Mixed continuum/atomistic models: The quasi-continuum method

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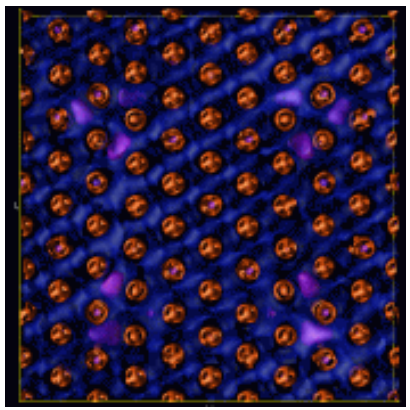
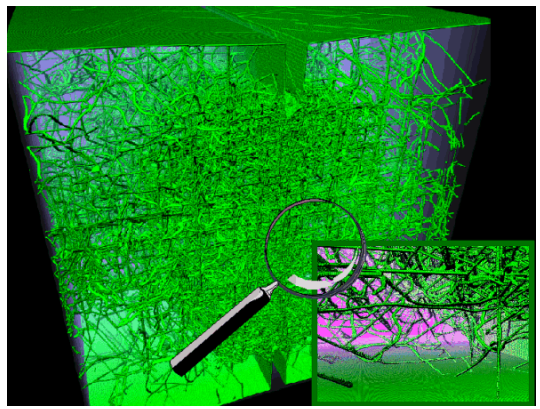
Limits of discrete models

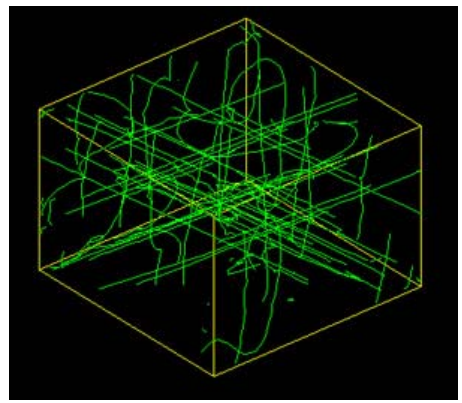
- First-principles calculations: Dislocation cores, dipoles, quadrupoles… ~ 10^3 atoms (T. Arias ’00)
- Molecular dynamics: Empirical potentials… ~ 10^9 atoms (F. Abraham ’03)
- Linear elasticity: Dislocation dynamics, L ~ 10^6b, ε ~ 1% (Bulatov et al. ’03)



Ta quadrupole
(T. Arias ´00)

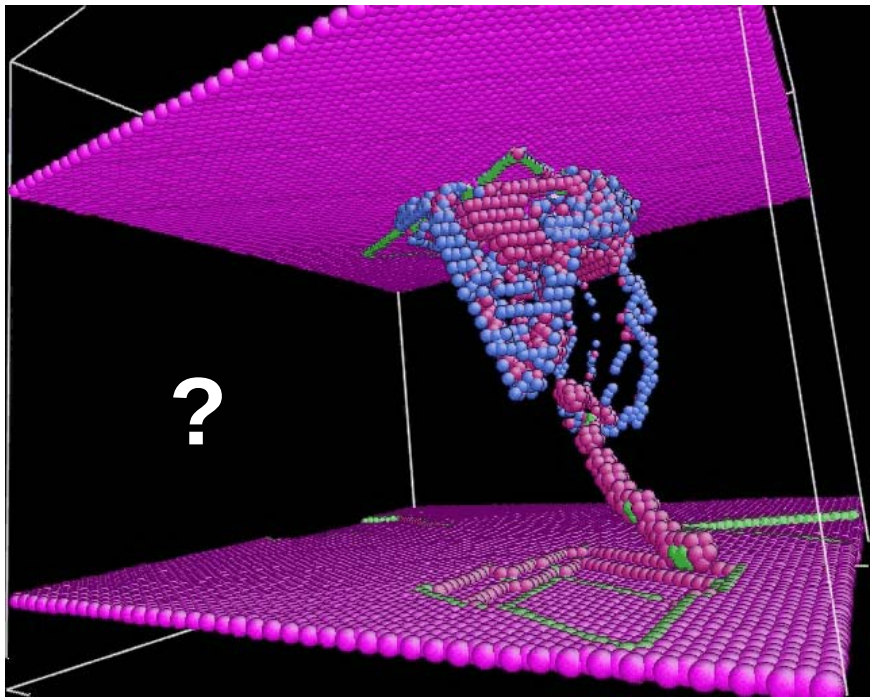


FCC ductile fracture
(F.F. Abraham ´03)



FCC dislocation dynamics
(M. Rhee et al.´02)

Au (111) nanoindentation – MD analysis



Li, J., K.J. Van Vliet, T. Zhu, S. Yip, S. Suresh, "Atomistic mechanisms governing elastic limit and incipient plasticity in crystals", *Nature*, **418**, (2002), 307.

- Early stages of indentation mediated by a defects → Need atomistics
- But elastic (long range) field important → large cells
- Indenter sizes ~ 70 nm, film thickness ~ 1 μm → large cells
- The vast majority of atoms in MD calculations move according to smooth elastic fields → MD wasteful!
- Mixed continuum/ atomistic description.

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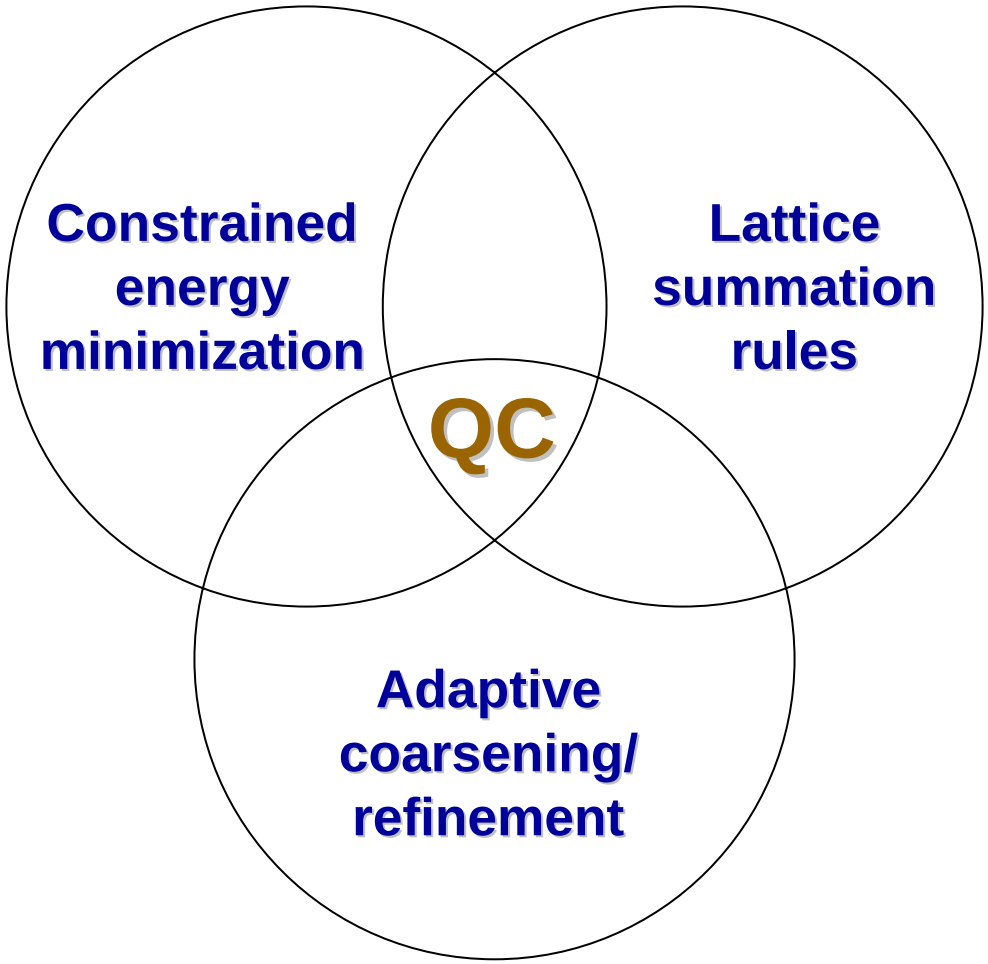
Multiscale continuum/atomistic models

- Objective: One model which bridges atomistic and continuum descriptions seamlessly, i.e., contains atomistic and continuum limits as special cases.
- All physics should be defined at the fundamental (atomistic) level (e.g., empirical potentials, DFT).
- Coarse-graining should not introduce additional physics or assumptions (e.g., random noise, viscosity, thermostats, thermodynamic equilibrium…).
- Coarsening/refinement should be:
  - ***Inhomogeneous*** *(e.g., full atomistics within defect cores, continuum-like behavior away from defects)*
  - ***Adaptive****, i.e., local resolution should be provided by the method itself as part of the solution.*

The quasicontinuum (QC) method, T=0

Tadmor, Ortiz and Phillips,*Phil. Mag. A*, **76** (1996) 1529.

Knap and Ortiz, *J. Mech. Phys. Solids*, **49** (2001) 1899.



Lattice statics – Problem definition

- Reference configuration: Atoms arranged as a subset of a *simple Bravais lattice*.
- $\mathcal{L} \subset \mathbb{Z}^3 \equiv$ Enumeration of atoms in ensemble.
- Atom positions in reference configuration:

$$\boldsymbol{X}(\boldsymbol{l}) = l^i \boldsymbol{a}_i, \quad \boldsymbol{l} \in \mathcal{L}$$

- Positions of atoms *after deformation*:

$$\boldsymbol{q} \equiv \{\boldsymbol{q}(\boldsymbol{l}), \boldsymbol{l} \in \mathcal{L}\} \in \mathbb{R}^{3N} \equiv X$$

- $X \equiv$ *Configuration space* of ensemble.

Lattice statics - Problem definition

- We wish to determine the equilibrium configurations of the ensemble at zero temperature.
- Total energy: $E(\boldsymbol{q}), \quad \boldsymbol{q} \in X, \quad t \in \mathbb{R}$
- Problem:

$$\inf_{\boldsymbol{q} \in X} E(\boldsymbol{q})$$

- Difficulties:
  - i) N very large $\sim 10^{23}$
  - ii) $E(\boldsymbol{q})$ highly nonconvex $\Rightarrow$ lattice defects, defect structures.

QC - Reduction

- Representative atoms: $\mathcal{L}_h \subset \mathcal{L}$

  $N_h = \text{card}(\mathcal{L}_h) \ll N$

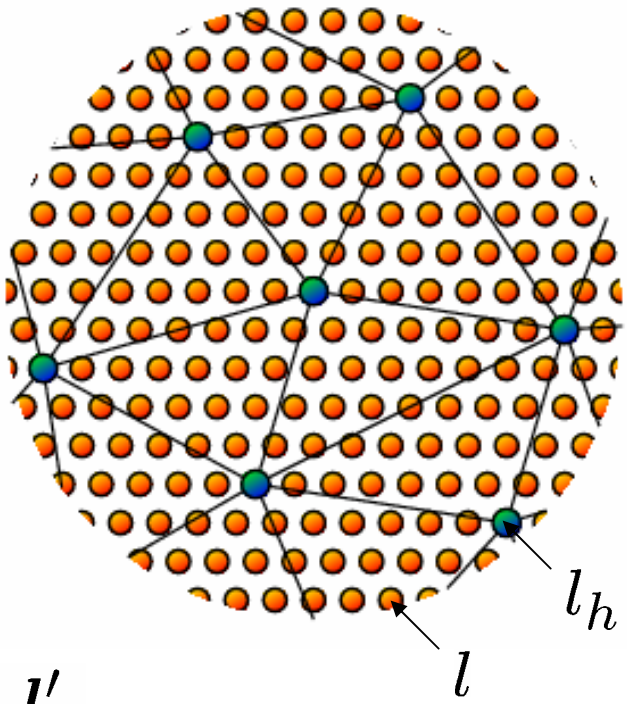
- Introduce triangulation $\mathcal{T}_h$ of $\mathcal{L}_h$

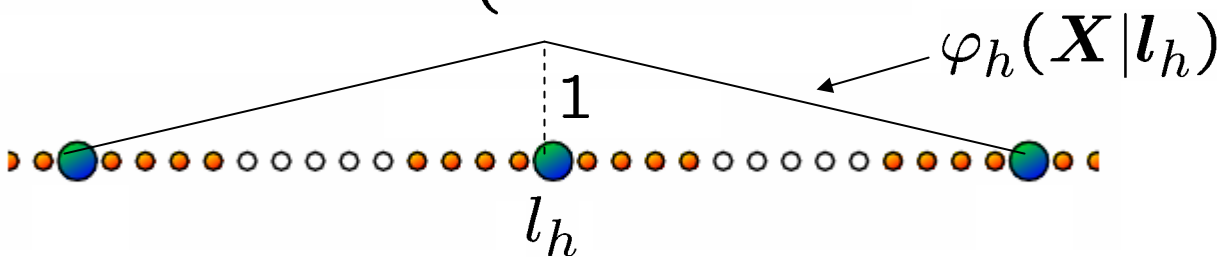
- Basis functions: For $\boldsymbol{l}_h \in \mathcal{L}_h$,

  i) $\varphi_h(\boldsymbol{X}|\boldsymbol{l}_h)$ continuous.

  ii) Linear over simplices $K \in \mathcal{T}_h$

  iii) $\varphi_h(\boldsymbol{X}(\boldsymbol{l}_h)|\boldsymbol{l}'_h) = \begin{cases} 1, & \text{if } \boldsymbol{l}_h = \boldsymbol{l}'_h \\ 0, & \text{otherwise} \end{cases}$

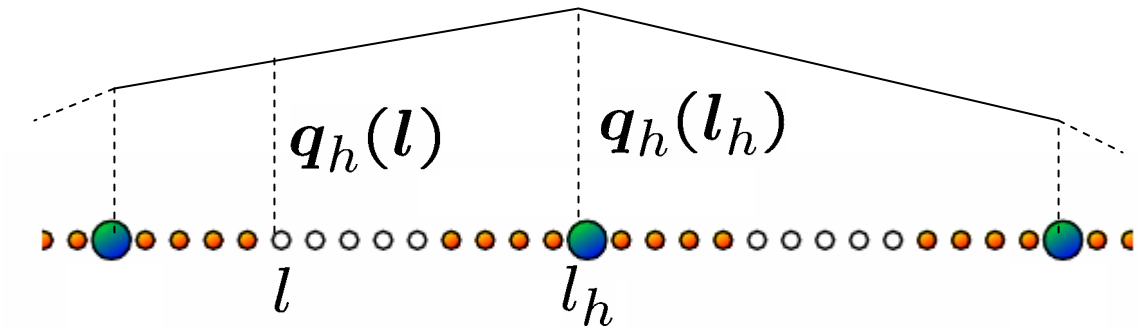




QC - Reduction

- Interpolation: Let $\varphi_h(\boldsymbol{l}|\boldsymbol{l}_h) = \varphi_h(\boldsymbol{X}(\boldsymbol{l})|\boldsymbol{l}_h)$. Then

$$\boldsymbol{q}_h(\boldsymbol{l}) = \sum_{\boldsymbol{l}_h \in \mathcal{L}_h} \varphi_h(\boldsymbol{l}|\boldsymbol{l}_h)\boldsymbol{q}_h(\boldsymbol{l}_h)$$



- For each triangulation $\mathcal{T}_h$, the collection of all interpolated configurations $\boldsymbol{q}_h$ defines a linear subspace X_h of X of dimension $3N_h$.

QC - Reduction

- Reduced problem: $\inf_{q \in X_h} E(q)$

- Reduced equilibrium equations:

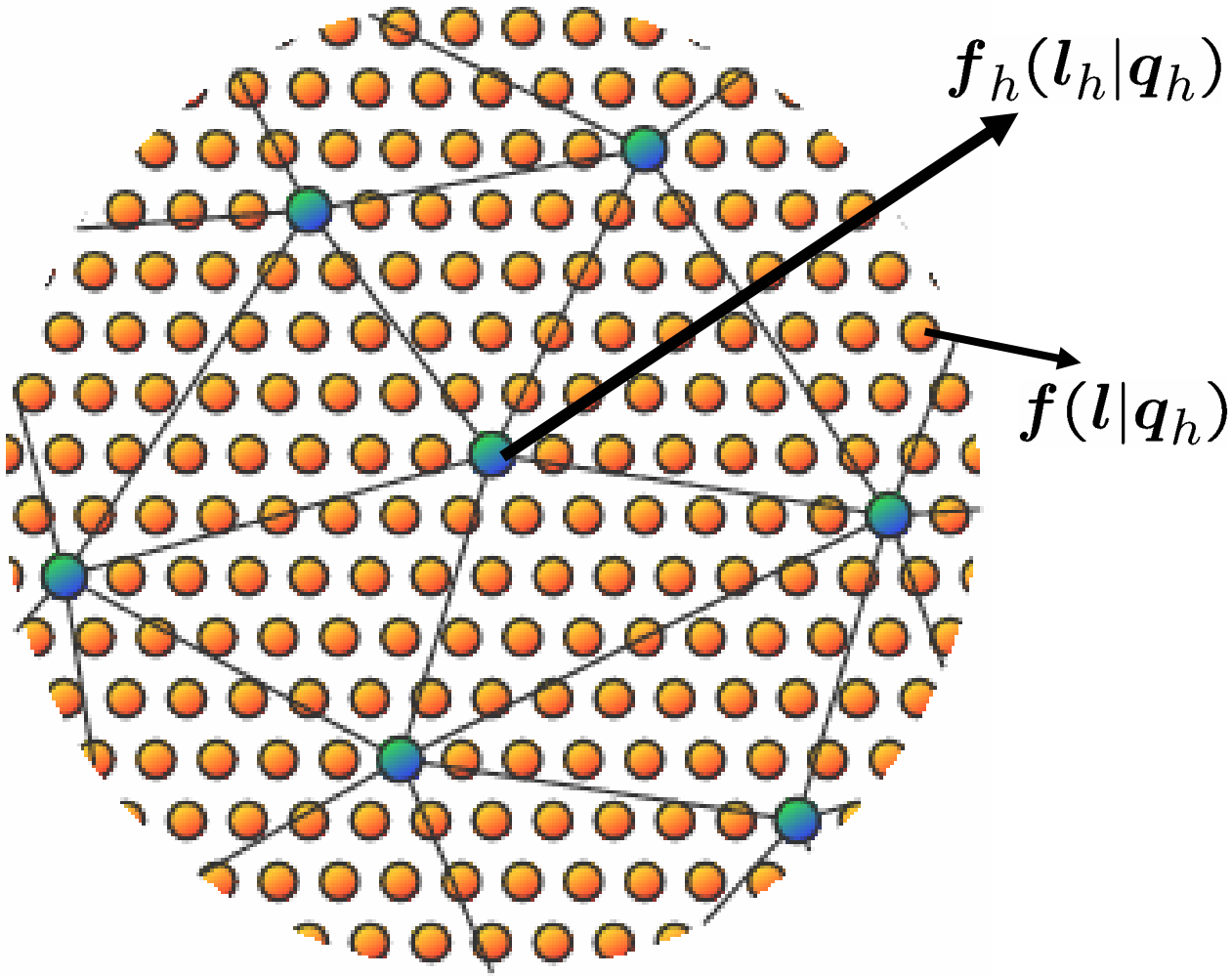
$$f_h(l_h|q_h) = \sum_{l \in \mathcal{L}} f(l|q_h)\varphi_h(l|l_h) = 0$$

where: $f(l|q_h) = \dfrac{\partial E}{\partial q(l)}(q_h)$

- Number of equilibrium equations $= 3N_h = \dim(X_h)$

- But: Calculation of $f_h(l_h|q_h)$ entails sum over entire lattice $\mathcal{L}$!

QC - Reduction

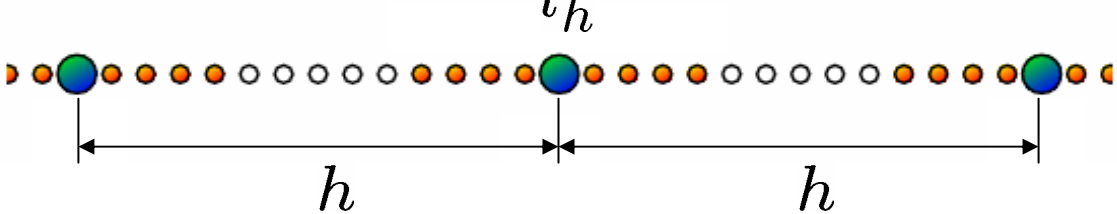


QC – Lattice summation rules

- Problem: Approximate lattice sum $S = \sum_{\boldsymbol{l} \in \mathcal{L}} f(\boldsymbol{l})$
- Summation rule: Let $\mathcal{S}_h \subset \mathcal{L}$. Then

$$S \approx S_h = \sum_{\boldsymbol{l} \in \mathcal{S}_h} n_h(\boldsymbol{l}) f(\boldsymbol{l})$$

- Example: *Node-based summation rules*, $\mathcal{S}_h = \mathcal{L}_h$, weights chosen such that $\varphi(\boldsymbol{l}|\boldsymbol{l}_h)$ summed exactly for all $\boldsymbol{l}_h \in \mathcal{L}_h$.
- Monatomic chain: $n_h(l_h) = \begin{cases} h, & \text{if } l_h \text{ interior} \\ (h+1)/2, & \text{otherwise} \end{cases}$



QC – Reduced equations

- Combine interpolation and lattice summation rule:

$$\boldsymbol{f}_h(\boldsymbol{l}_h|\boldsymbol{q}_h) = \sum_{\boldsymbol{l}\in\mathcal{S}_h} n_h(\boldsymbol{l})\boldsymbol{f}(\boldsymbol{l}|\boldsymbol{q}_h)\varphi_h(\boldsymbol{l}|\boldsymbol{l}_h) = \boldsymbol{0}$$

- All operations are now $O(N_h)$ provided $\mathrm{card}(S_h)$ is $O(N_h)$.

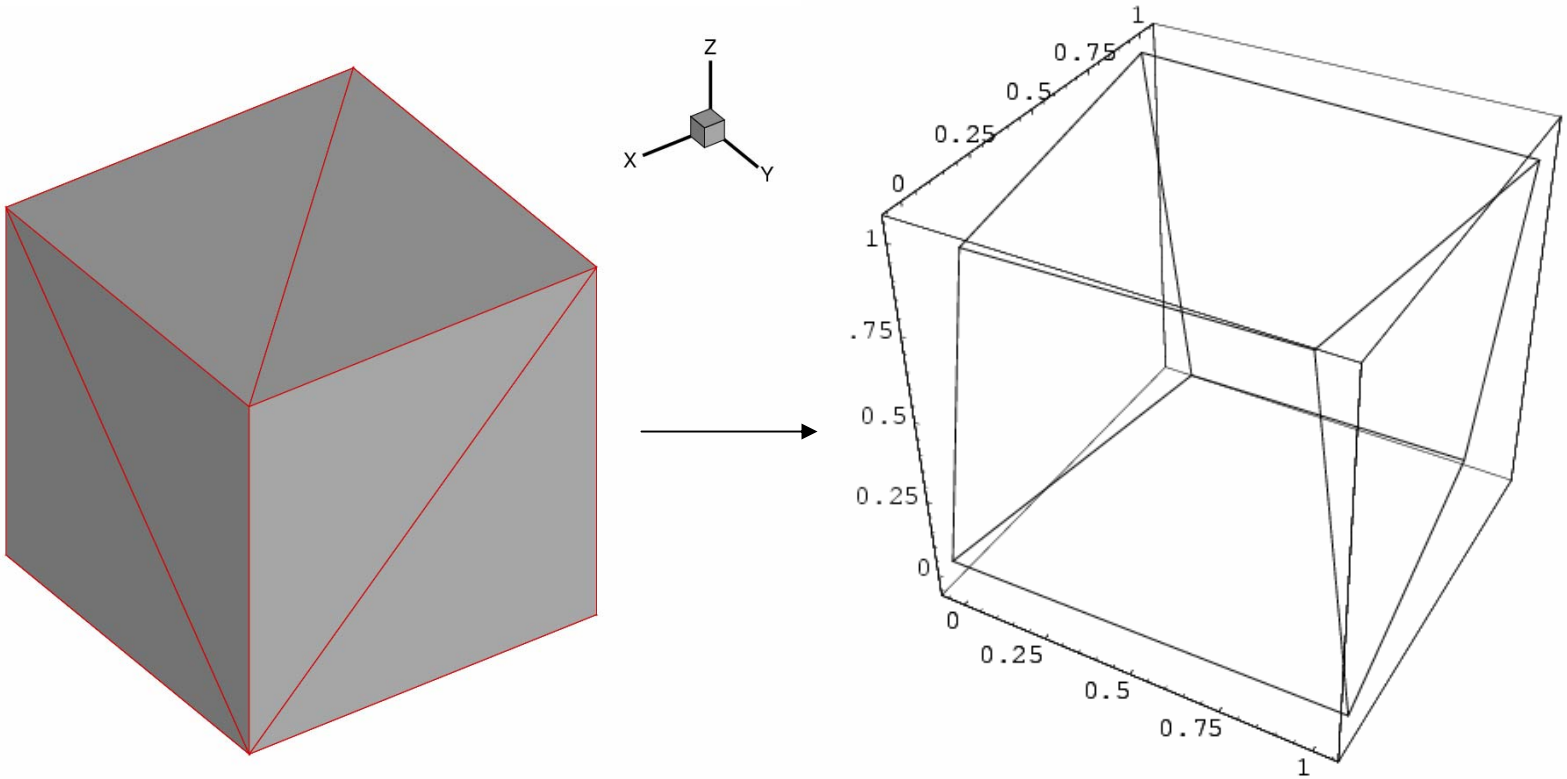
- Example: For node-based summation rule,

$$\boldsymbol{f}_h(\boldsymbol{l}_h|\boldsymbol{q}_h) = \sum_{\boldsymbol{l}'_h\in\mathcal{L}_h} n_h(\boldsymbol{l}'_h)\boldsymbol{f}(\boldsymbol{l}'_h|\boldsymbol{q}_h)\varphi_h(\boldsymbol{l}'_h|\boldsymbol{l}_h) = \boldsymbol{0}$$

- Questions: Convergence, accuracy?

Lattice summation rules - Stability

- Node-based summation rule *undersamples* the ensemble and is *unstable*.



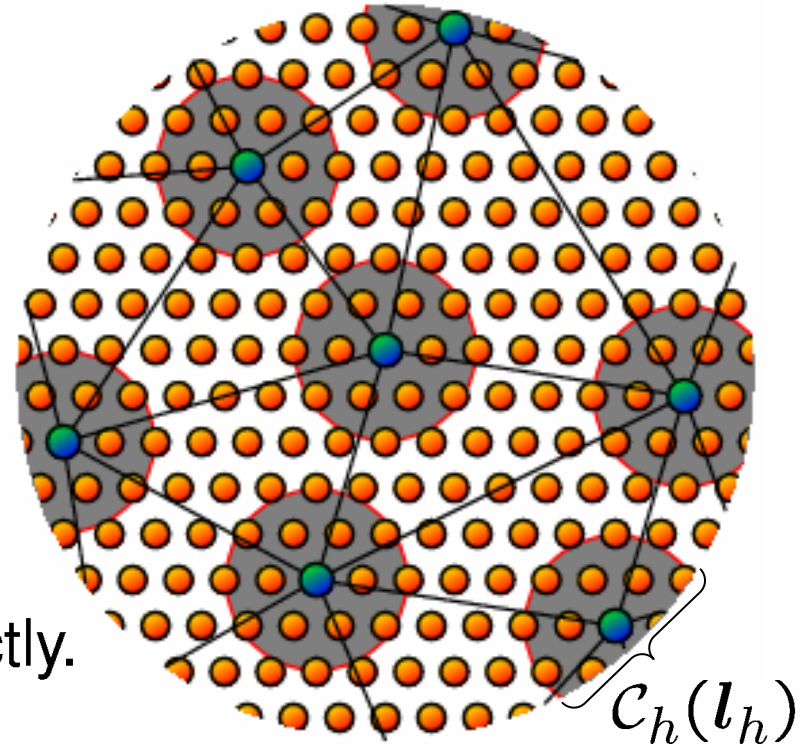
Zero-energy mode of 32x32 Lennard-Jones fcc cluster resulting from node-based summation rule.

Cluster-based lattice summation rules

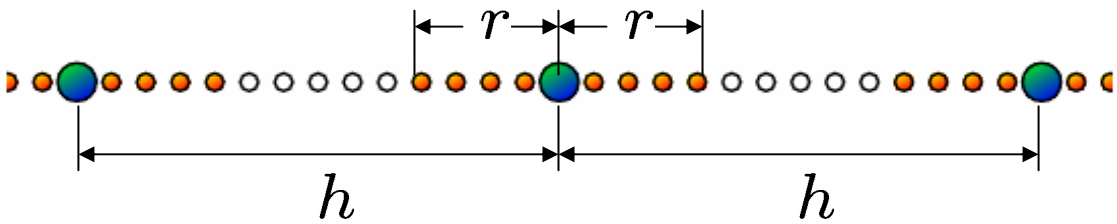
- $\mathcal{C}_h(\boldsymbol{l}_h) \equiv$ Cluster of lattice sites centered at $\boldsymbol{l}_h$
- Cluster summation rule:

$$S_h = \sum_{\boldsymbol{l}_h \in \mathcal{L}_h} n_h(\boldsymbol{l}_h) \Big\{ \sum_{\boldsymbol{l} \in \mathcal{C}(\boldsymbol{l}_h)} f(\boldsymbol{l}) \Big\}$$

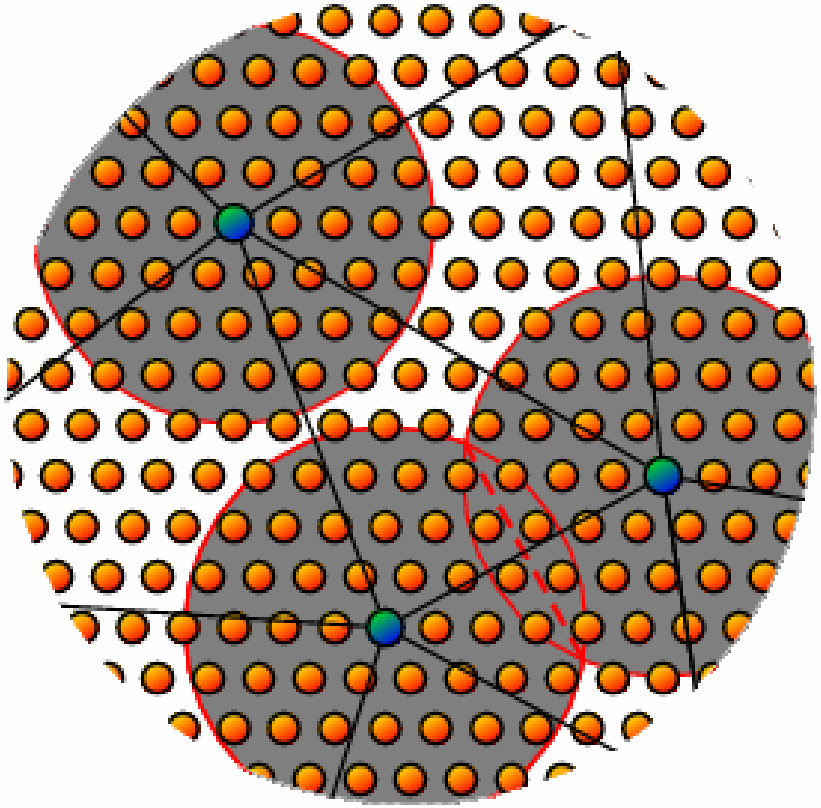
$n_h(\boldsymbol{l}_h)$ s. t. $\varphi(\boldsymbol{l}|\boldsymbol{l}_h)$ summed exactly.



- Monatomic chain: $n_h(l_h) = h/(1+2r)$



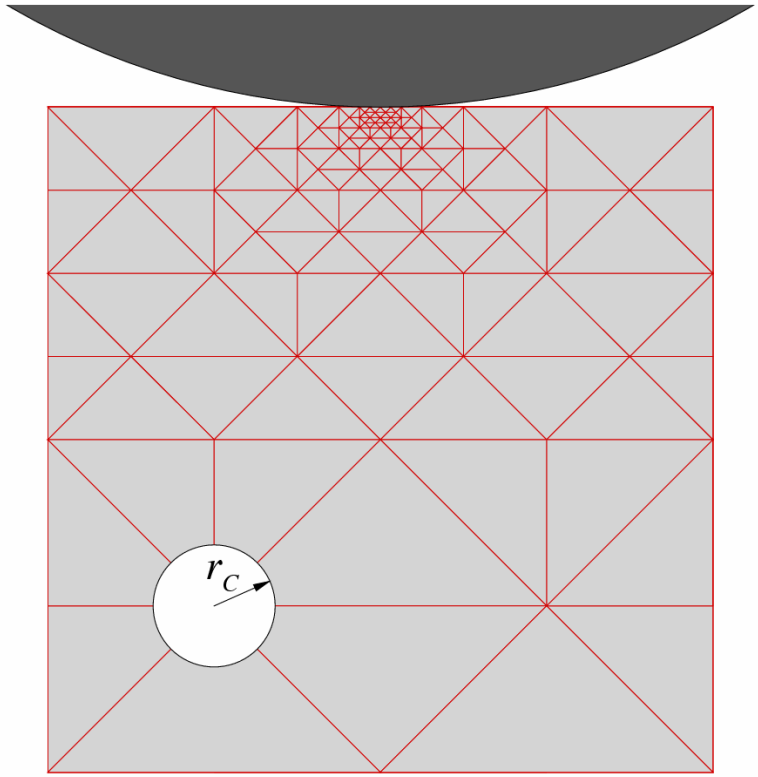
Cluster-based lattice summation rules

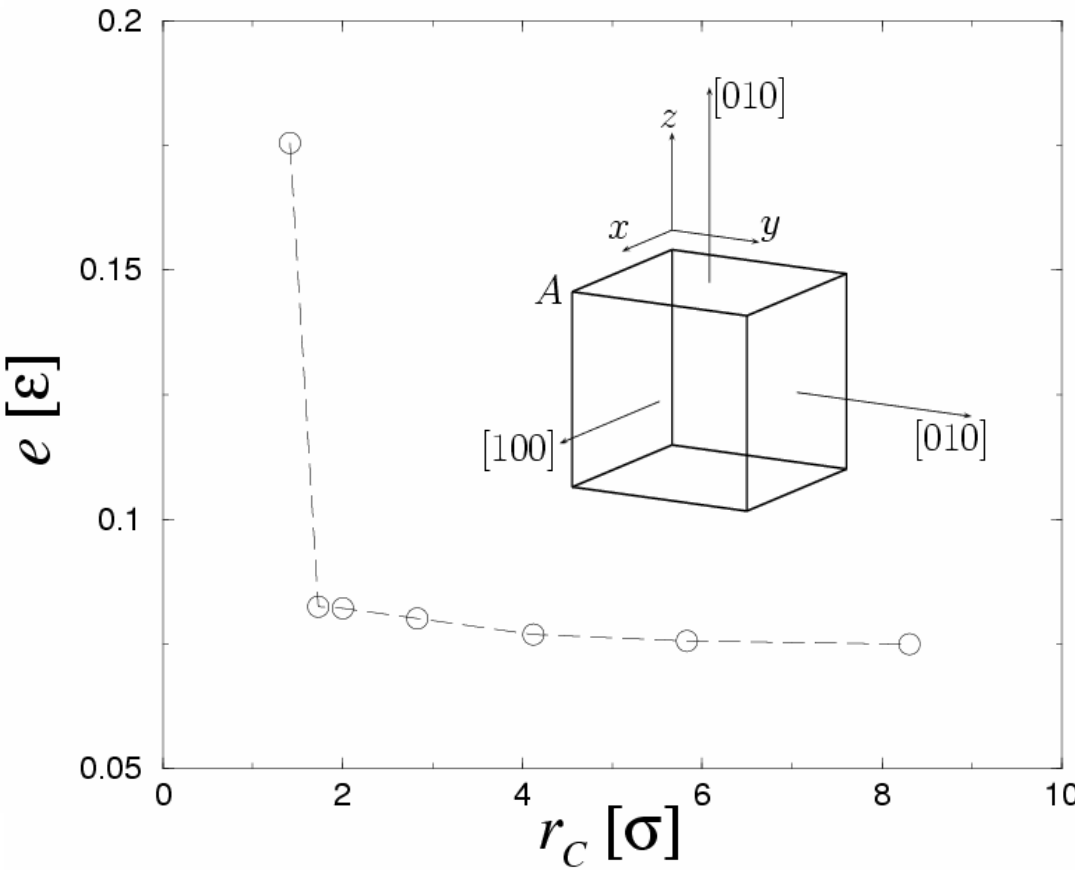


Truncation scheme for overlapping clusters

- $\mathcal{L}_h \to \mathcal{L} \Rightarrow X_h \to X$ and $\inf E_h \to \inf E$

Cluster sums - Effect of cluster size





Effect of cluster size on energy error for 0.1σ indentation of 64x64x64 fcc cell sample of Lennard-Jones crystal.

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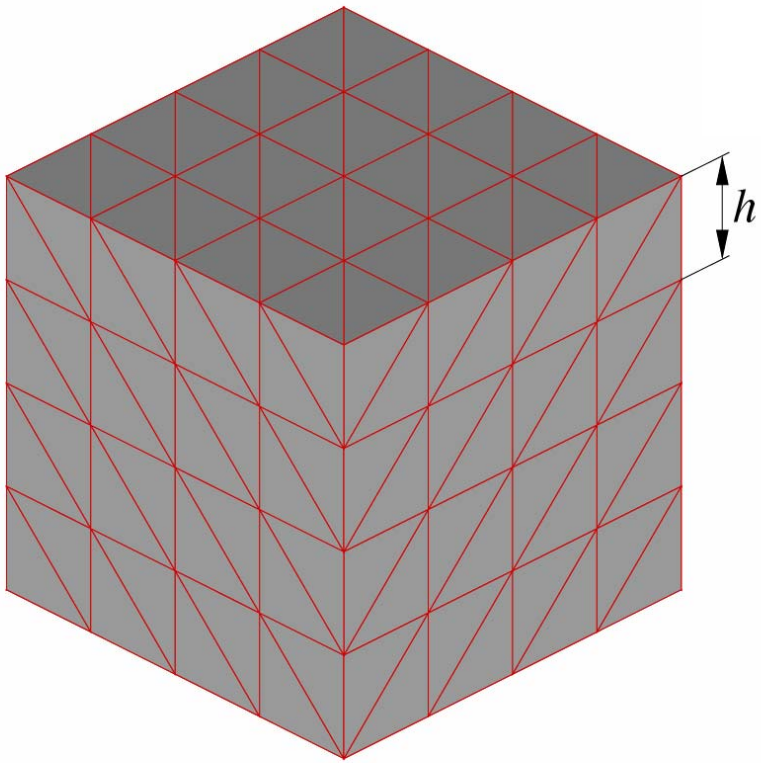
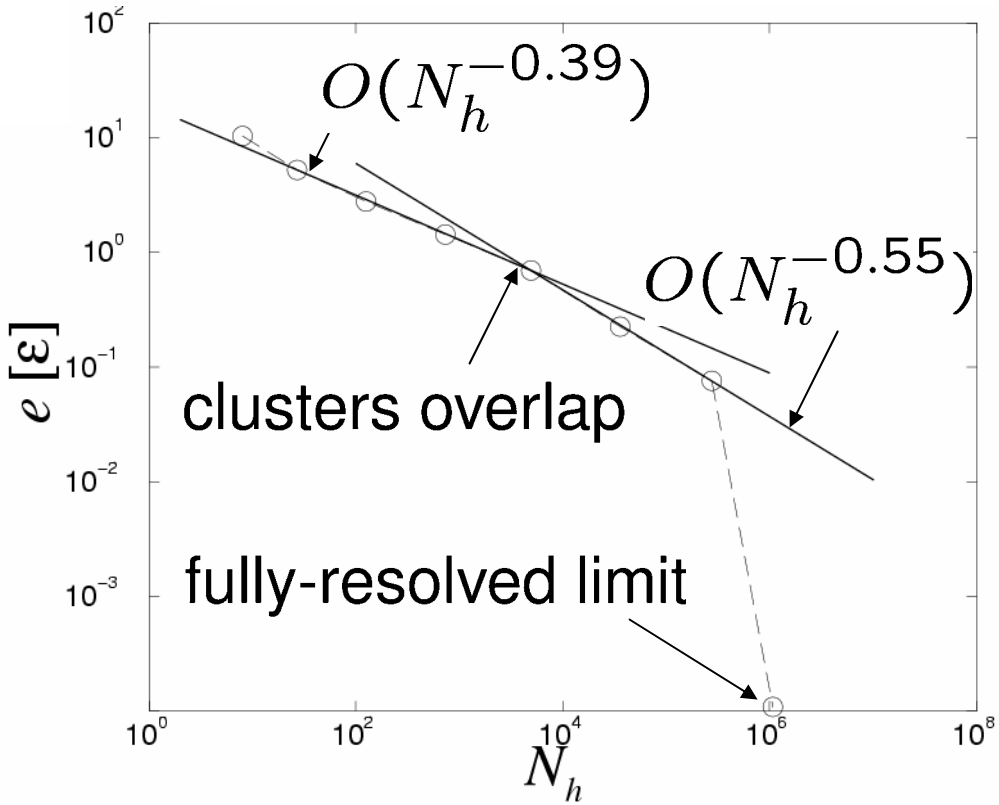
QC - Convergence

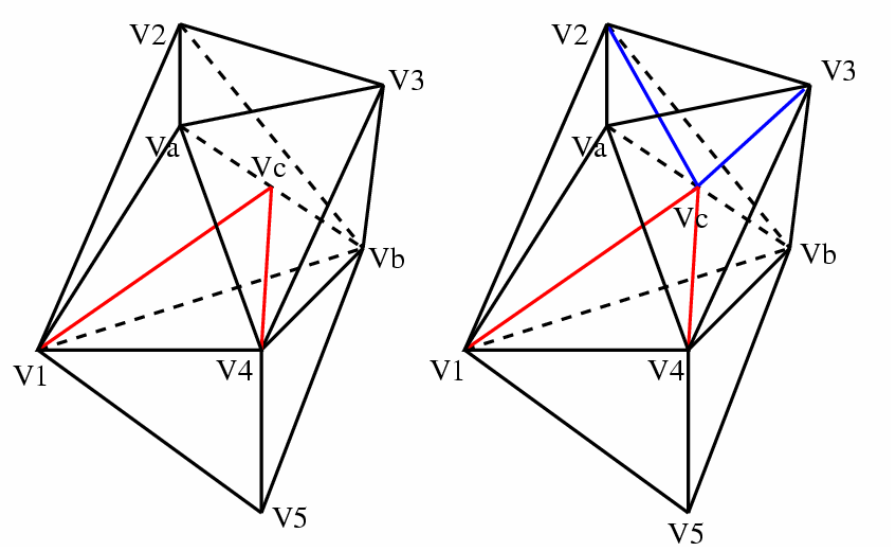




Convergence of energy error under regular refinement of fcc cell sample of Lennard-Jones crystal under point load

QC - Adaptivity

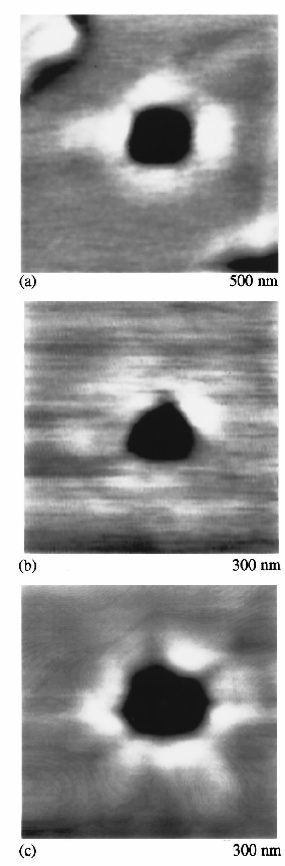
- $\boldsymbol{E}(K) \equiv$ Lagrangian strain in simplex $K \in \mathcal{T}_h$
- Refinement criterion: *Bisect* K if $|\boldsymbol{E}(K)| \geq \text{TOL}\dfrac{b}{h(K)}$

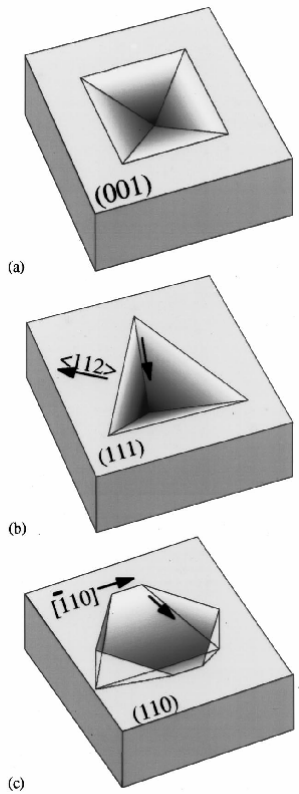


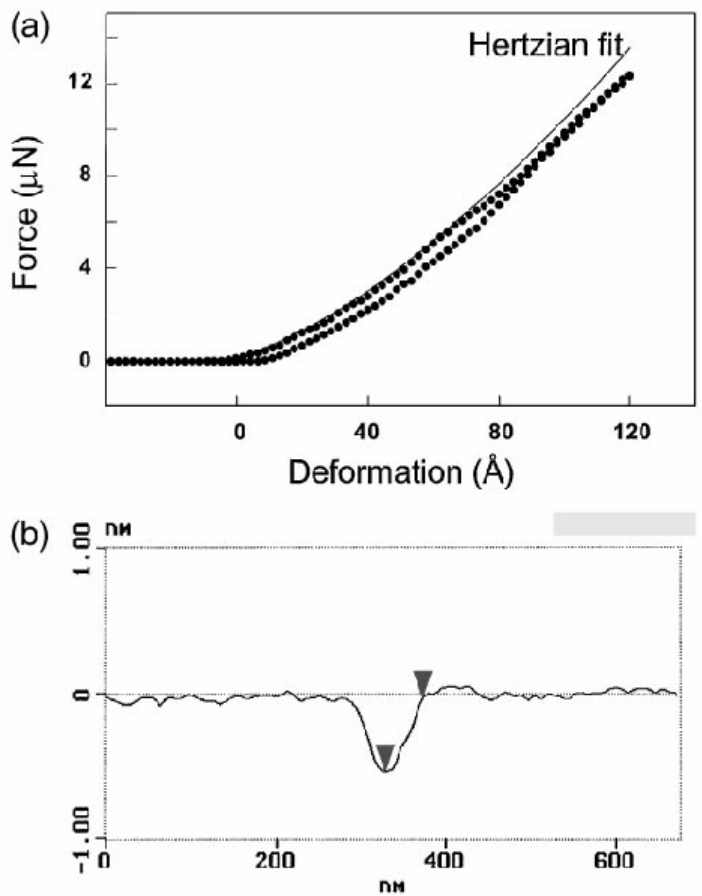
Longest-edge bisection of tetrahedron (1,4,a,b) along longest edge (a,b) and of ring of tetrahedra incident on (a,b)

- General statement: $\inf_{\boldsymbol{q} \in X_h,\, \mathcal{T}_h} E(\boldsymbol{q}, \mathcal{T}_h)$

Nanoindentation of [001] Au

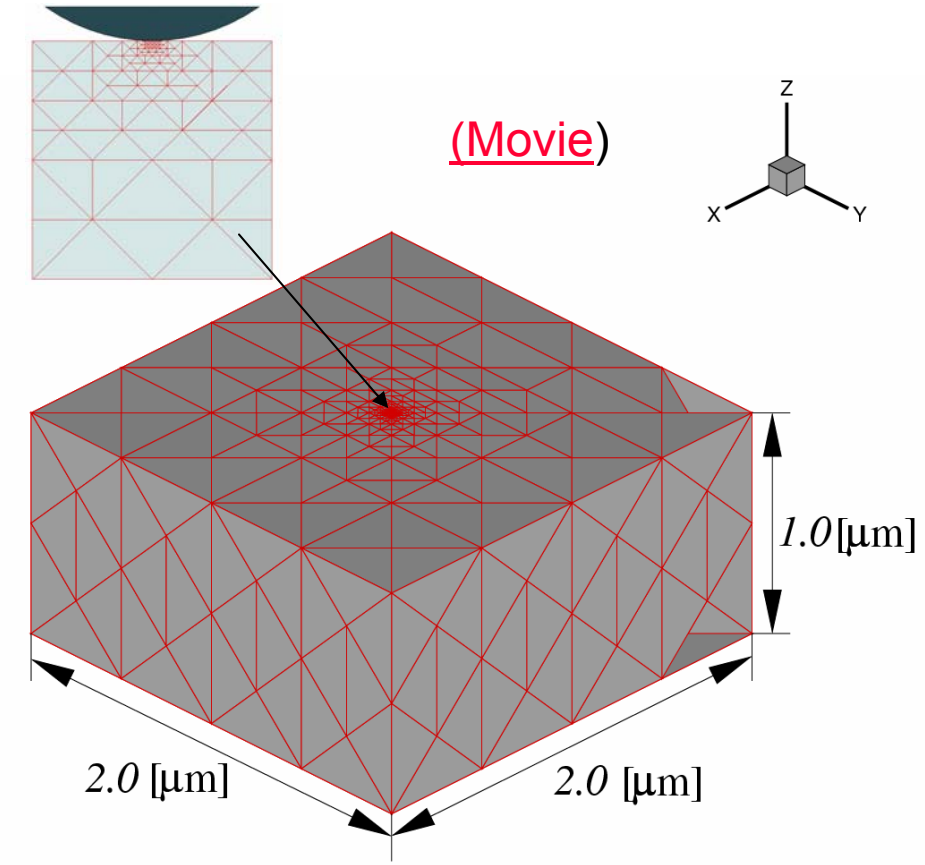






(Kiely and Houston, Phys. Rev. B, 1998)

Example - Nanoindentation of [001] Au

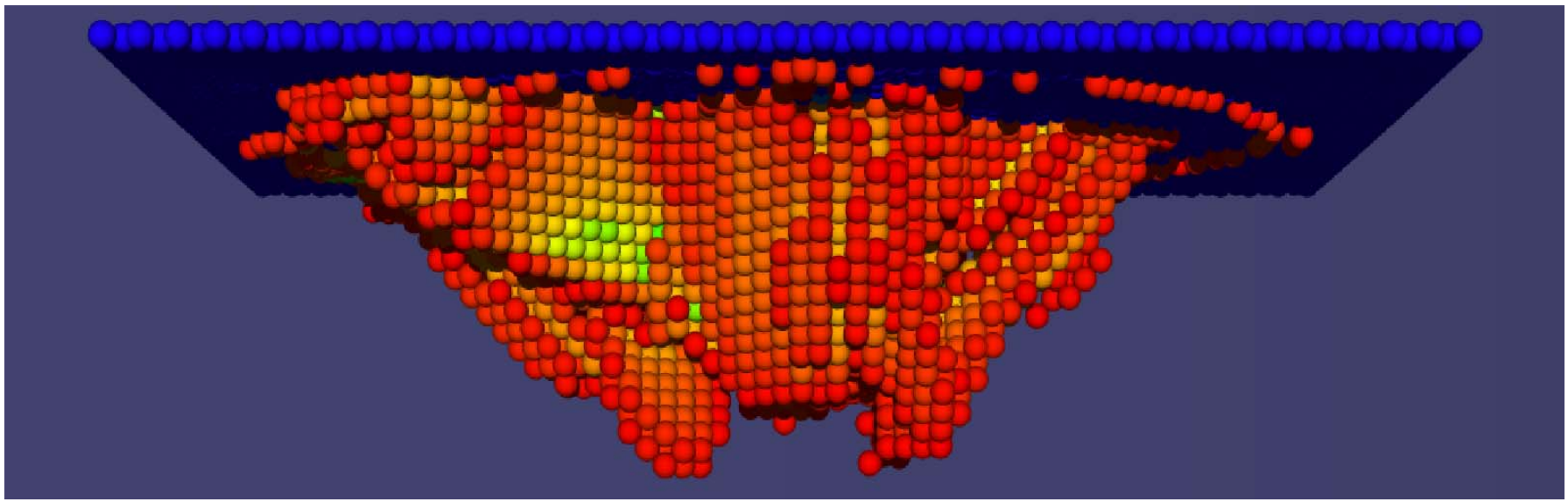


- Nanoindentation of [001] Au, 2x2x1 micrometers
- Spherical indentor, R=7 and 70 nm
- Johnson EAM potential
- Total number of atoms ~ 0.25 10^12
- Initial number of nodes ~ 10,000
- Final number of nodes ~ 100,000

Detail of initial computational mesh

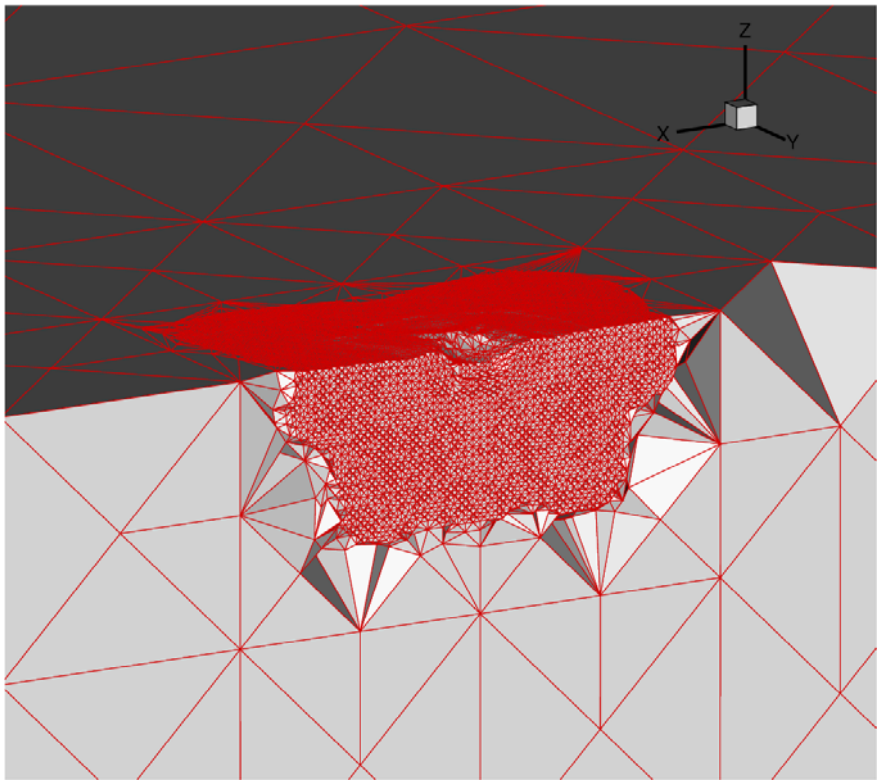
(Knap and Ortiz, *PRL* **90** 2002-226102)

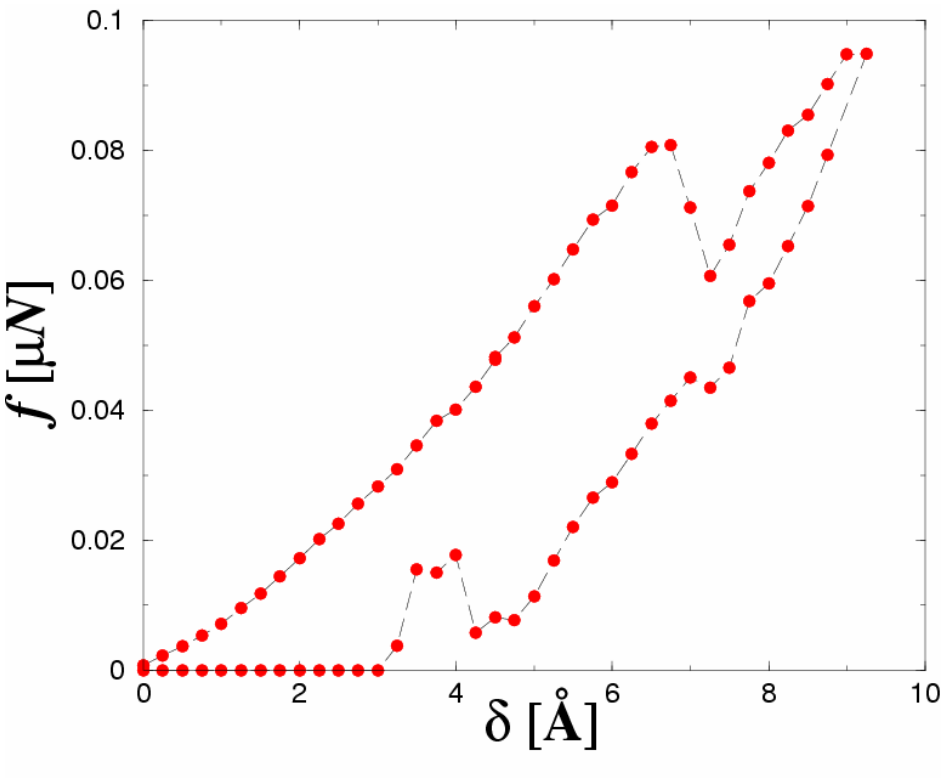
Nanoindentation - [001] Au



7 nm indenter, depth = 0.92 nm

Nanoindentation - [001] Au





7 nm indenter, depth = 0.92 nm

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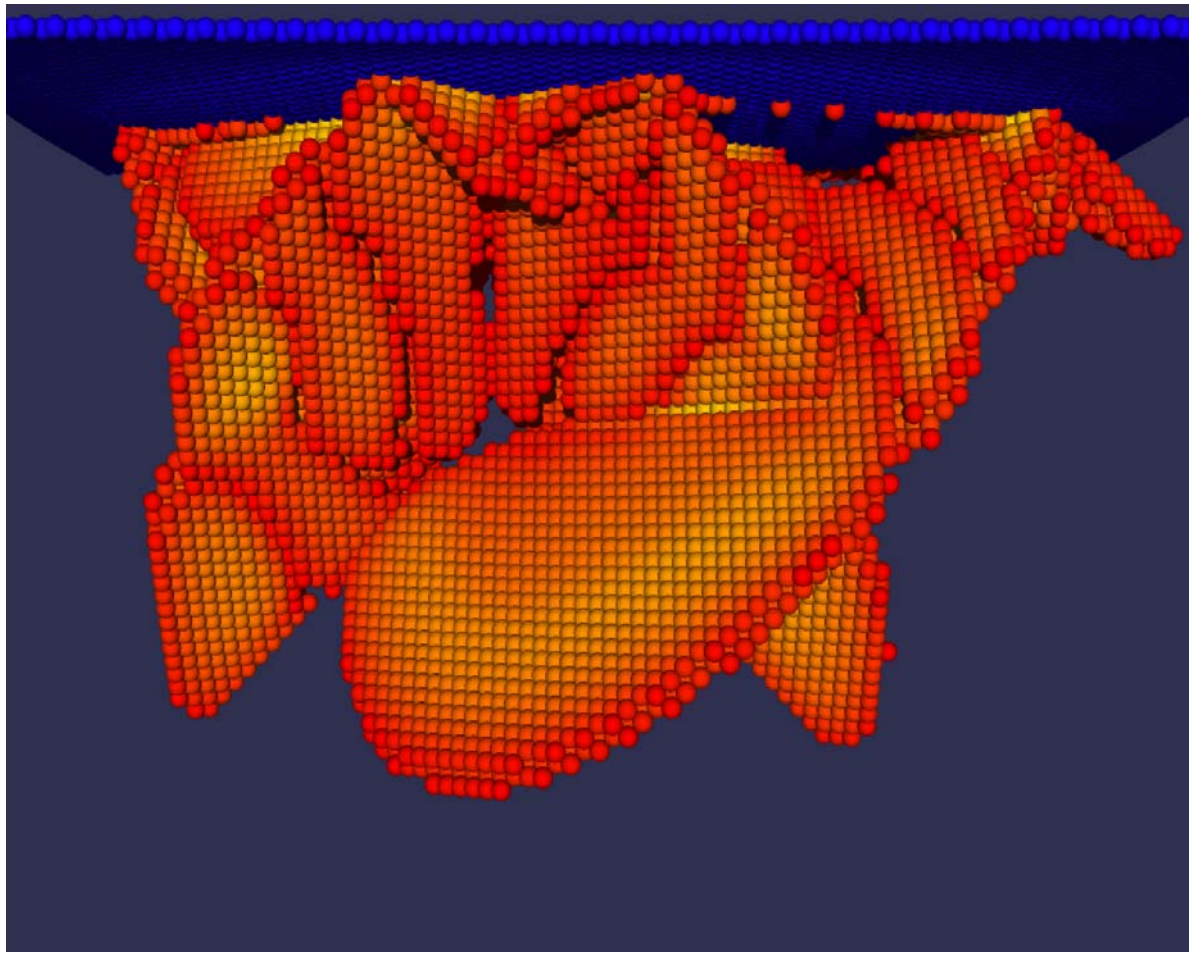
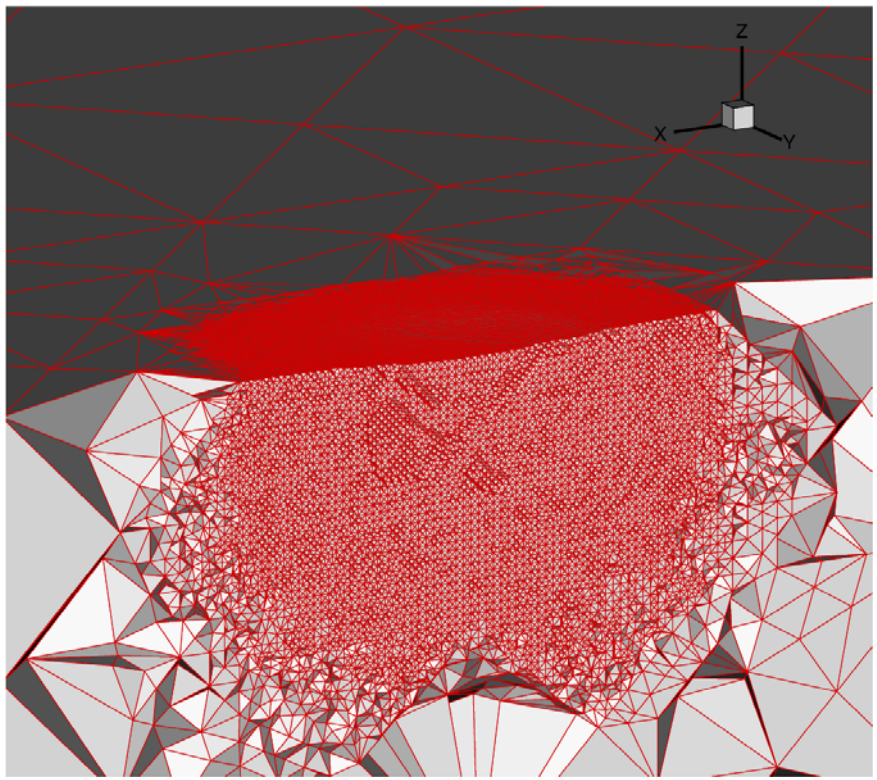
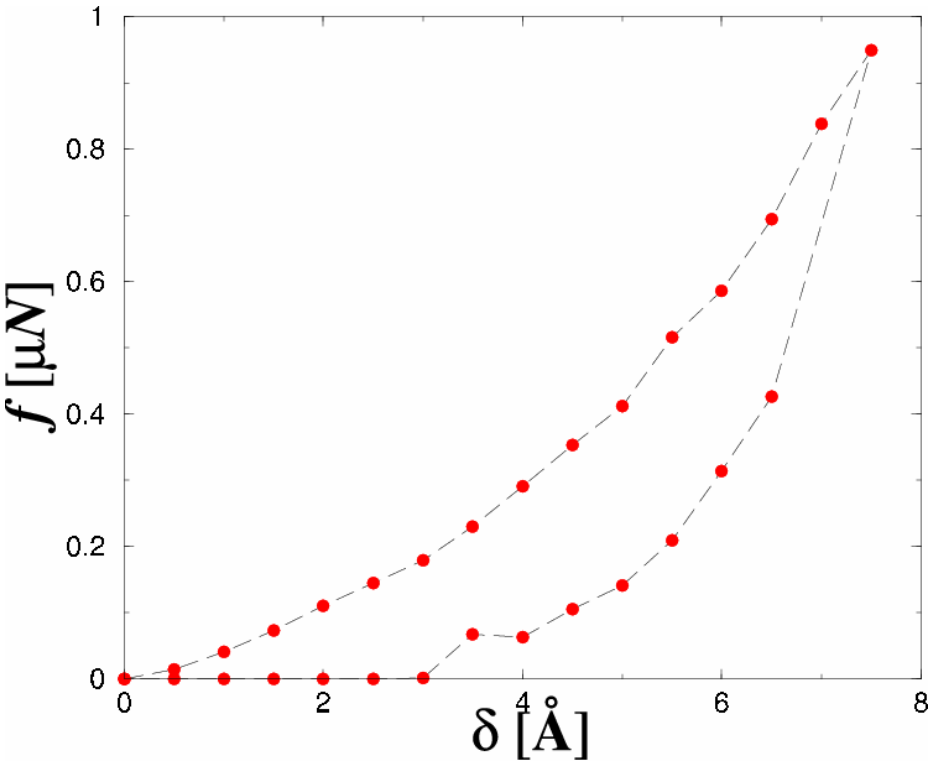
Nanoindentation - [001] Au



70 nm indenter, depth = 0.75 nm

Nanoindentation - [001] Au





70 nm indenter, depth = 0.75 nm

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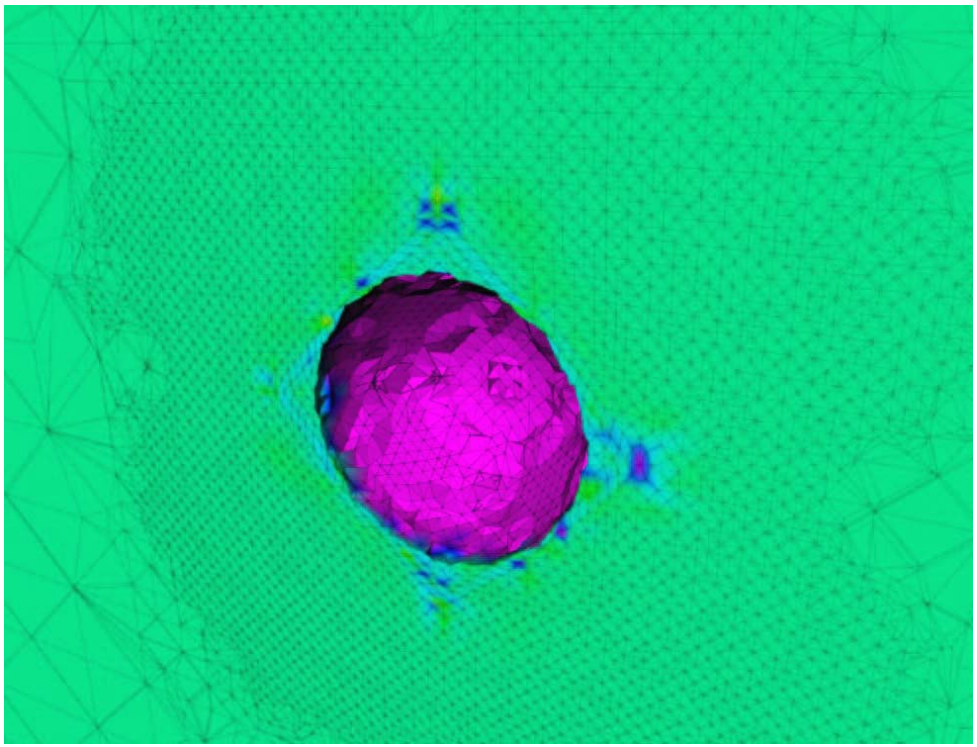
Nanovoid cavitation in Al

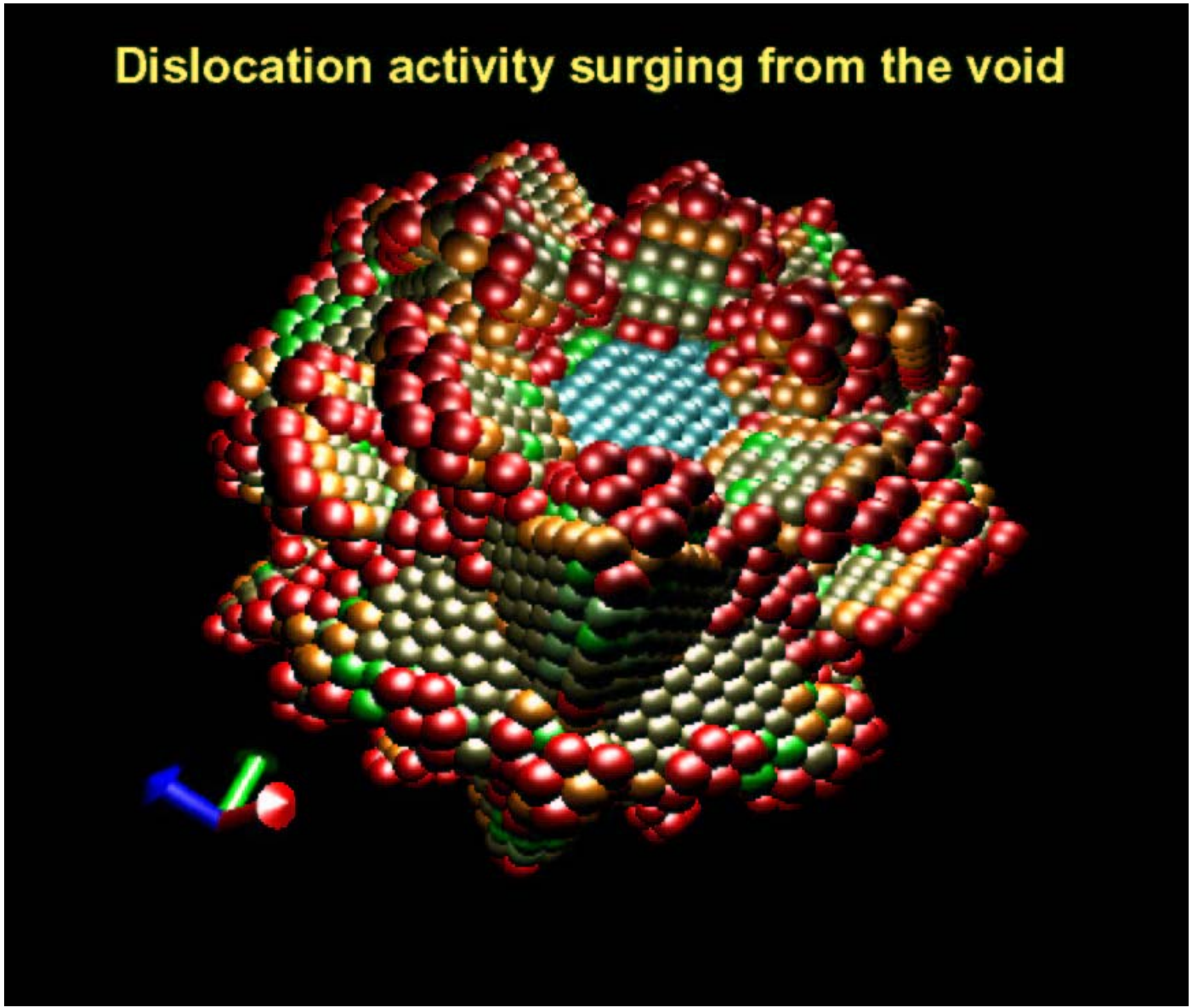


Close-up of internal void

- 72x72x72 cell sample
- Initial radius R=2a
- Ercolessi and Adams (*Europhys. Lett.* **26**, 583, 1994) EAM potential.
- Total number of atoms ~16×10^6
- Initial number of nodes ~ 34,000

(Marian, Knap and Ortiz ´03)

Nanovoid cavitation in Al



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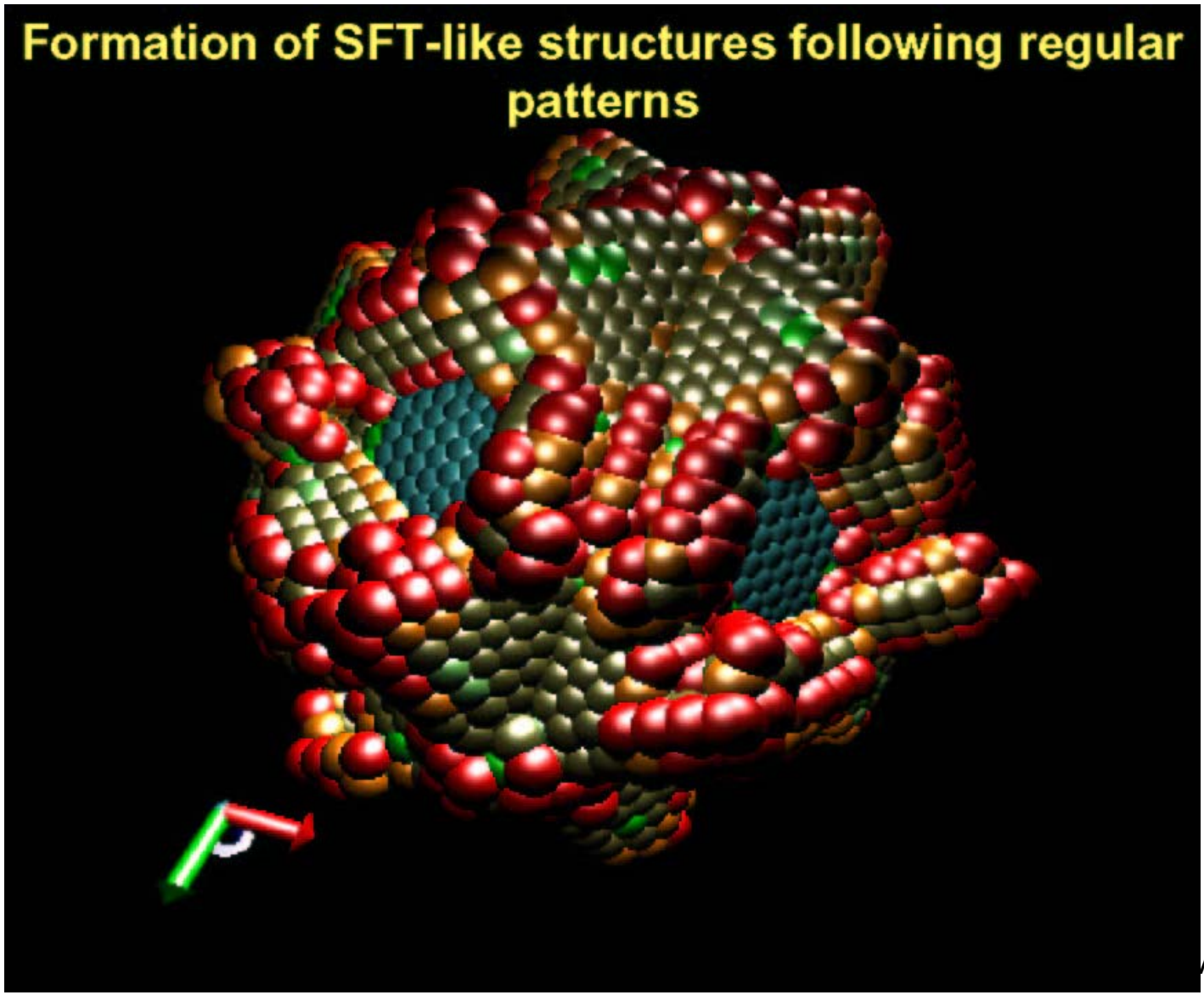
Nanovoid cavitation in Al



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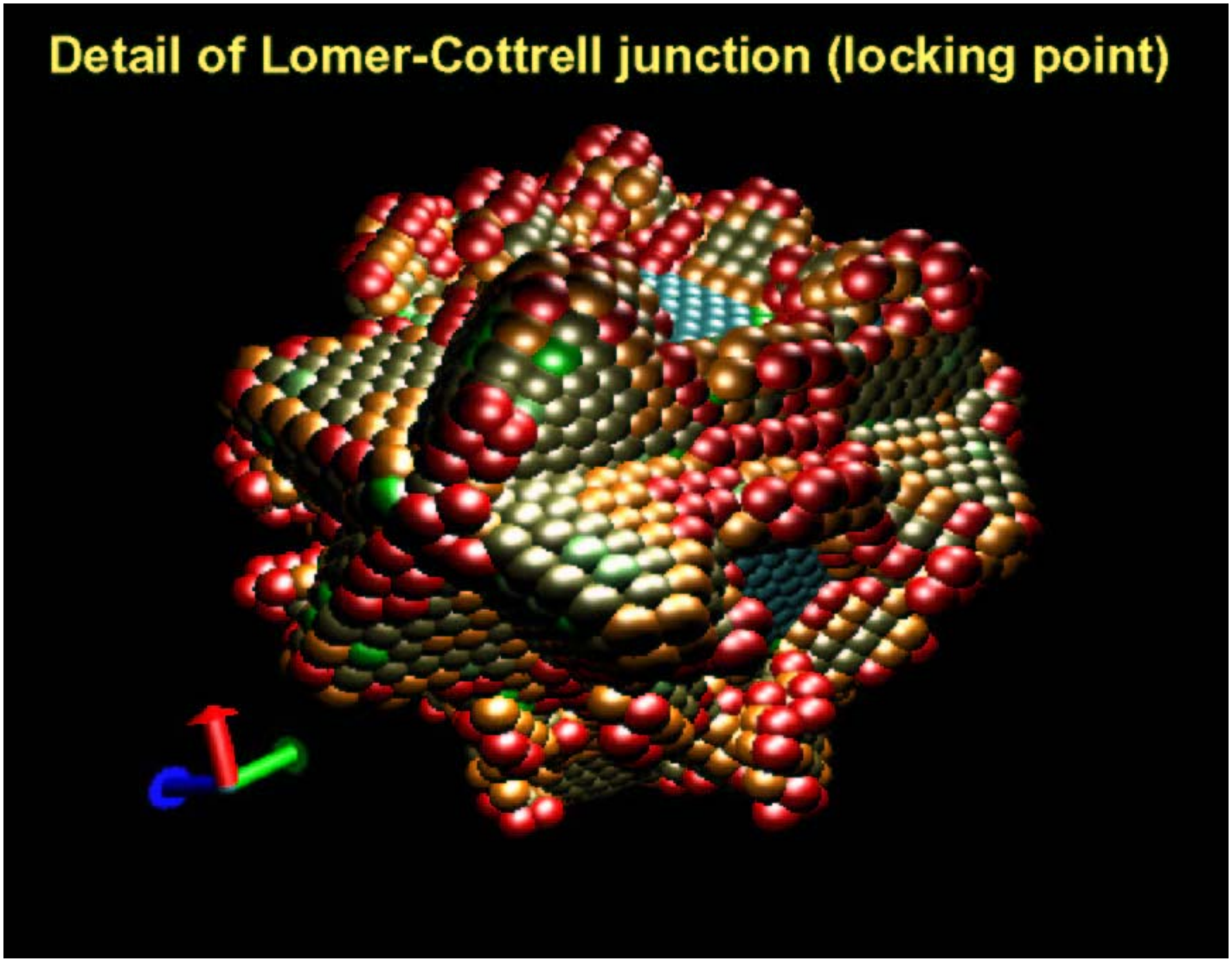
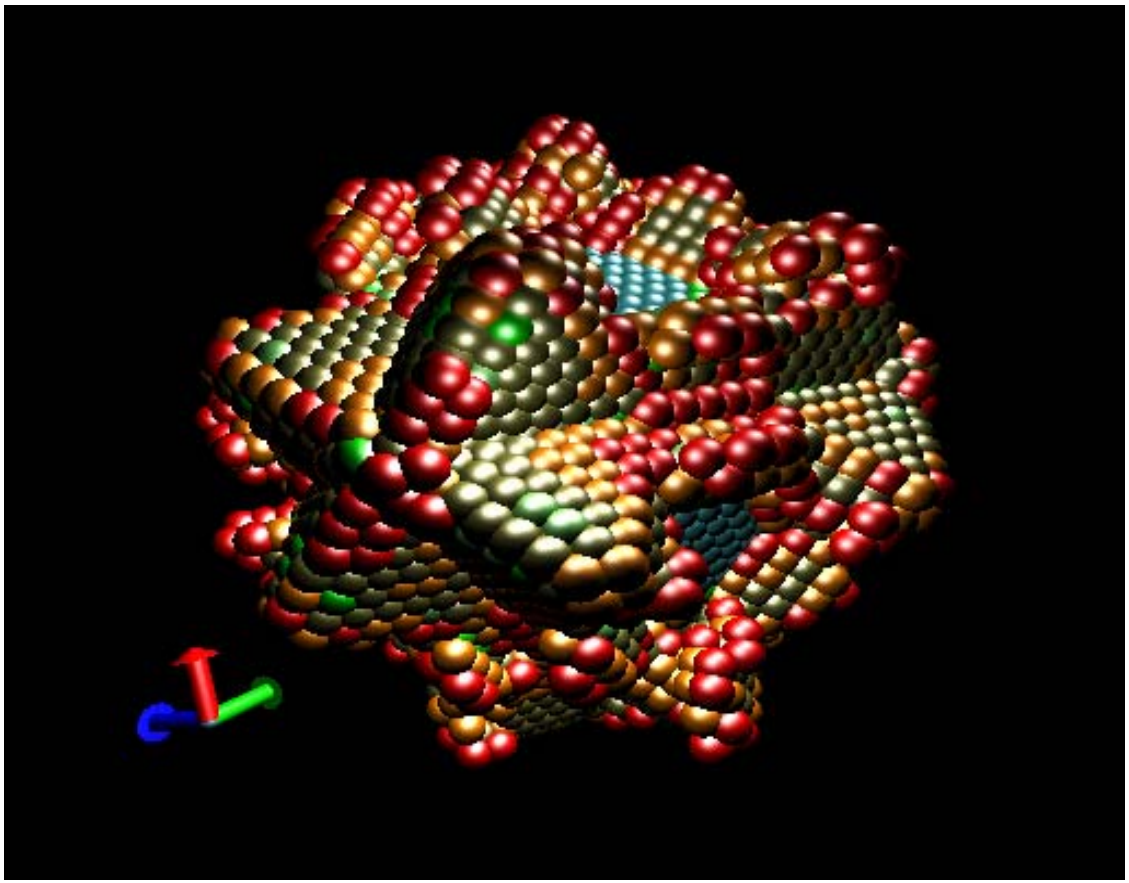
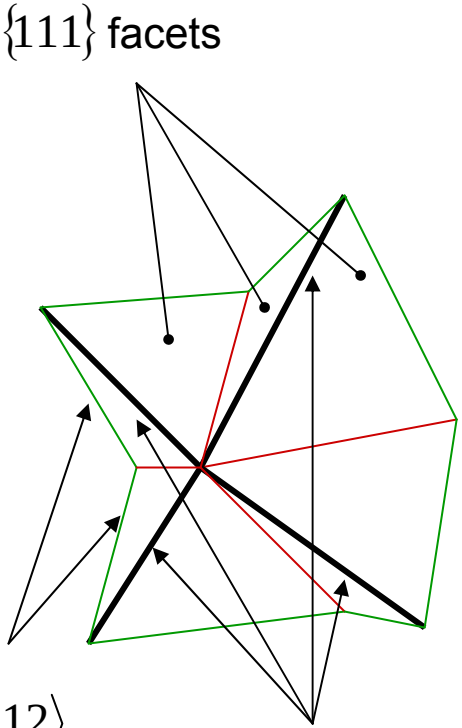
Nanovoid cavitation in Al



Nanovoid cavitation in Al





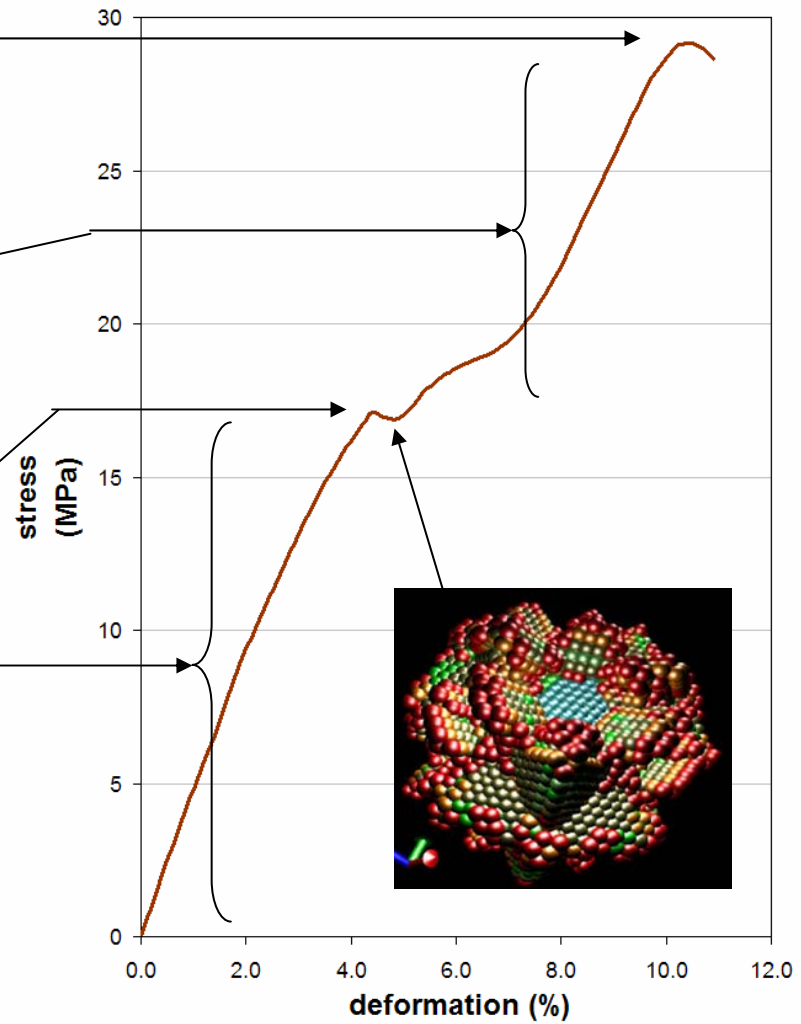
Nanovoid cavitation in Al

2nd yield point:
(being investigated)

Hardening regime:
dislocation locking

1st yield point

Initial elastic regime,
following the interatomic
potential's shape



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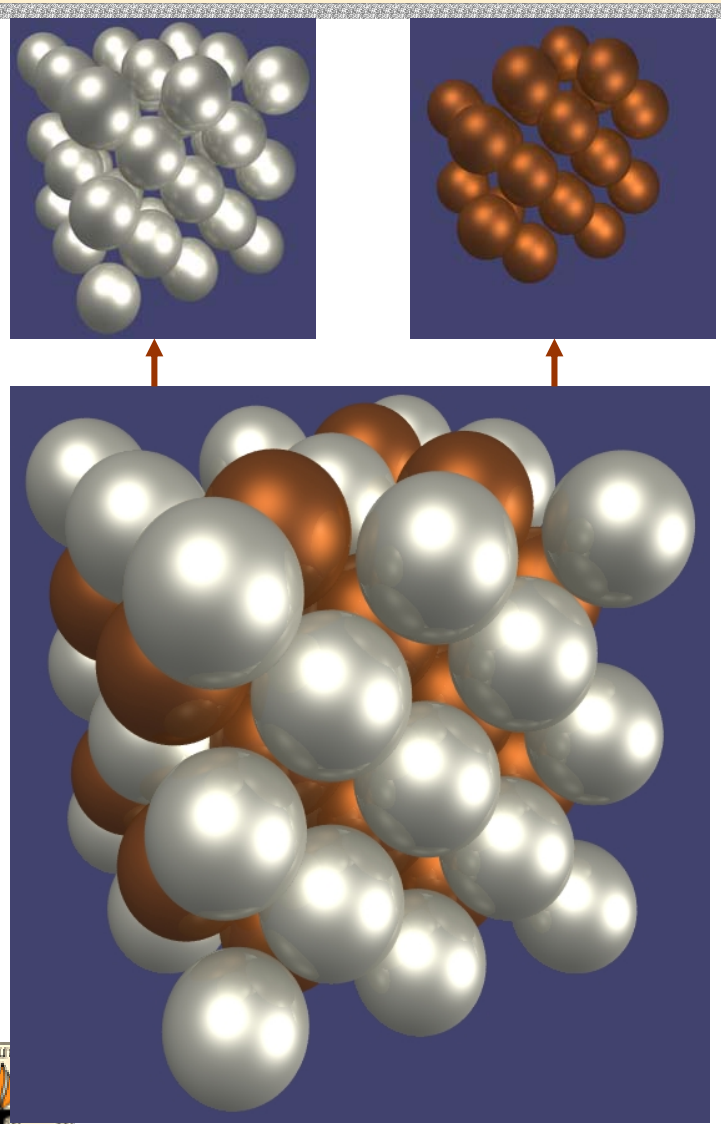
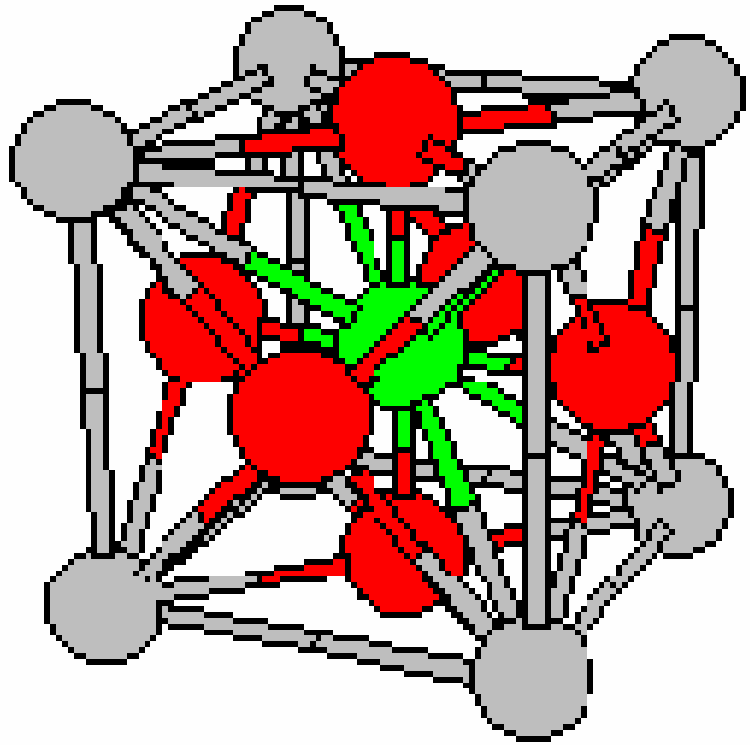
Complex lattices





- Approach: Interpolate each sublattice independently.
- $BaTiO_3$: 5 sublattices, meshes, **Ba, Ti, Ox, Oy, Oz.**

Complex lattices

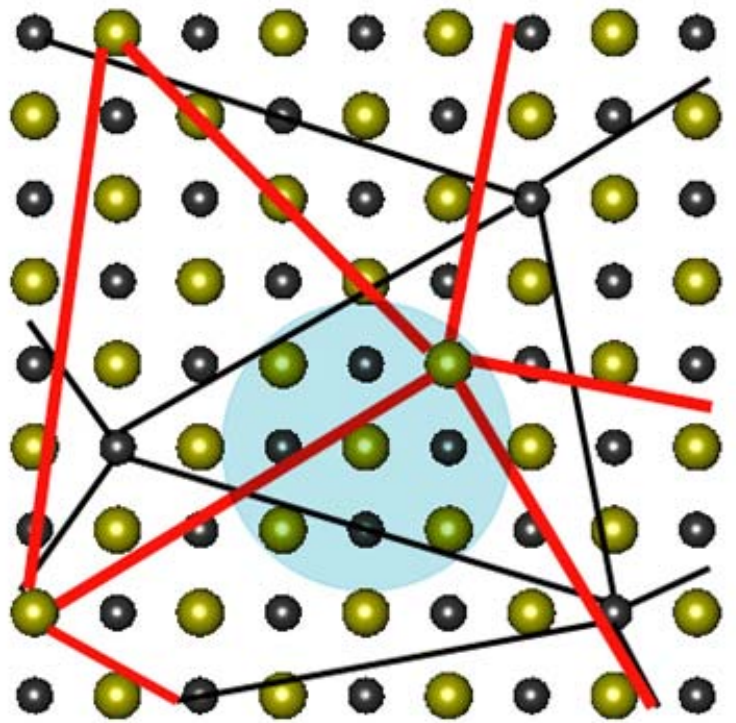
- Kinematics:

$$q_h^A(l) = \sum_{l_h \in \mathcal{L}_h^A} \phi_h^A(l|l_h) q_h^A(l_h)$$

$$q_h^B(l) = \sum_{l_h \in \mathcal{L}_h^B} \phi_h^B(l|l_h) q_h^B(l_h)$$

- Constrained minimization:

$$\min_{(q_h^A, q_h^B) \in X_h} E(q_h^A, q_h^B)$$



- Cluster summation rules:

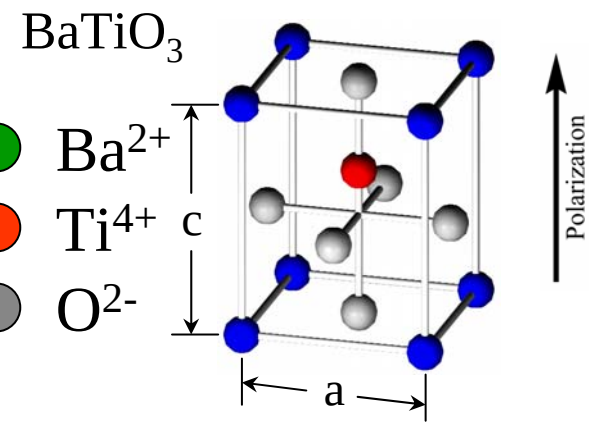
$$E(q_h^A, q_h^B) \approx \sum_{l_h \in \mathcal{L}_h^A \cup \mathcal{L}_h^B} n_h(l_h) \left(\sum_{l \in \mathcal{C}(l_h)} E(l|q_h^A, q_h^B) \right)$$

Charge redistribution

- Charge interpolation:

$$Q_h^A(l) = \sum_{l_h \in \mathcal{L}_h^A} \phi_h^A(l|l_h) Q_h^A(l_h)$$

$$Q_h^B(l) = \sum_{l_h \in \mathcal{L}_h^B} \phi_h^B(l|l_h) Q_h^B(l_h)$$



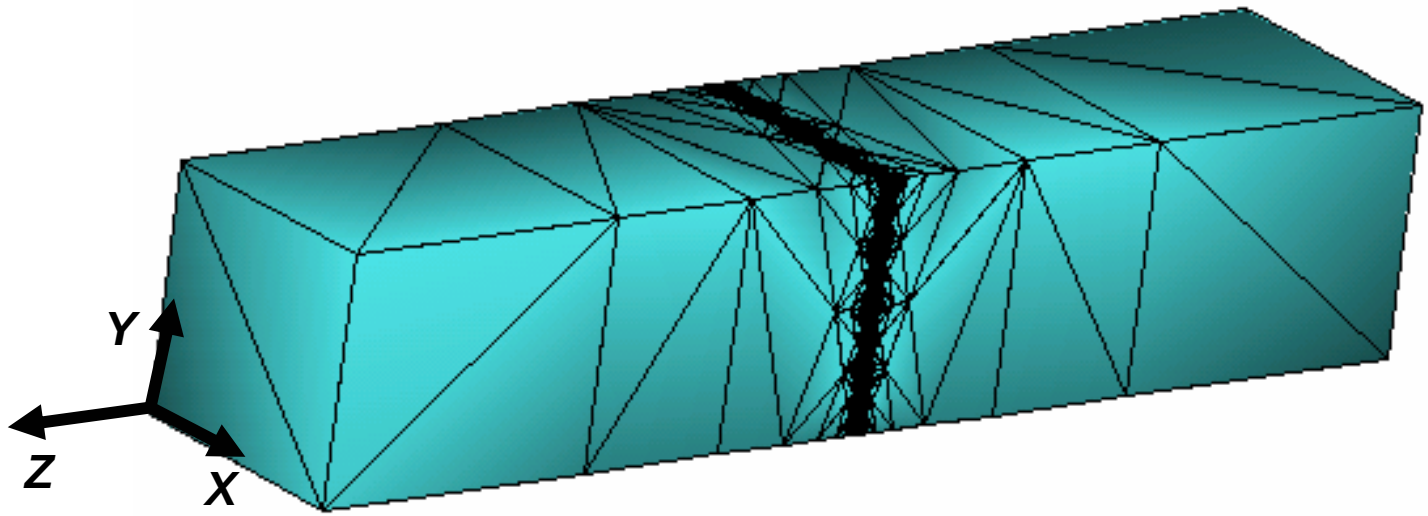
Tetragonal (room temp)

- Constrained minimization:

$$\min_{\{(q_h^A,Q_h^A),(q_h^B,Q_h^B)\} \in X_h} E((q_h^A, Q_h^A), (q_h^B, Q_h^B))$$

- Charge summation rules: *Spherically truncated cluster summation rule* (D. Wolf *et al.*, *J. Chem. Phys.*, 1999)

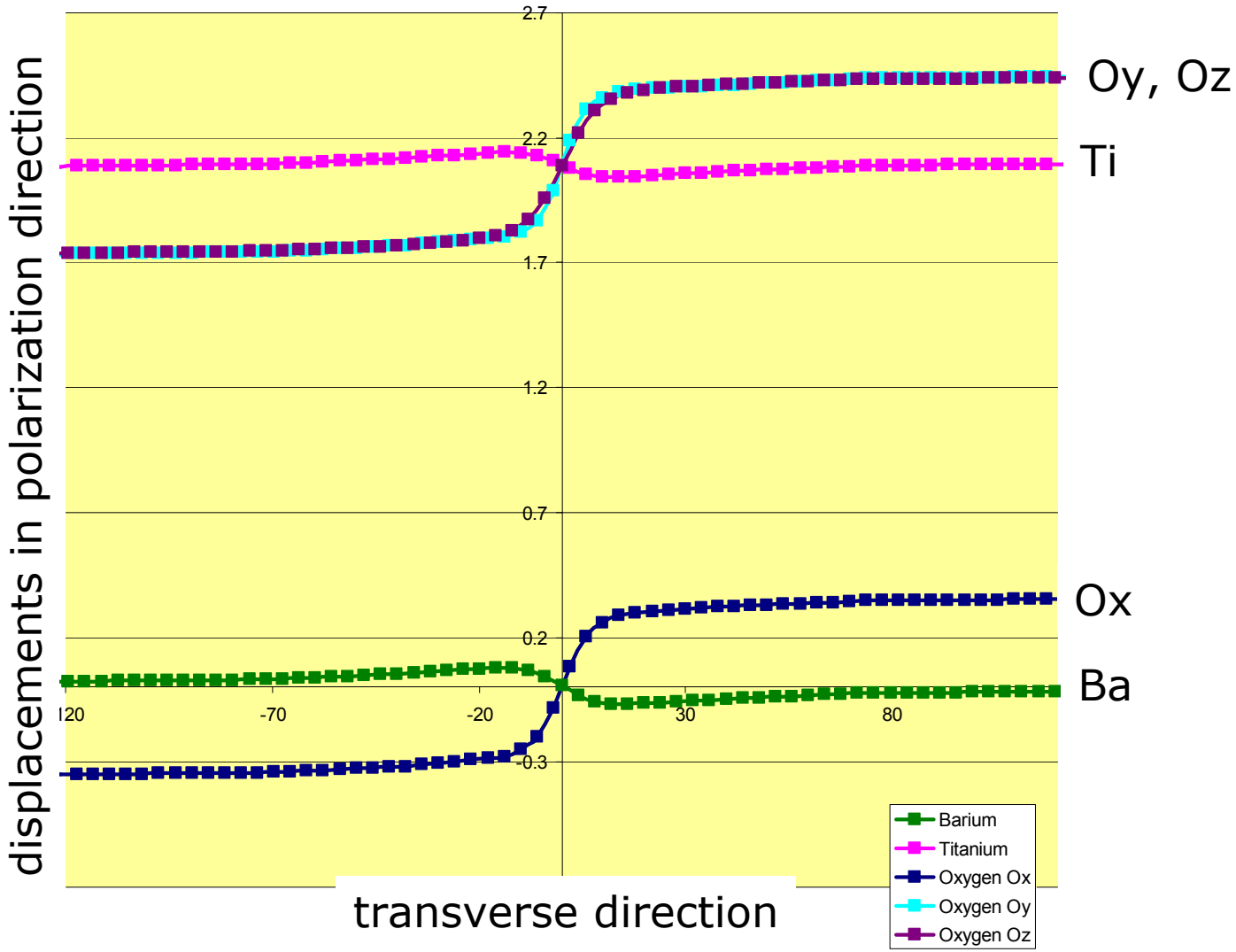
$BaTiO_3$ – 180° wall



- Polarization in X-direction
- Nominal number of atoms ~ $11x10^6$
- 65x65x513 unit cells
- Atomistic resolution: 9 cells
- Goddard *et al.* polarizable Reax FF

(Kowalesky, Knap and Ortiz ´03)

$BaTiO_3$ – 180° wall



180°-wall: Displacements (close up)

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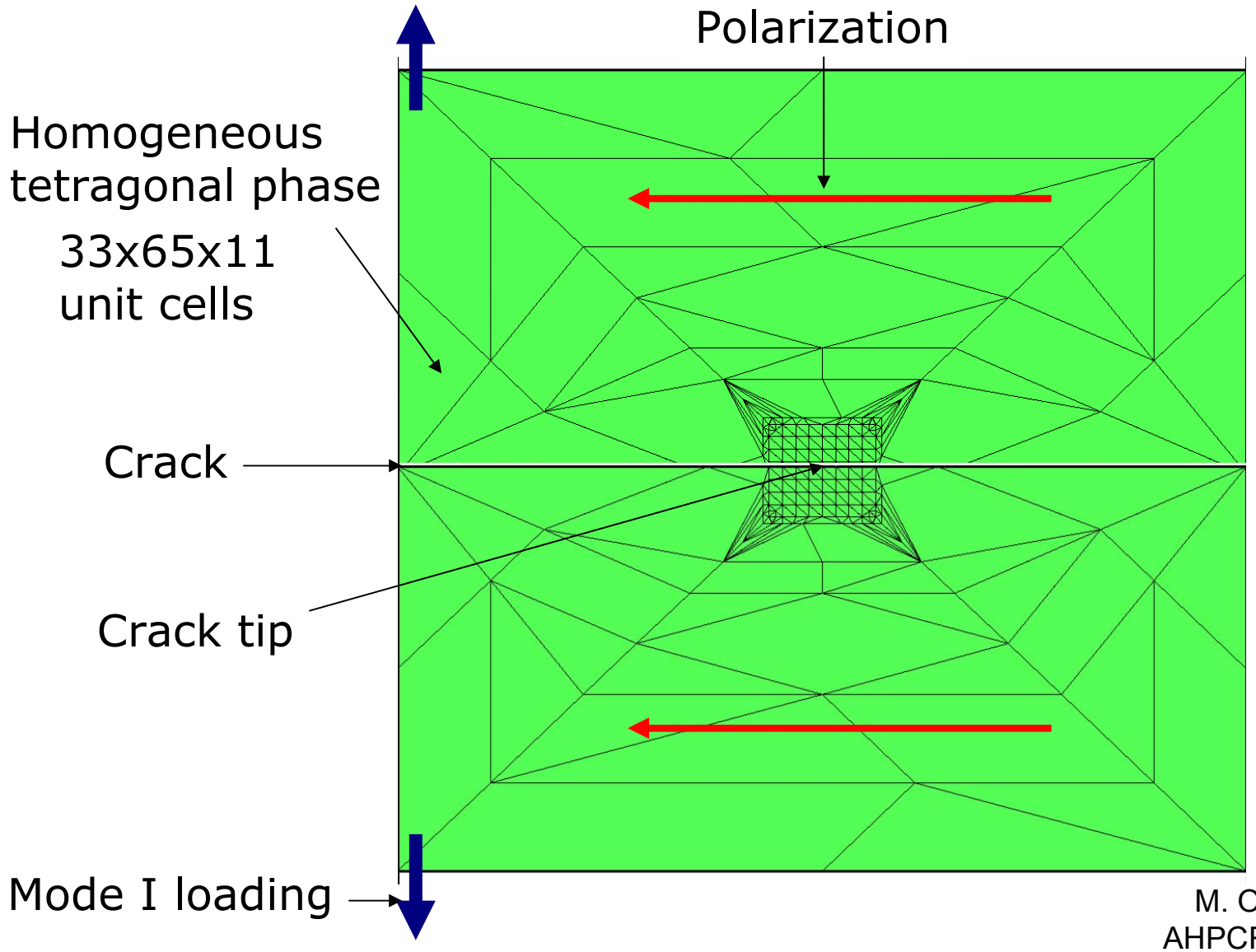
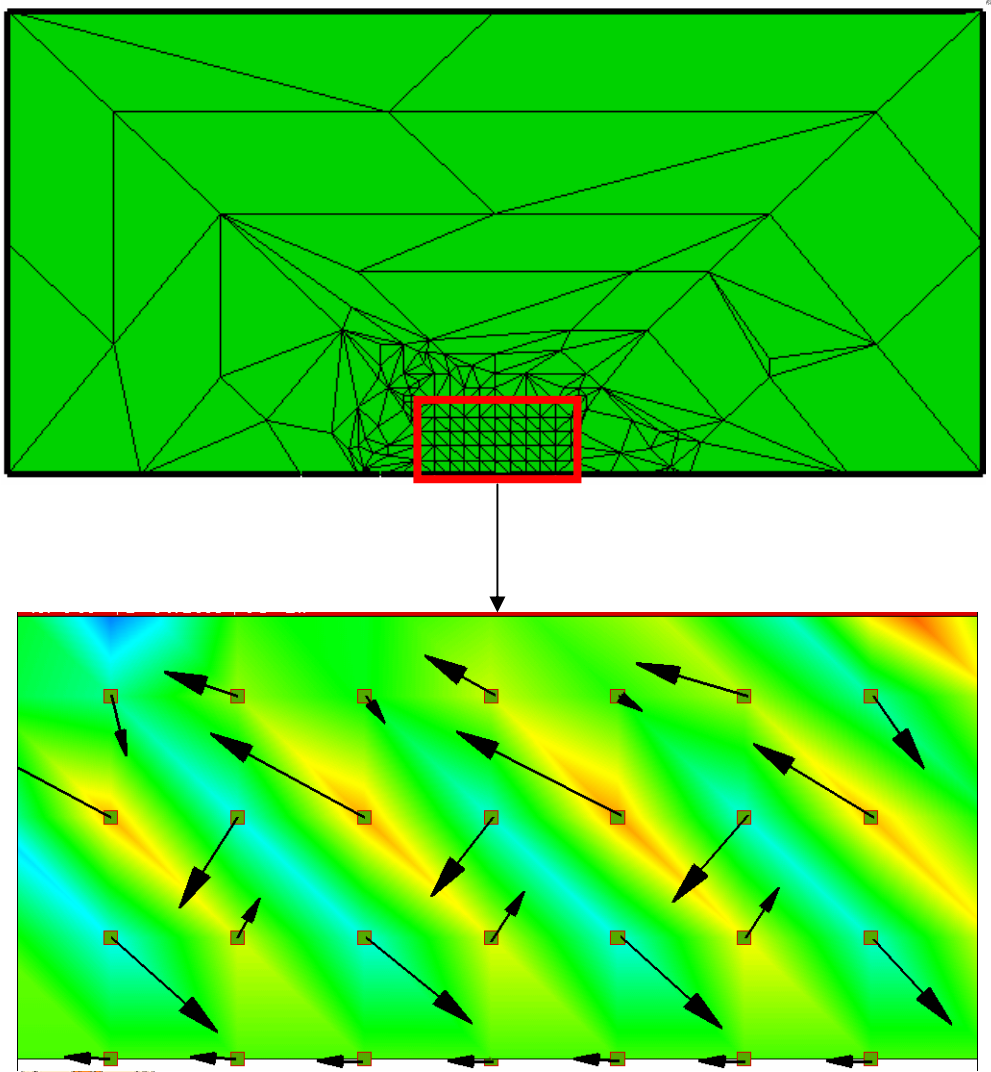
$BaTiO_3$ – Tetragonal crack



$BaTiO_3$ – Tetragonal crack

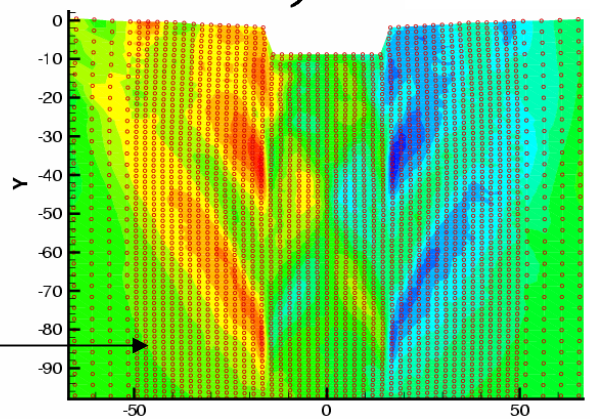


- Polarization field after three loading steps, showing domains and 90° walls
- Domain switching under cyclic loading?
- Misfit strains under cyclic loading?
- Bond breaking (Reax FF), crack growth?
- Crack-growth rates?

Dynamics

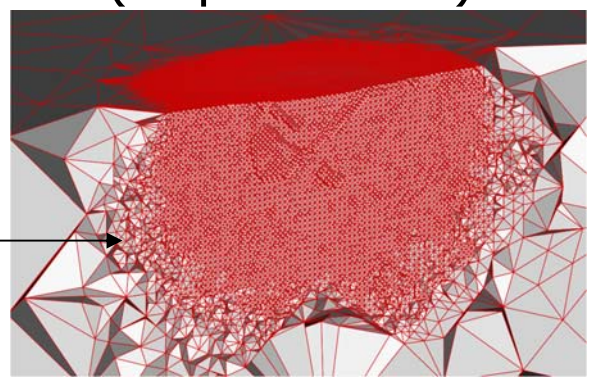
- Action integral: $I[\boldsymbol{q}] = \int_a^b \left\{ \frac{m}{2} |\dot{\boldsymbol{q}}|^2 - E(\boldsymbol{q}) \right\} dt$
- Hamilton's principle: $\delta I[\boldsymbol{q}] = 0$
- Galerkin reduction: $X \to X_h$,

  $\boldsymbol{M}_h \ddot{\boldsymbol{q}}_h + f_h(\boldsymbol{q}_h) = \boldsymbol{0}$



Shenoy, Ortiz and Phillips (unpublished)

- Limitations:
  - i) Thermal component is wiped out.
  - ii) Intermal reflections (need absorbing boundaries).



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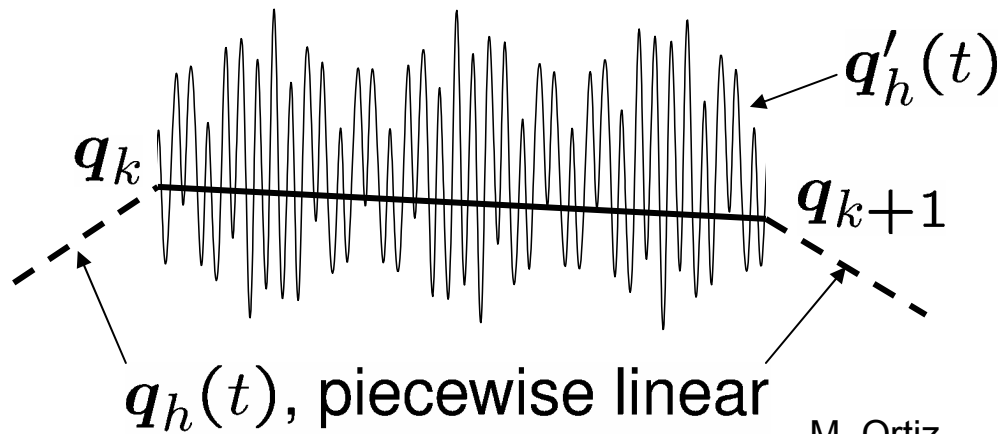
Finite temperature

- Course-Grained Molecular Dynamics (Rudd & Broughton, Phys. Rev. B 1998).
- Einstein model (Shenoy and Phillips, 1999):

$$F_h = E_h + \sum_{K \in \mathcal{T}_h} n_h(K) 3 k_B T \log \left(\frac{h \boldsymbol{D}^{1/6}(K)}{k_B T} \right)$$

- Weak convergence + separation of time scales (Bornemann ´97):

$$L_d(\boldsymbol{q}_k, \boldsymbol{q}_{k+1}) \approx \int_{t_k}^{t_{k+1}} L\Big(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t)\Big)\, dt$$



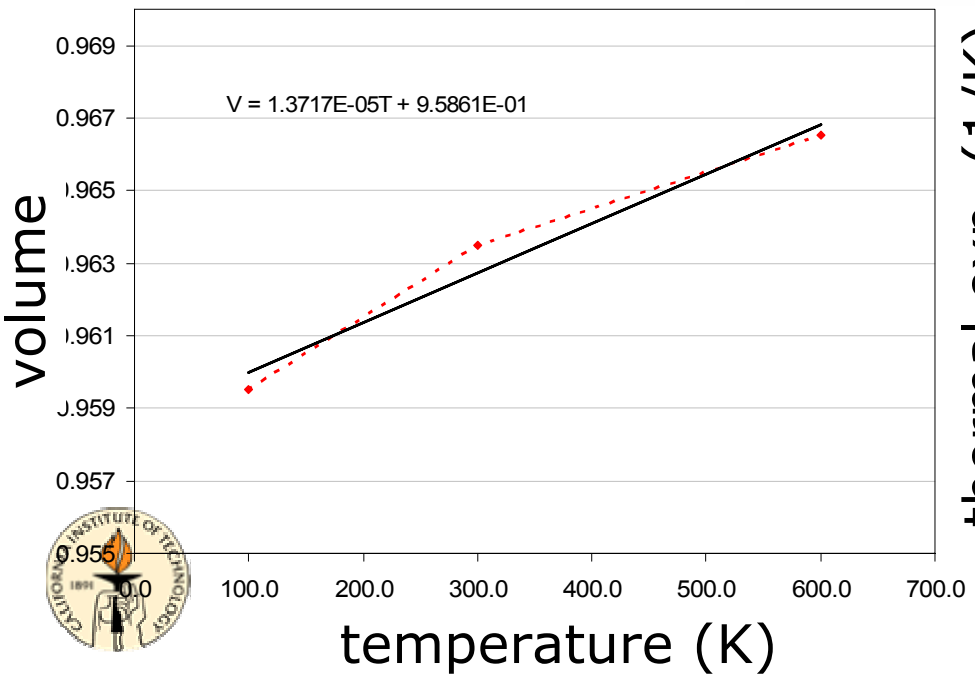
Finite temperature

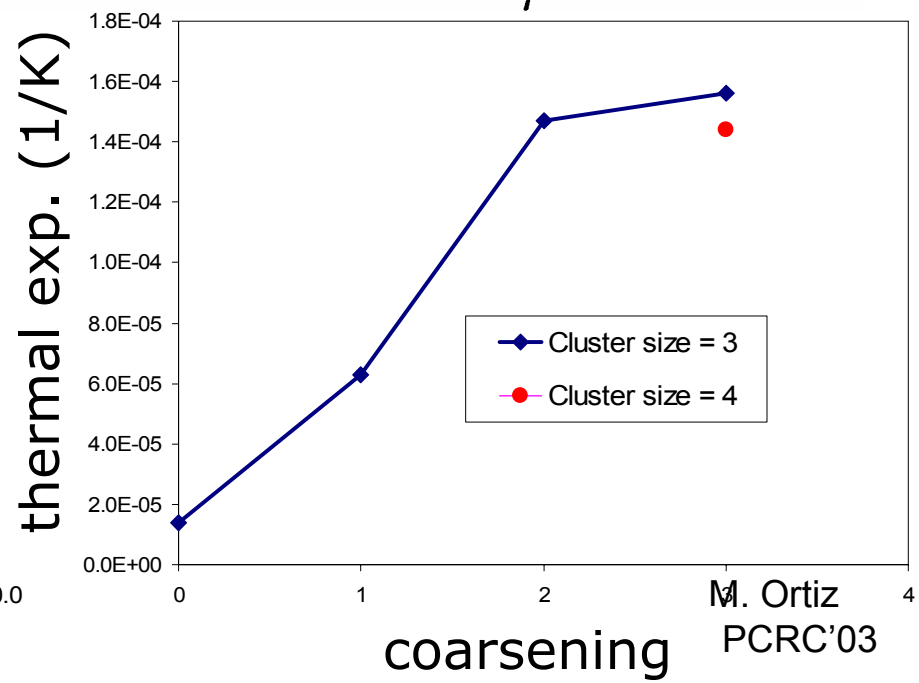
- Langevin dynamics (Marian, Knap and Ortiz ´03):

$$\boldsymbol{M}_h\ddot{\boldsymbol{q}}_h + \tau^{-1}\boldsymbol{M}_h\dot{\boldsymbol{q}}_h = \boldsymbol{f}_h(\boldsymbol{q}_h) + \boldsymbol{R}_h(t)$$

$$\boldsymbol{R}_h(\boldsymbol{l}_h, t) = \sum_{\boldsymbol{l}\in\mathcal{L}} \boldsymbol{R}(\boldsymbol{l}, t)\varphi_h(\boldsymbol{l}|\boldsymbol{l}_h)$$

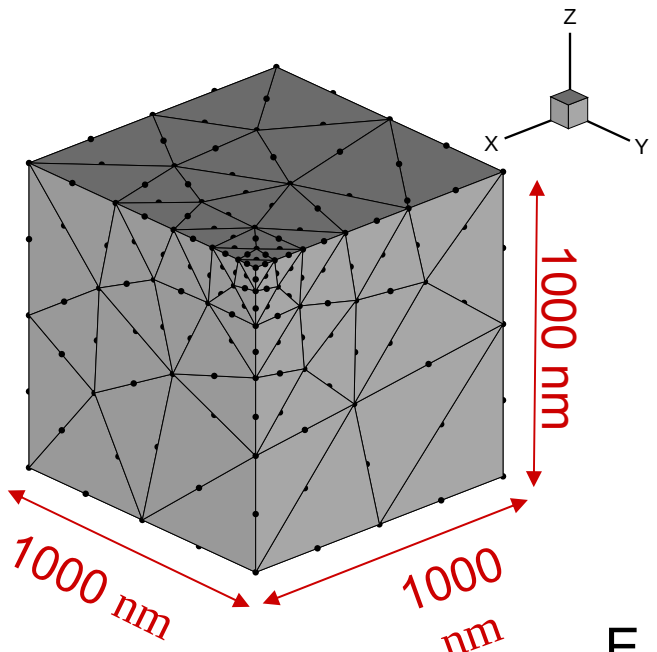
$$\langle \boldsymbol{R}(\boldsymbol{l}, t)\rangle = \boldsymbol{0}, \quad \langle \boldsymbol{R}(\boldsymbol{l}, 0) \otimes \boldsymbol{R}(\boldsymbol{l}, t)\rangle = 2\frac{m^2}{\tau} k_B T \boldsymbol{I}\delta(t)$$

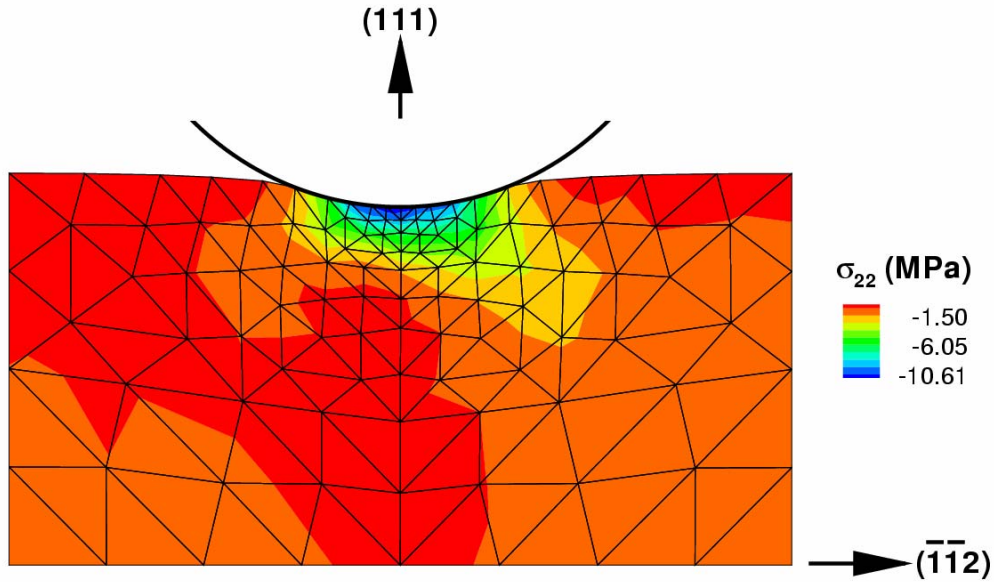




Coupling to quantum mechanics

CB rule: Smith, Tadmor and Kaxiras, *PRL* **84**, 2000, p. 1260)



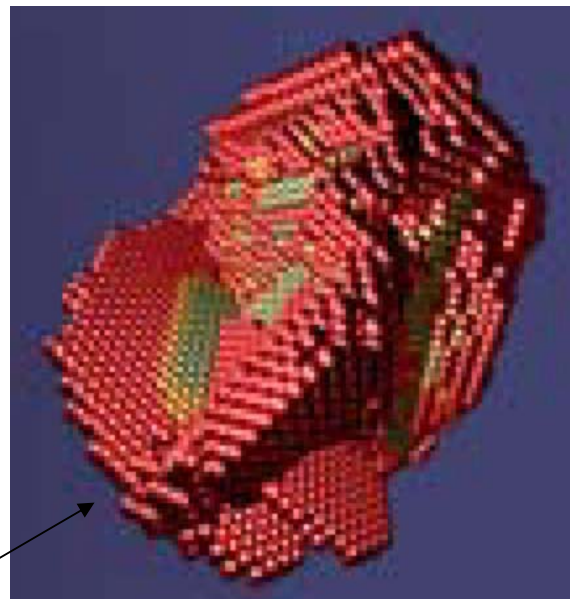


E.A. Carter, M. Fago, R. Hayes, M. Ortiz ´03

Structure: fcc Al crystal
Size: 2μm x 2μm x 1μm single crystal
Indenter radius: 0.75μm
Mesh: 105 elements ⇒ 420 QM calculations
Total # QM calculations: ⇒ 8 million

Concluding remarks

- Continuum/atomistic methods are useful for:
  - *Overcoming the size and time limitations of straight molecular dynamics*
  - *Building atomistic realism and fidelity into continuum boundary value problems*
- Outstanding issues:
  - *Mathematical analysis*
  - *Mesh optimization*
  - *Finite temperature*
  - *Transport properties:*
    - *Mass*
    - *Viscosity*
    - *Heat conduction*
  - *Dislocation dynamics*



Nanovoid cavitation
(Marian, Knap and Ortiz ´03)