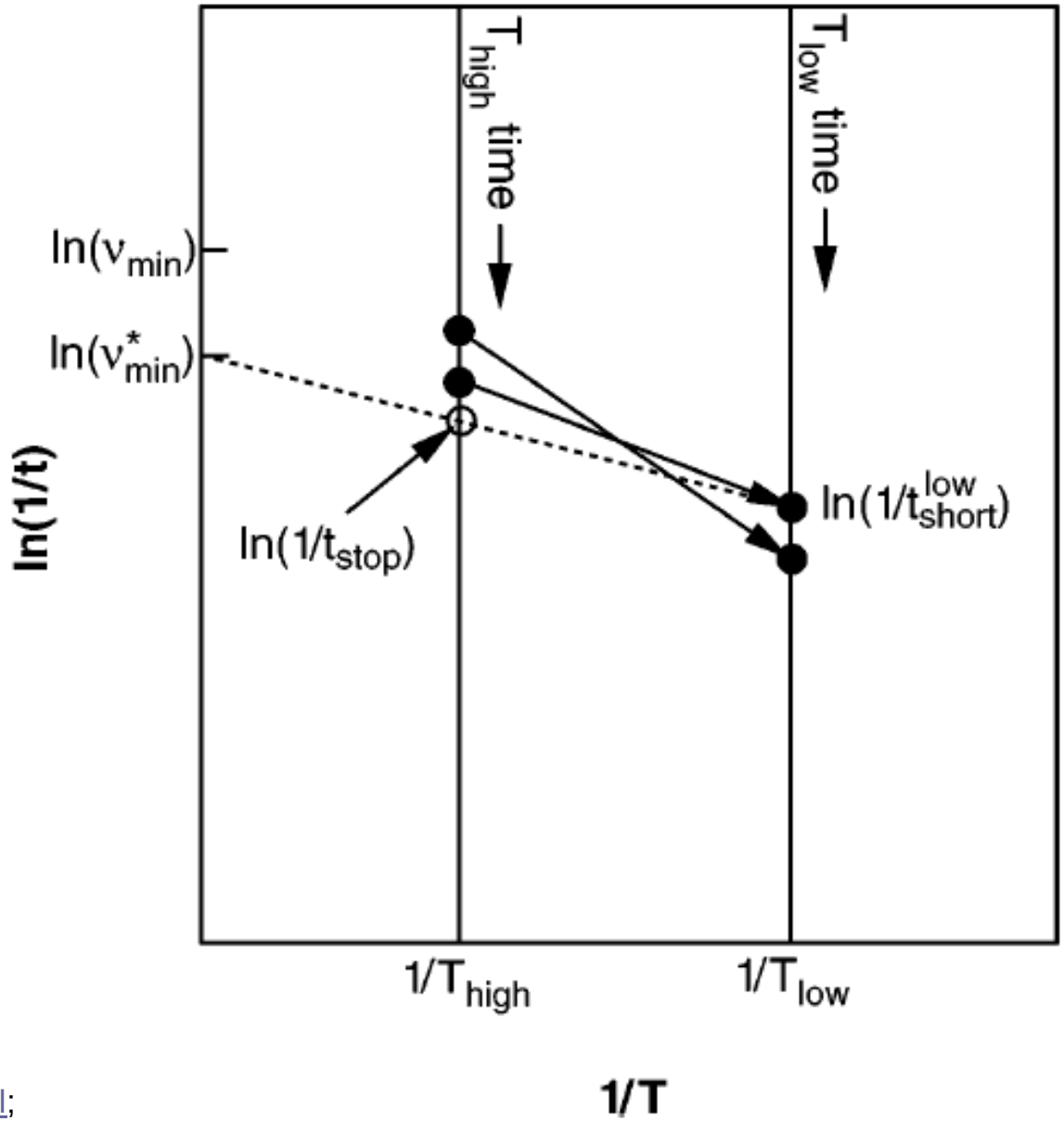
Using transition state theory, calculate when this event would have happened at low temperature

$$t_{high,stop} \equiv \frac{\ln(1/\delta)}{\nu_{min}} \left(\frac{\nu_{min} t_{low,short}}{\ln(1/\delta)} \right)^{T_{low}/T_{high}}$$

http://www.t12.lanl.gov/home/afv/publications.html;
http://www.t12.lanl.gov/home/afv/acceleratedynamics.html

Outlook: Bridging time scales

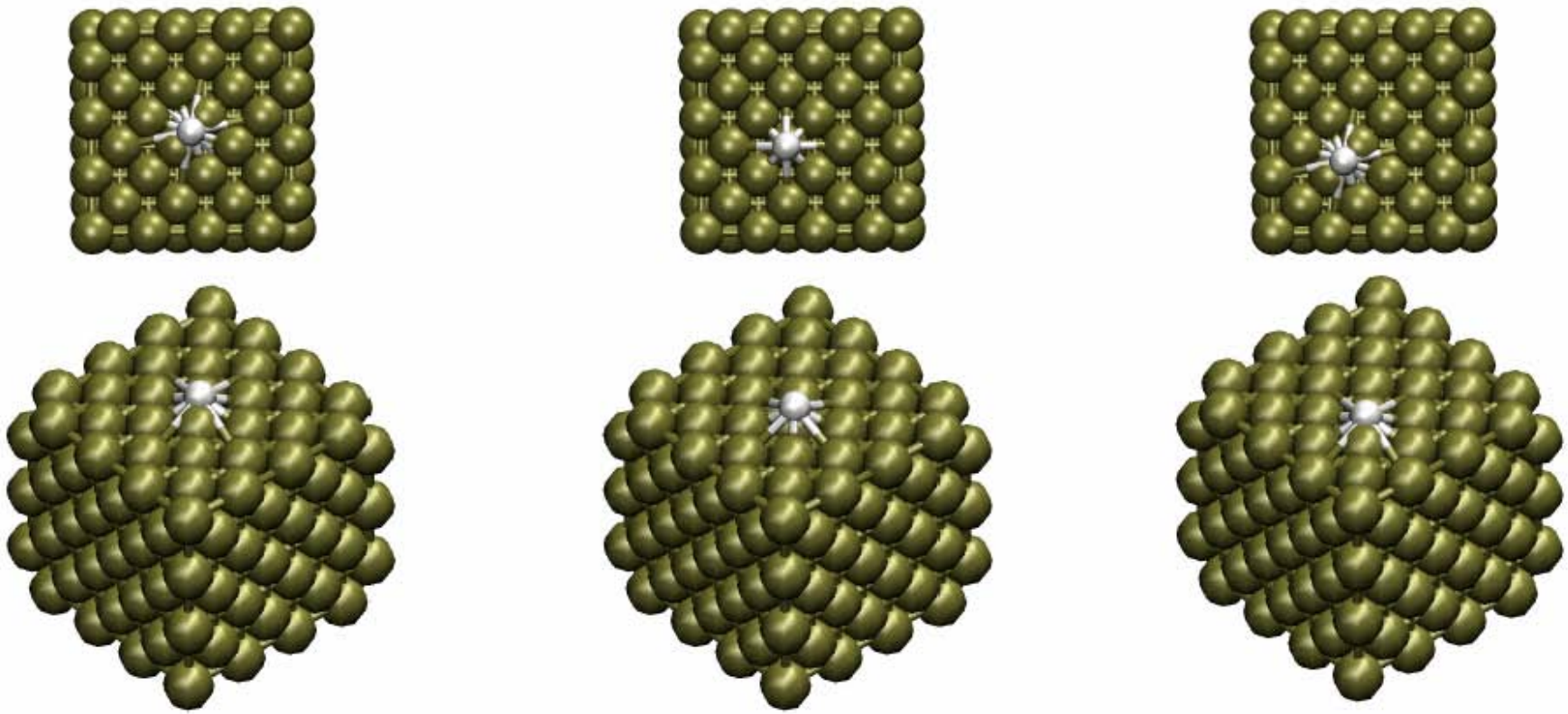
- Knowing time at high temperature allows to estimate dynamics at lower temperature



http://www.t12.lanl.gov/home/afv/publications.html;
http://www.t12.lanl.gov/home/afv/acceleratedddynamics.html

Diffusion of H on Pt: Reactive description with ReaxFF

TAD low temperature 400 K (high sampling temperature 1300 K)



State 1 → State 2 → State 3 (equiv. to state 1)

Δt = 1.33E-8 sec
AE = 0.512 eV

Δt = 2.131E-10 sec
AE = 0.252 eV

(Buehler, Goddard *et al.*, in collaboration with Art Voter, LANL)

ReaxFF interfaced with TAD through CMDF

Discussion and conclusion

- Concurrent scale-coupling techniques have evolved significantly in the past 10 years
- Now, robust and stable methods become available applicable to an increasingly wider range of problems
- Finite temperature applications remain a subject of ongoing research
- Concurrent multi-scale methods are readily available, and simulation codes can be downloaded from websites (e.g. www.qcmethod.com)
- However, using the codes can be quite difficult and results should be interpreted with care
- Some researchers think that concurrent coupling is difficult and associated with many numerical and physical difficulties, and therefore favor hierarchical methods as a cleaner way to convey information across the scales

Acknowledgements

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  - Catalin Picu (RPI)
  - Gang Lu (SUCN)
  - Dan Negrut (ANL)

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  - Avoids difficulties of finite temperature; established for 0K
- Coupled Atomistic/Discrete Dislocation method (CADD)
  - L. Shilkrot, R.E. Miller and W.A. Curtin, *Journal of the Mechanics and Physics of Solids* 2004; 52:755-787
- Bridging Domain method
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- Review articles:
  - W.A. Curtin and R.E. Miller, *Modelling and Simulation in Materials Science and Engineering* 2003; 11:R33-R68
  - W.K. Liu, E.G. Karpov. S. Zhang and H.S. Park, *Computer Methods in Applied Mechanics and Engineering* 2004; 193:1529-1578

Slide courtesy H. Park