Modeling the Solid State with Coupled Atomistic/Continuum Methods

Ronald E. Miller
Carleton University, Ottawa, Canada

KITP
June 7, 2012

Credits

Lead Actors

Collaborator on many things (QC, hot QC, comparisons):
Ellad Tadmor, U. Minnesota

Post-Docs:
Denis Saraev (PDF, currently at large)
Behrouz Shiari (PDF, now at NNIN Michigan)

Collaborators on CADD:
Leo Shilkrot (currently at large)
Bill Curtin (Brown and EPFL)

Collaborators on hot QC:
Laurent Dupuy, CEA
Frederic Legoll, University of Paris
W.K. Kim, PDF at U. Minnesota

Supporting Cast

Help with all the comparisons of methods:
Mitch Luskin, Univ. of Minnesota
Michael Parks, LANL
Catalin Picu, RPI
Dong Qian, U. Cincinnati

Producers

NSERC CRSNG

Ontario Premier's Research Excellence Awards (PREA)

Outline | Coupled Atomistic/Continuum Methods

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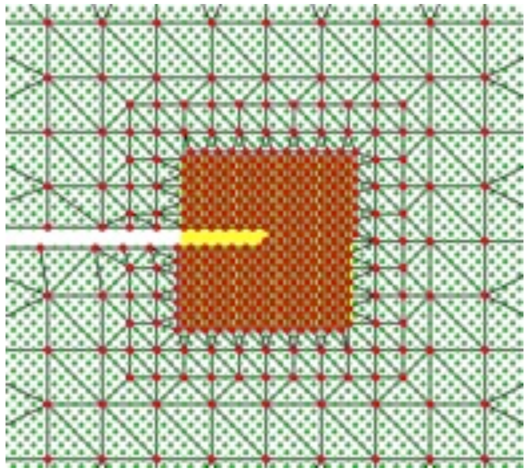
1. Static partitioned-domain methods for modeling crystalline solids
   - Overview of the essential ingredients of these coupling methods



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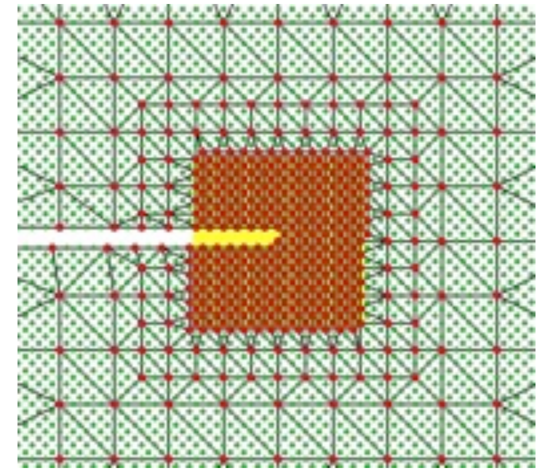
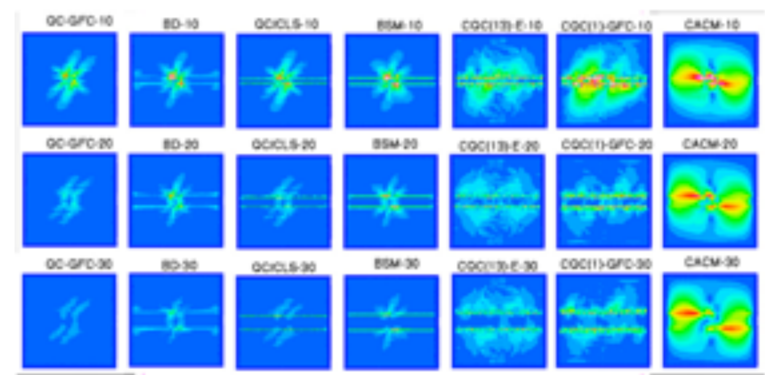


2. Relative accuracy and efficiency of 14 static methods from the literature



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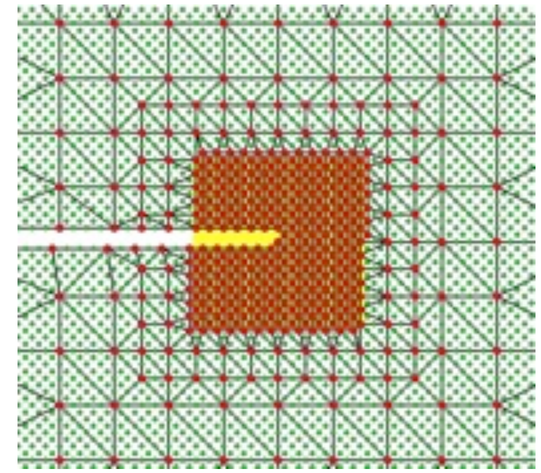

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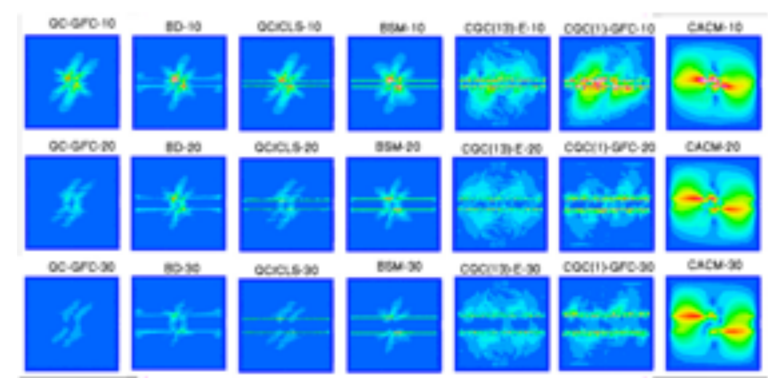
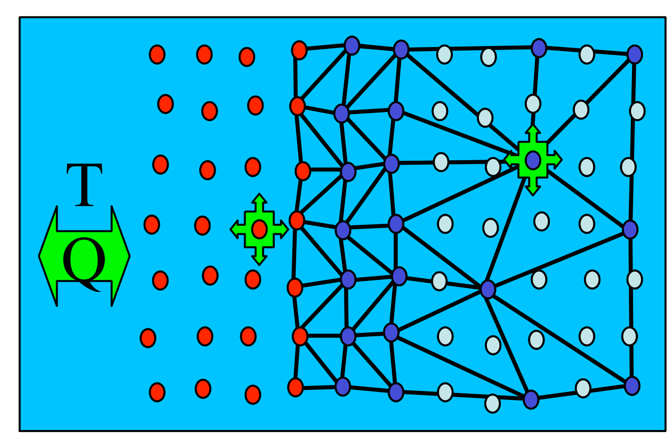


3. Extending these methods to finite Temperature



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about 200,000 Ni on Cu at zero K

...mulations of crystalline fracture and plasticity

MD simulations require relatively large systems

Nickel on Copper
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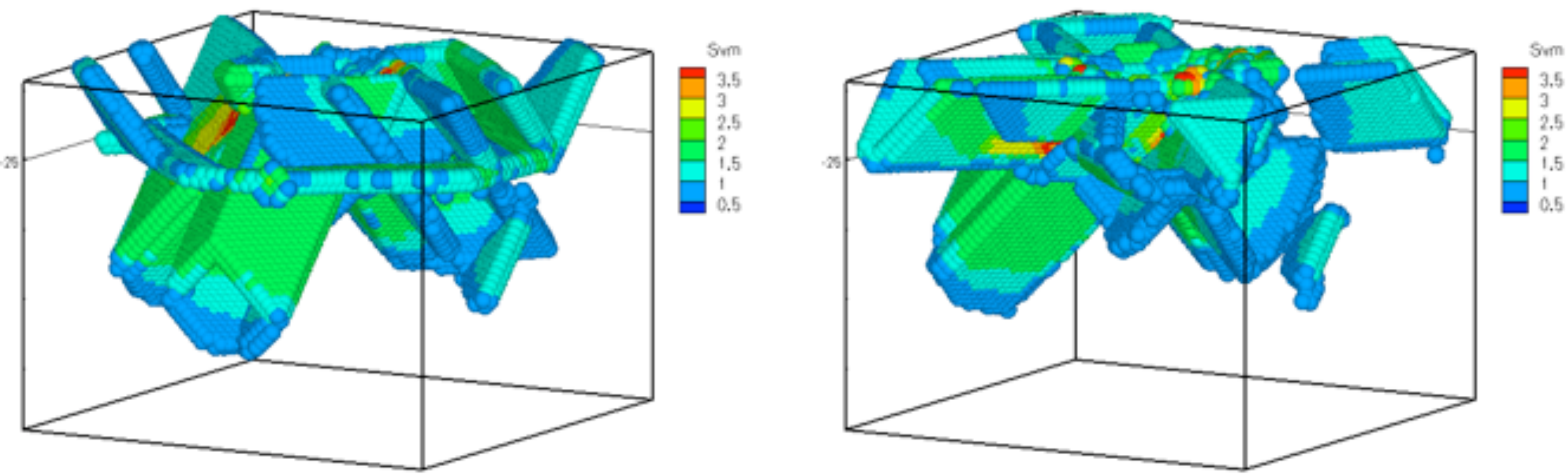

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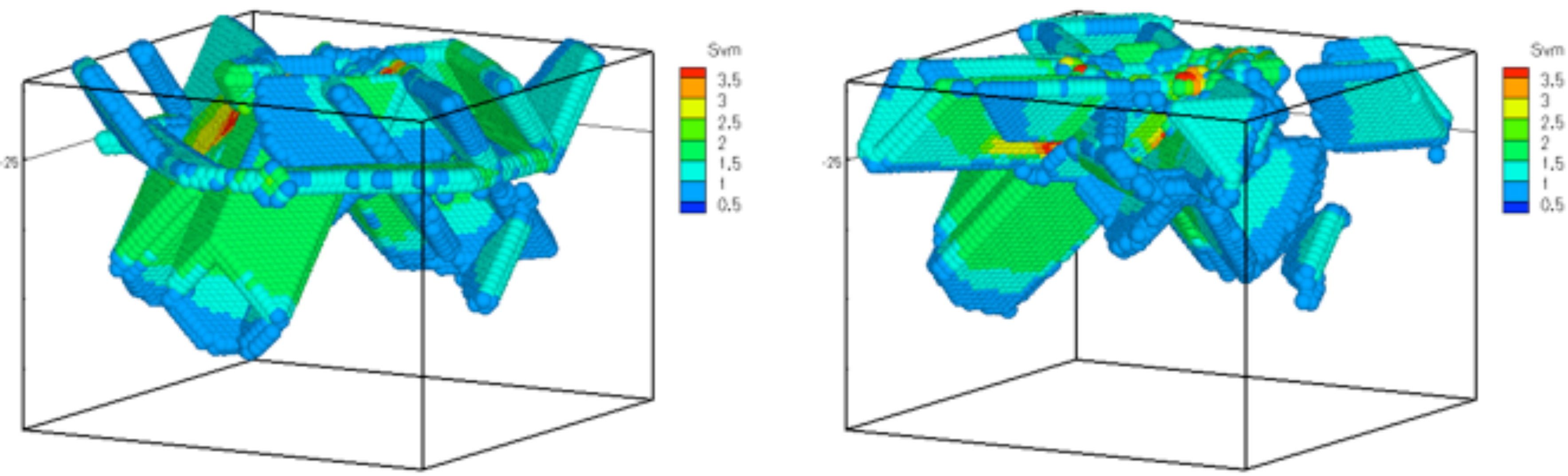

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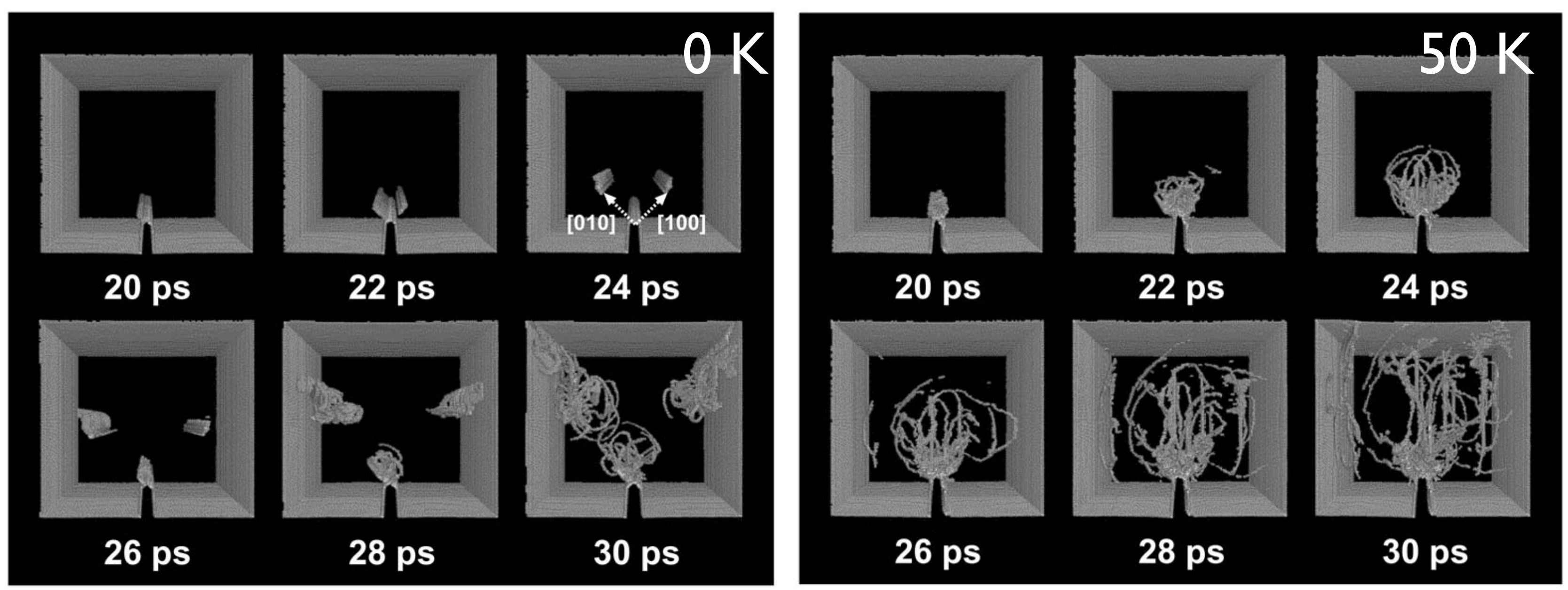
Aluminum



Kimizuki et al., *JCAMD*, 2003

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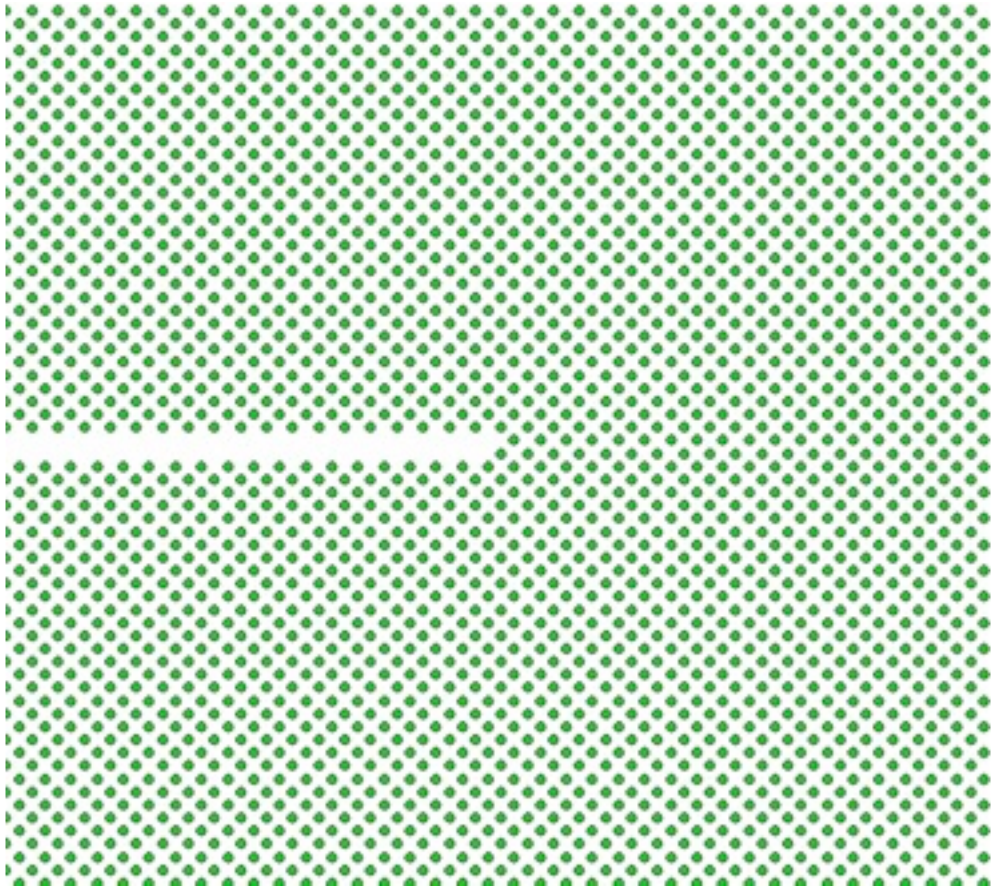

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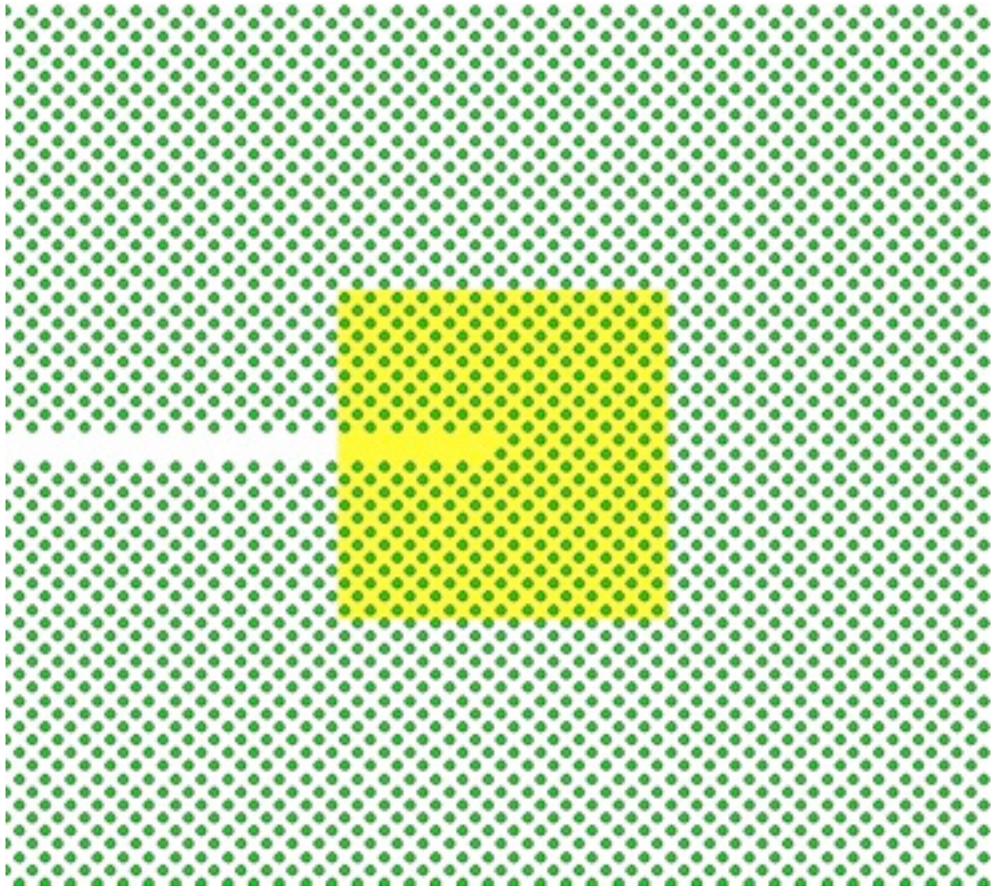

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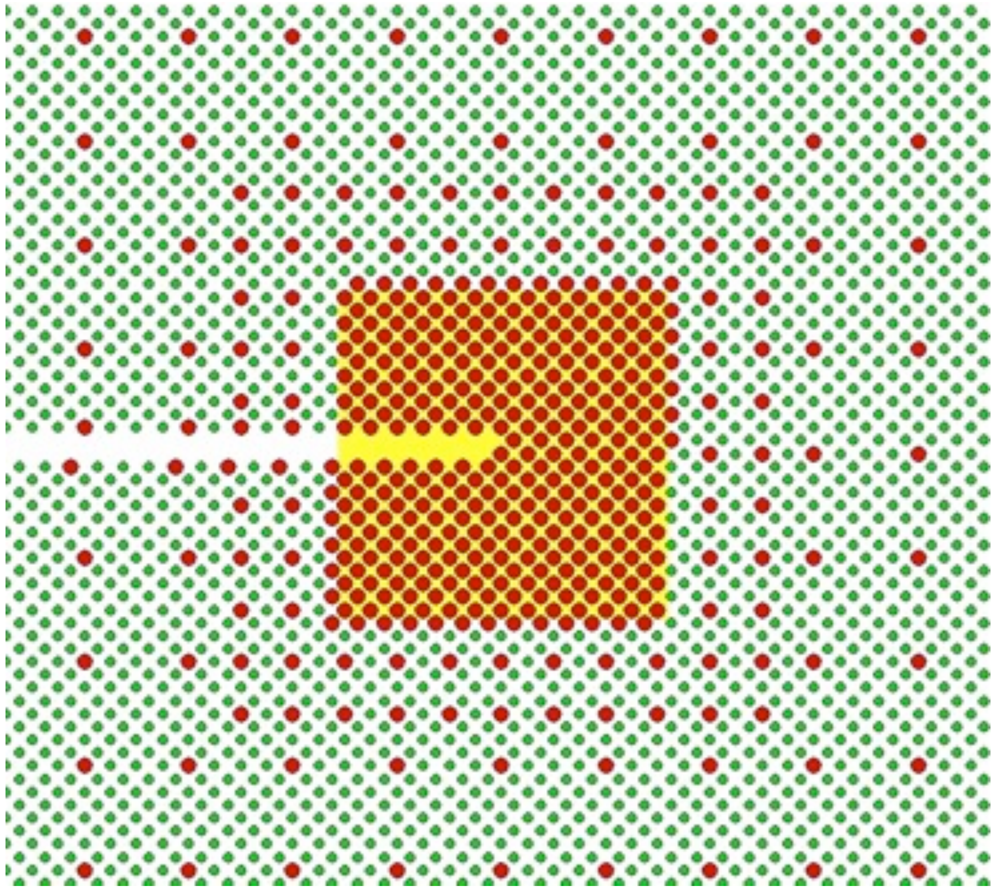

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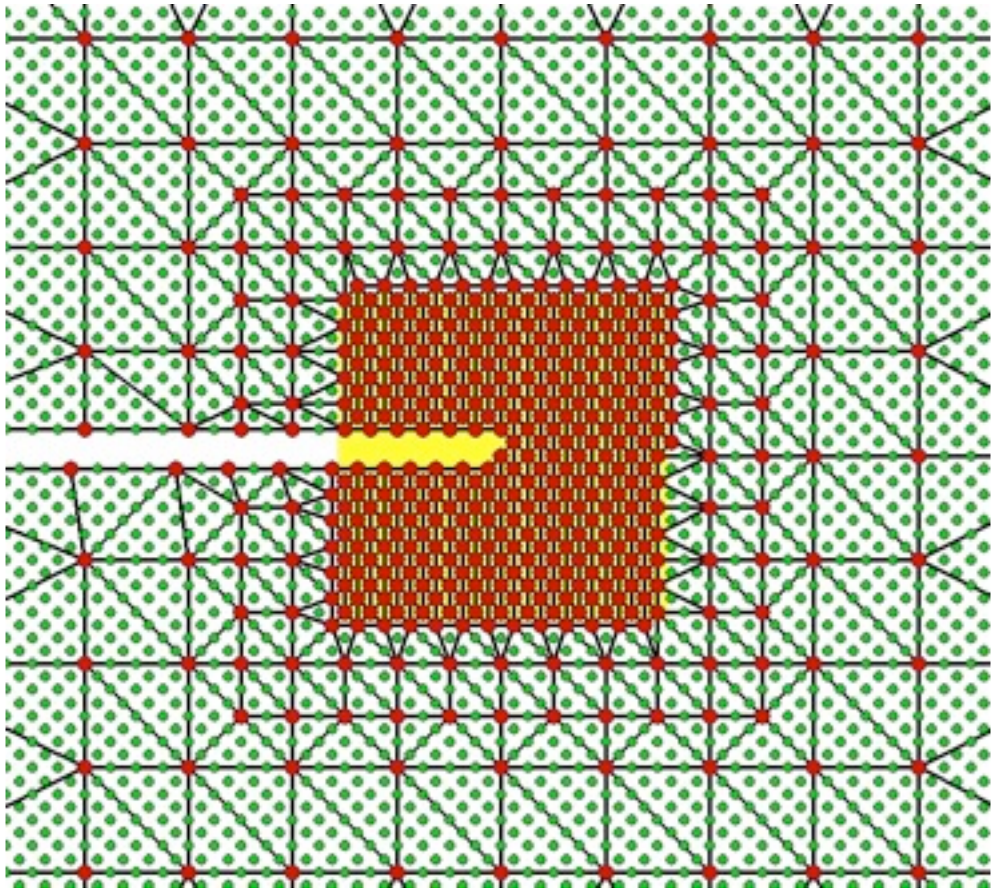

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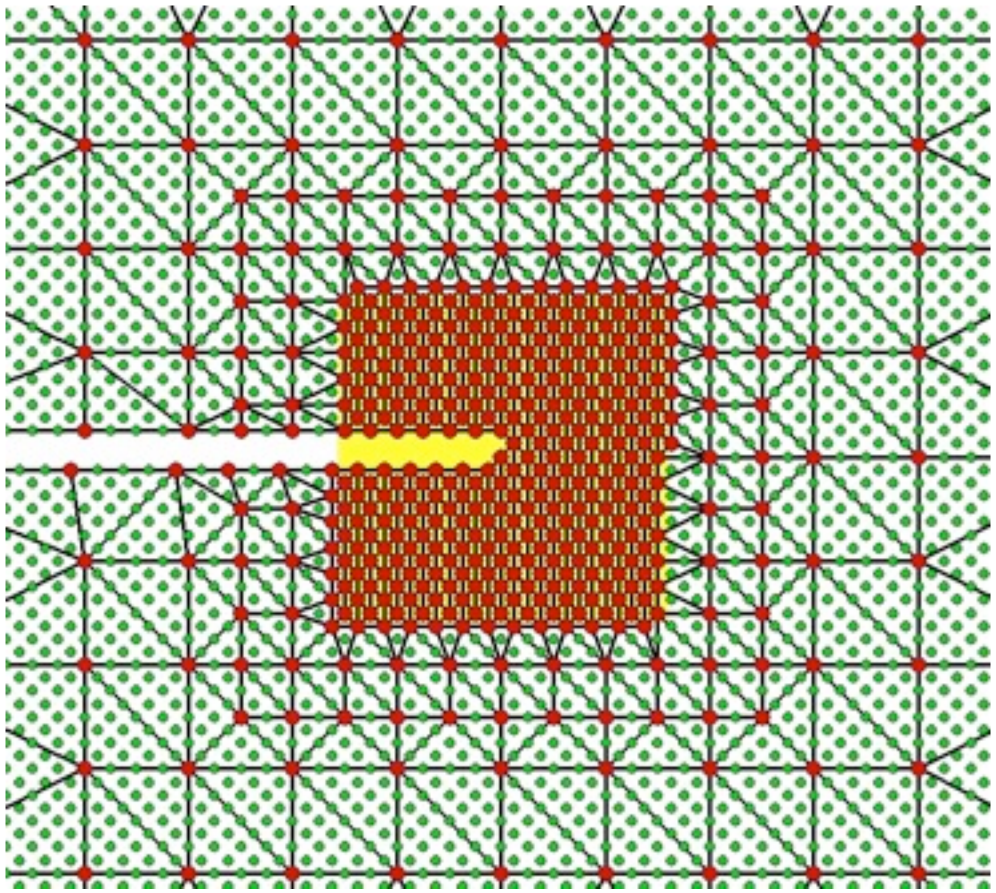
Positions of atoms found by interpolation

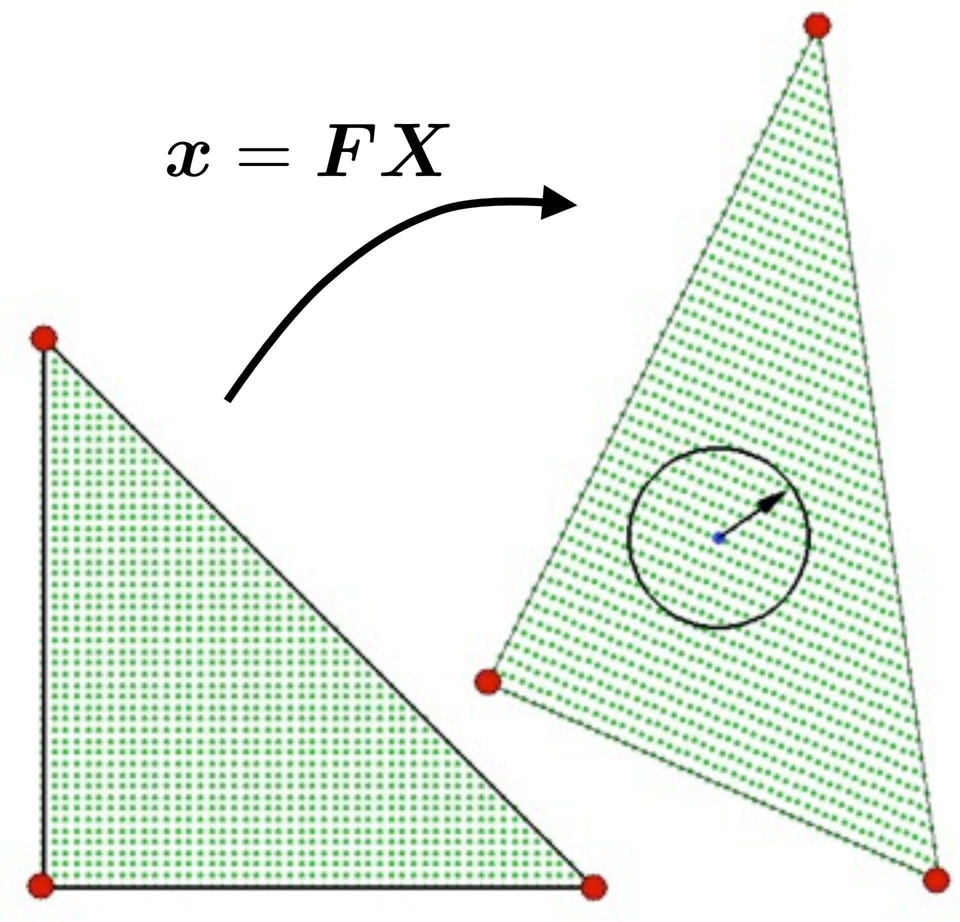
$$\boldsymbol{u}^{\alpha} = \sum_{i}^{\text{nodes}} S_i(\boldsymbol{X}^{\alpha})\boldsymbol{u}_i$$



The Quasicontinuum Method

Use the Cauchy-Born rule as the constitutive law

$$W(\boldsymbol{F}) = \frac{E^{\mathrm{CB}}(\boldsymbol{F})}{\Omega_0}$$



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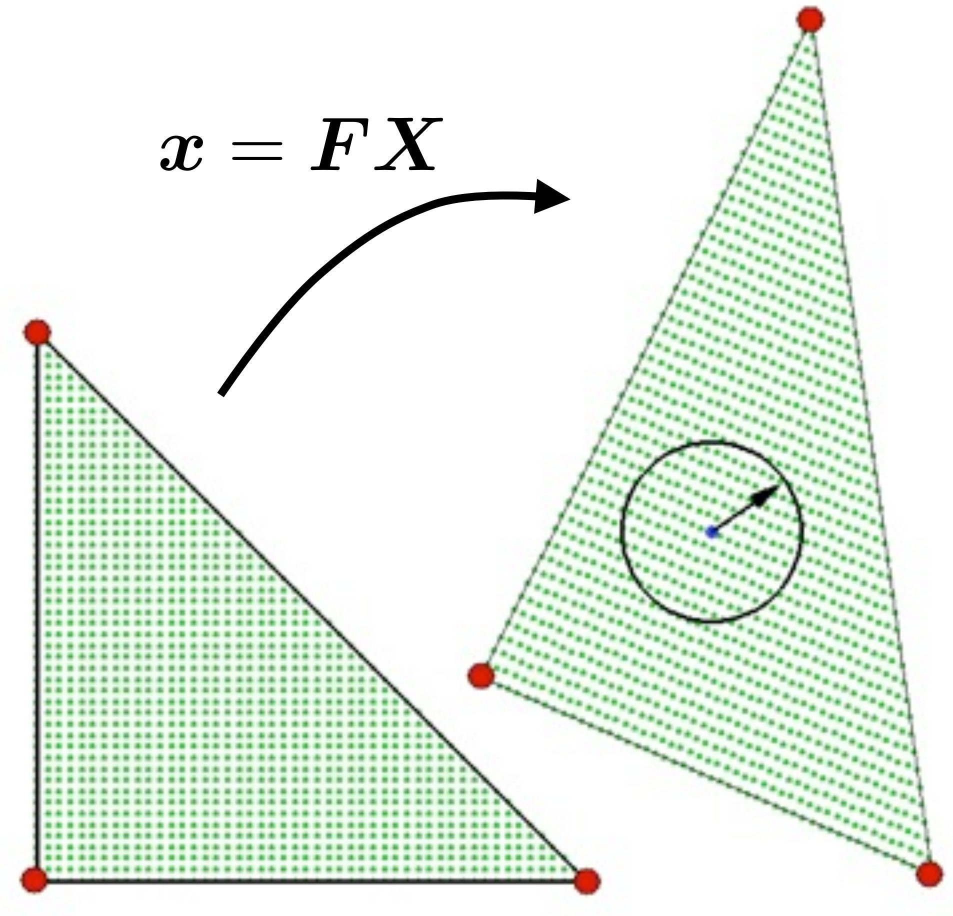

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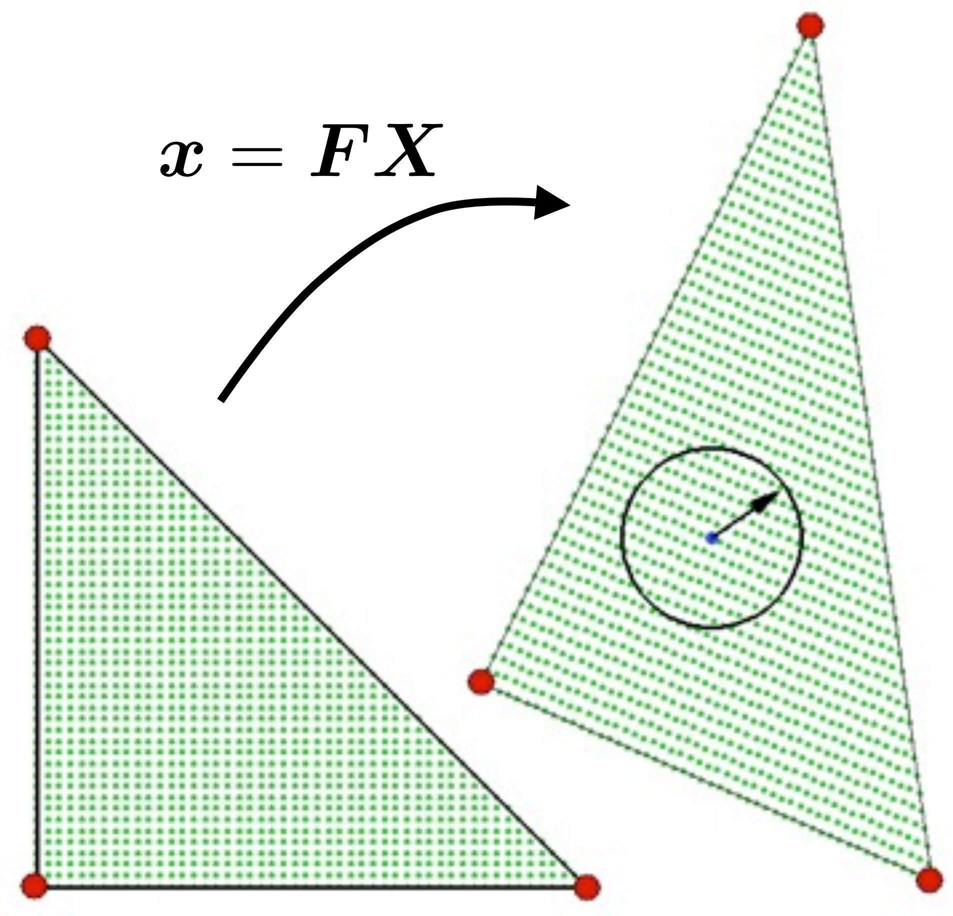

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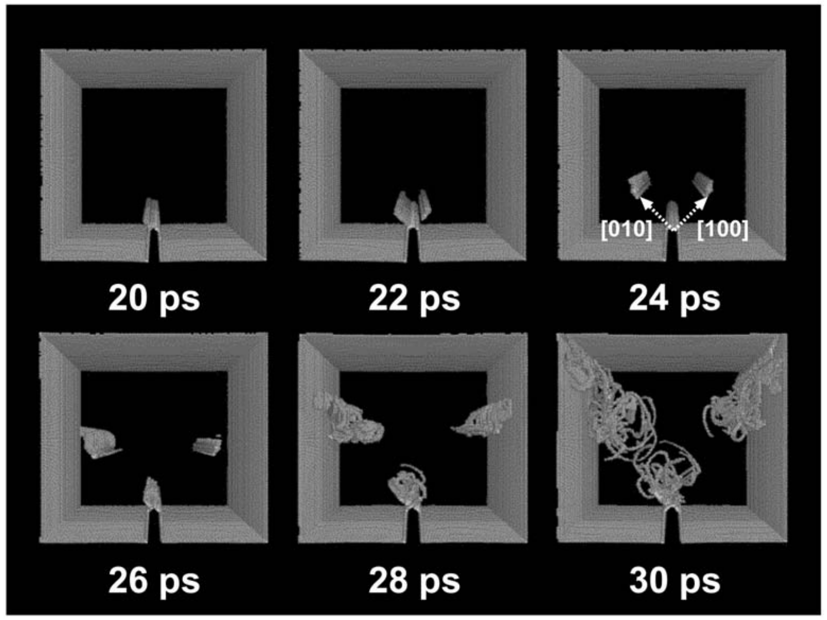
since

$$\frac{V^e}{\Omega_0} \approx n^e$$

Example: Fracture using the QC Method

Multiscale Goal:
To replace this...



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Tadmor, unpublished

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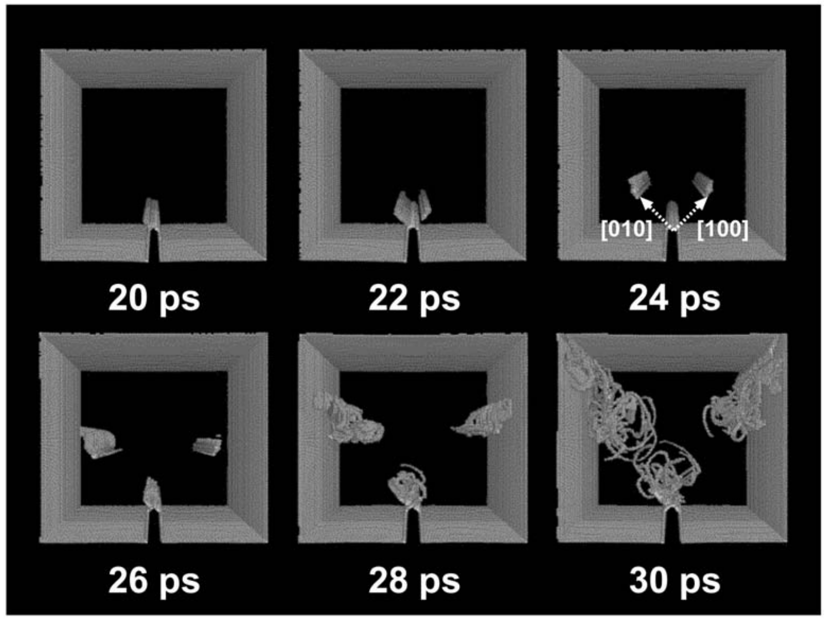

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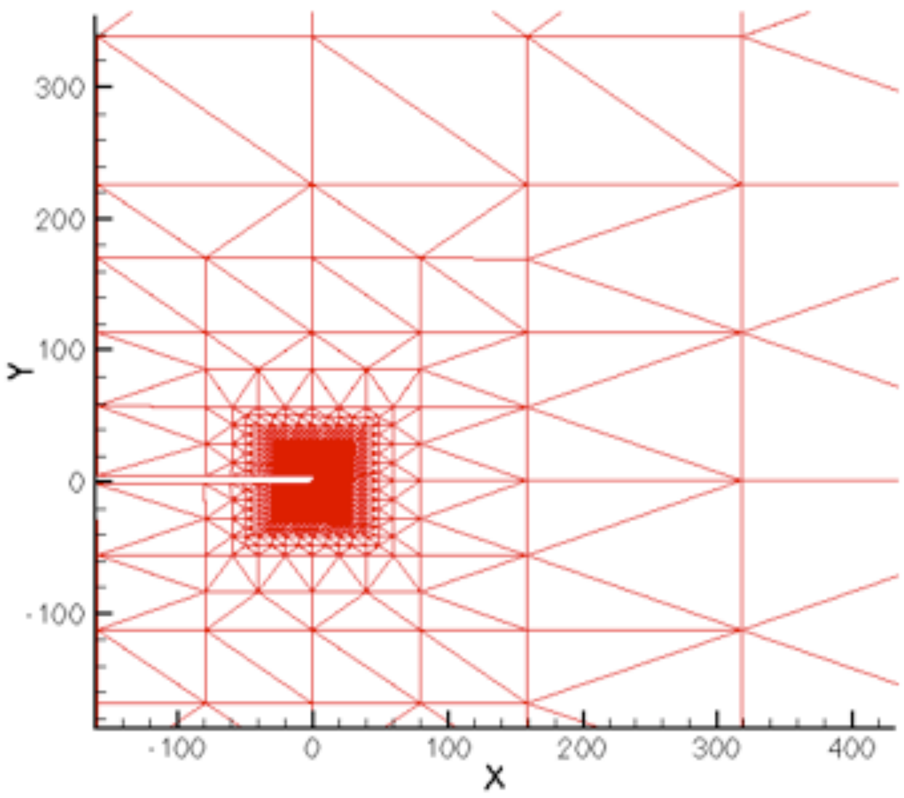

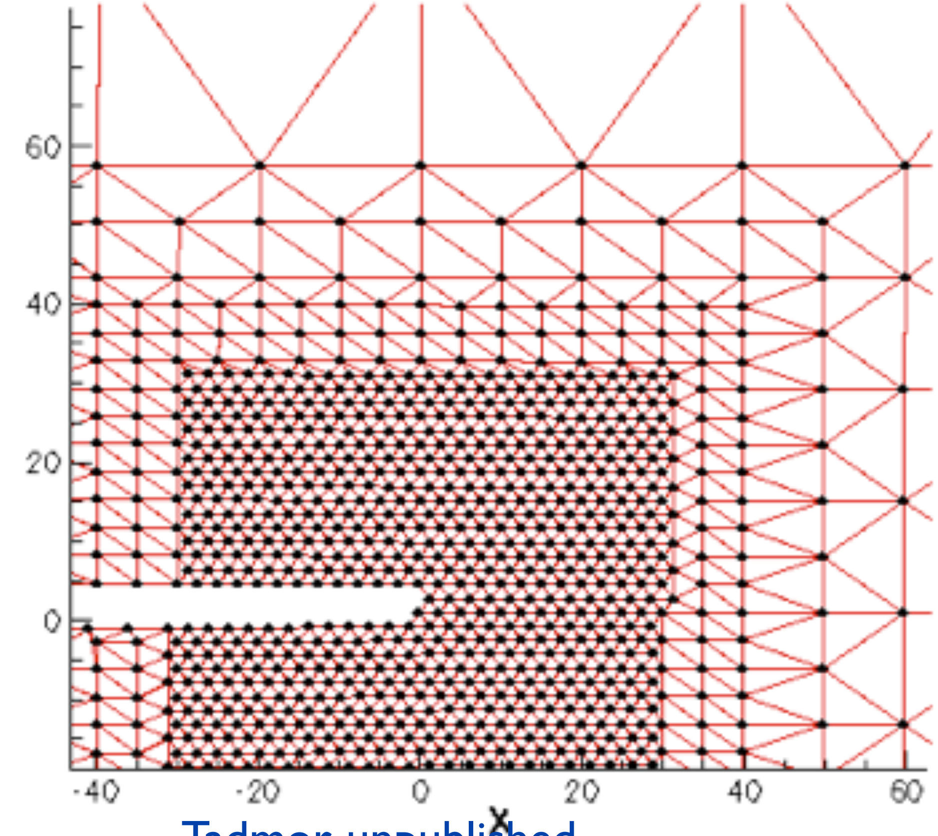

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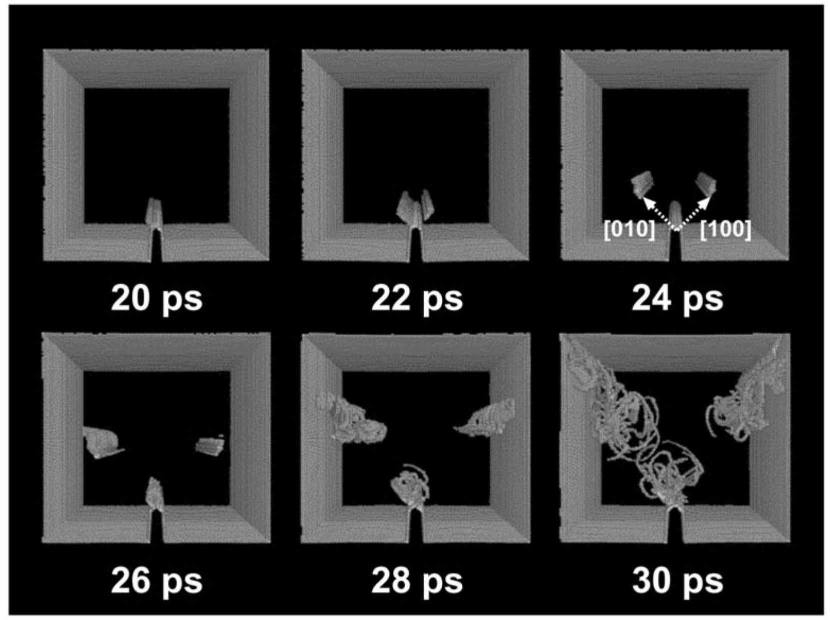

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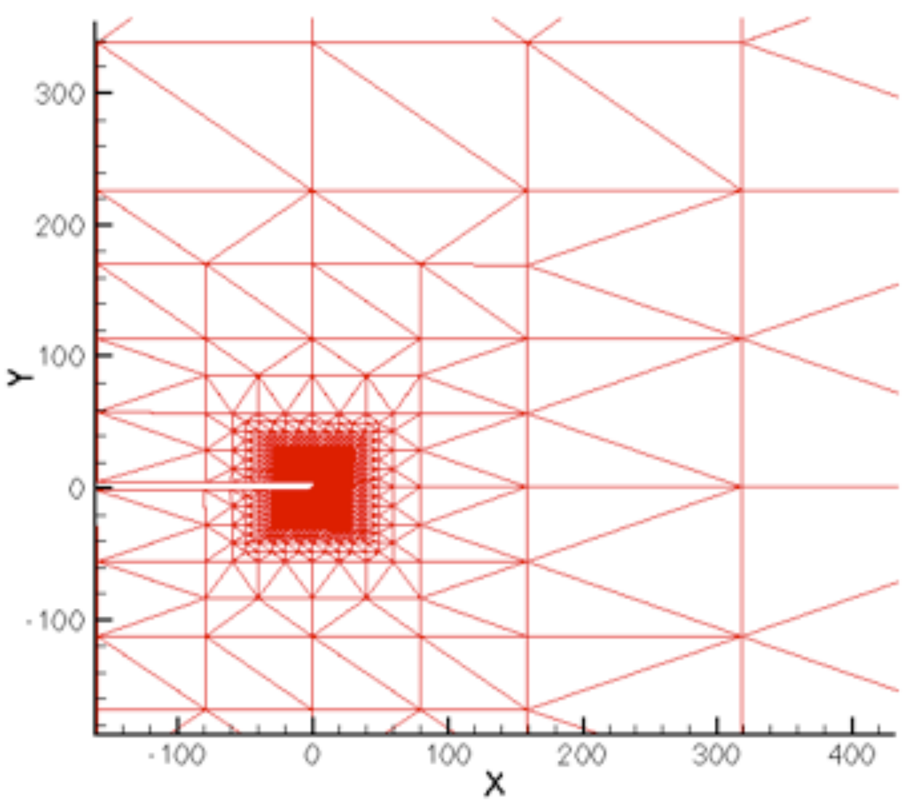

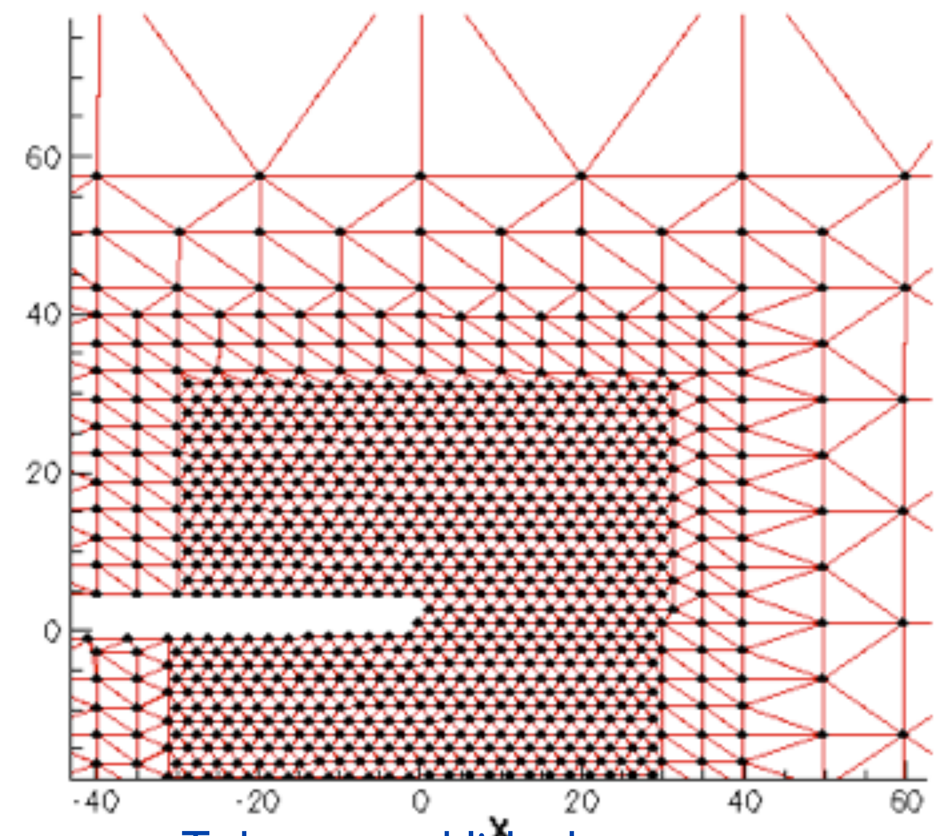

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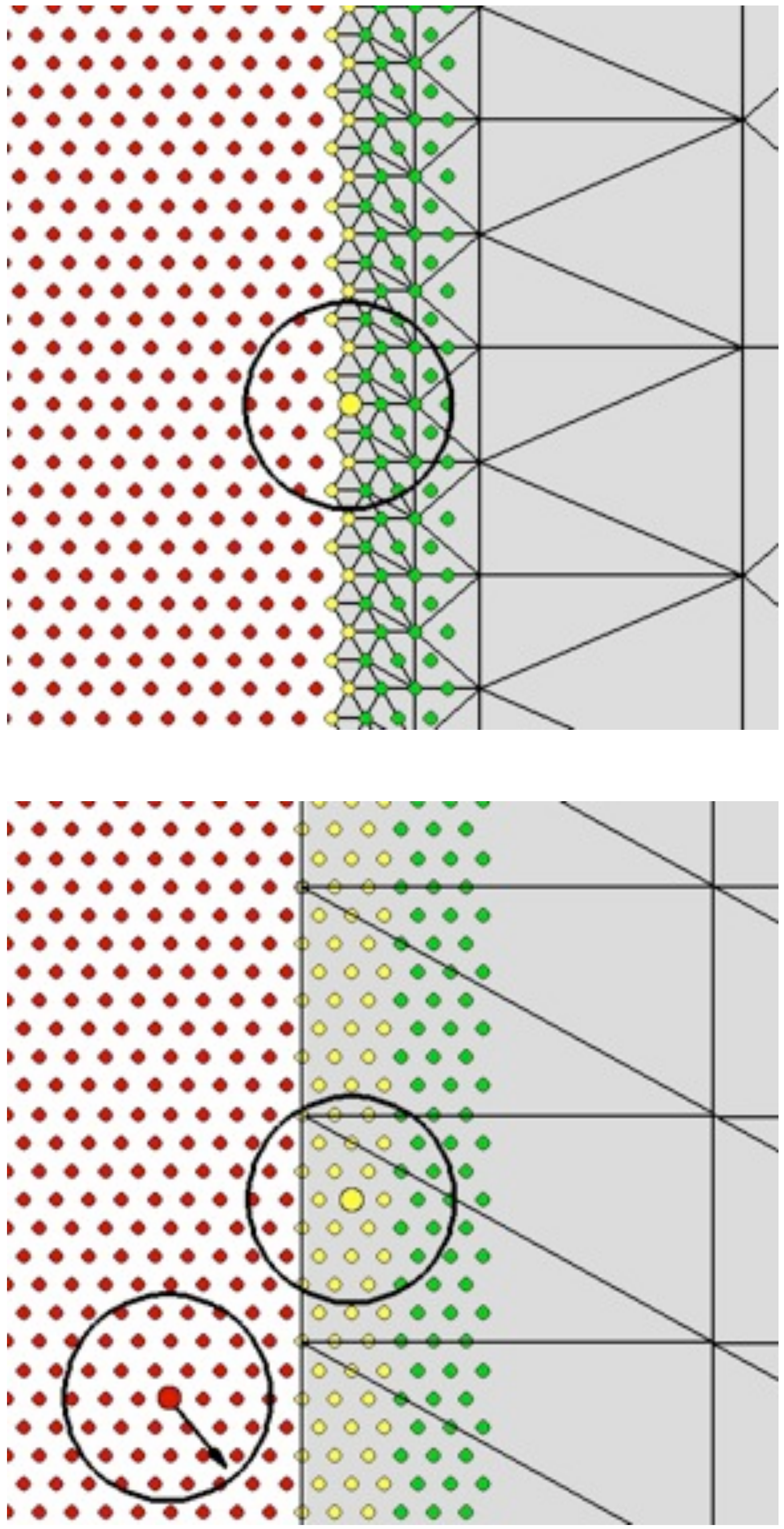
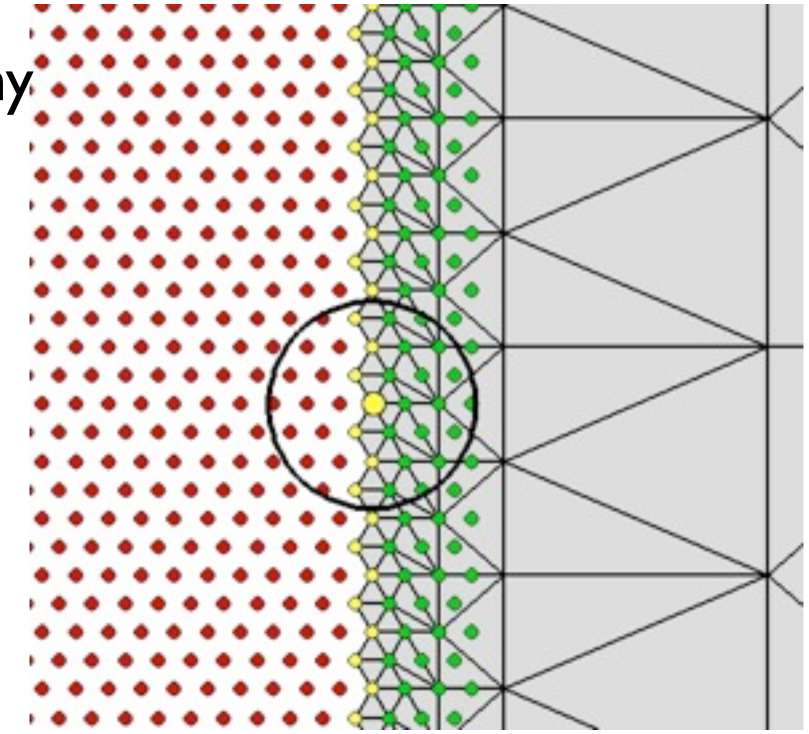
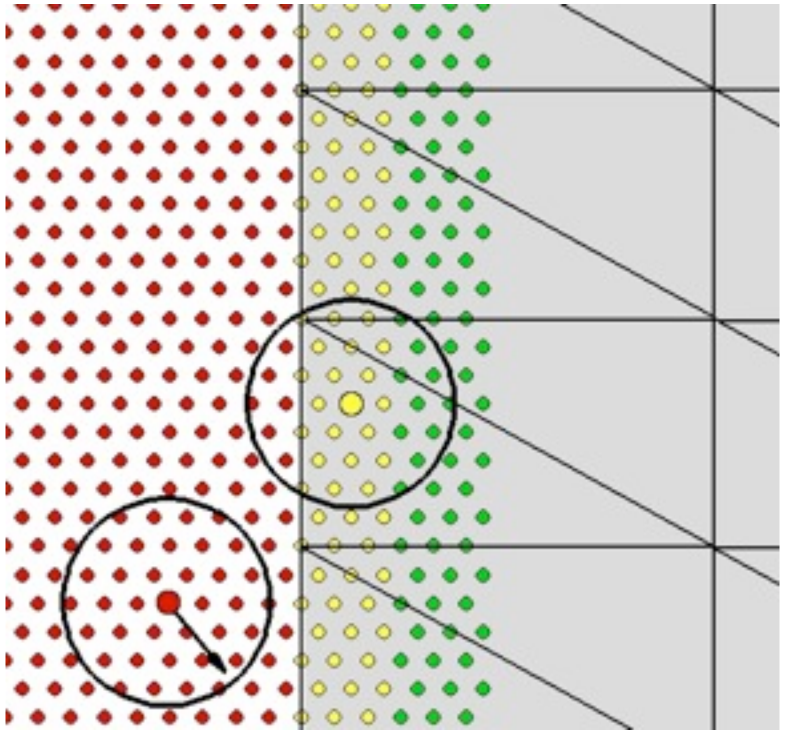
Coupled Atomistic/Continuum Models



Coupled Atomistic/Continuum Models

Since 1991 (*Kohlhoff et al., Phil. Mag. A*), there have been many different methods developed.





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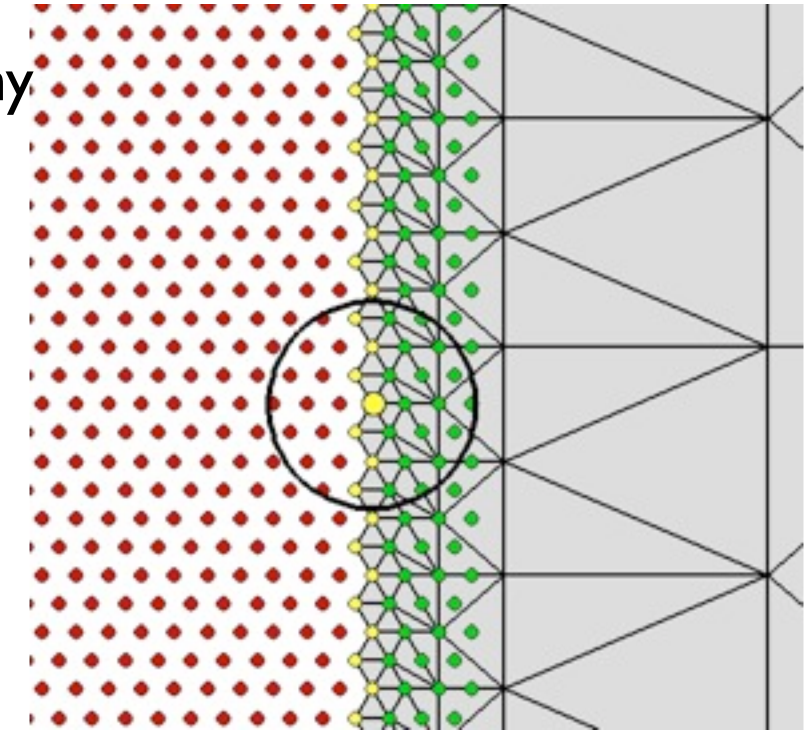

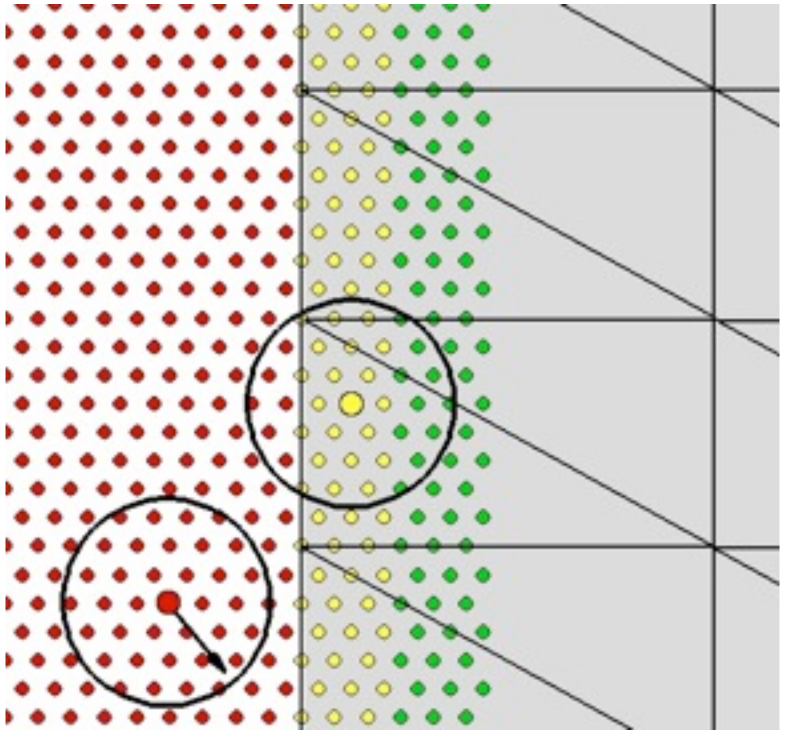

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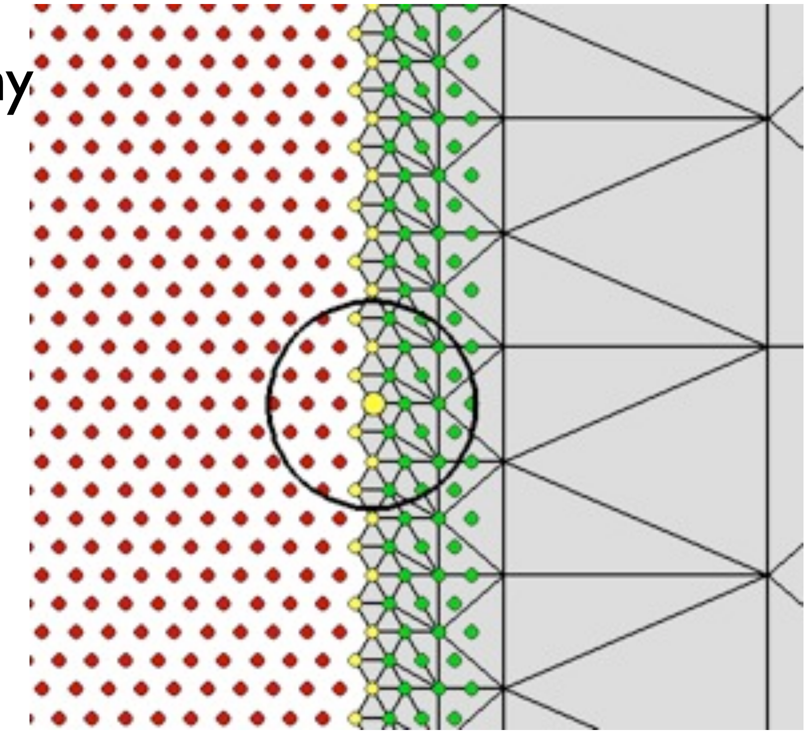

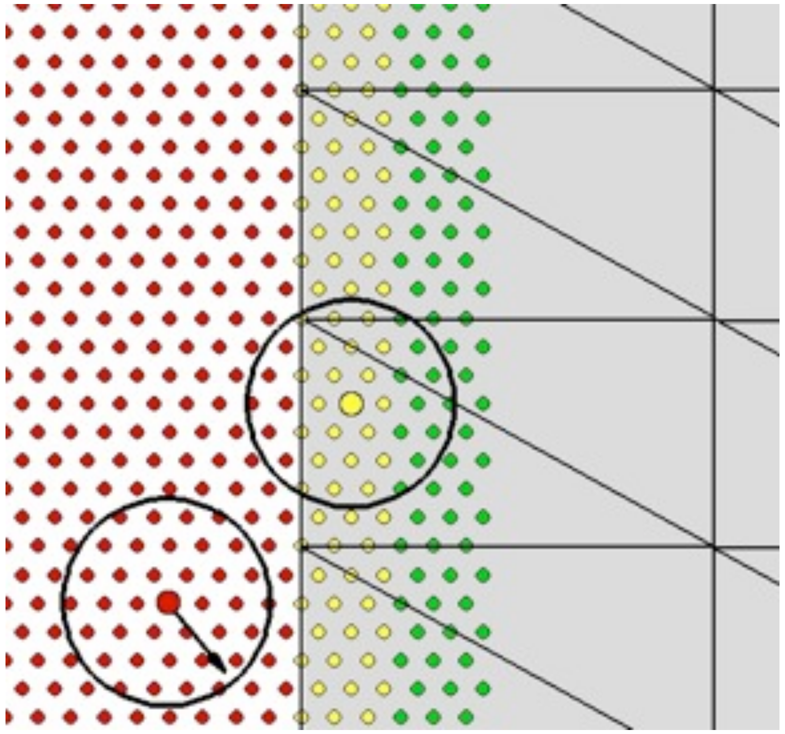

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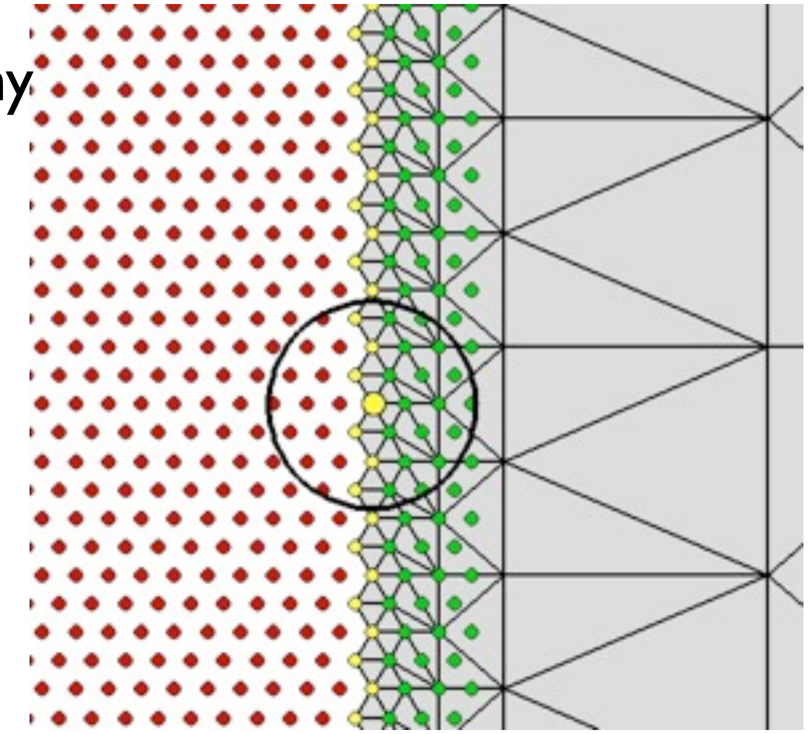

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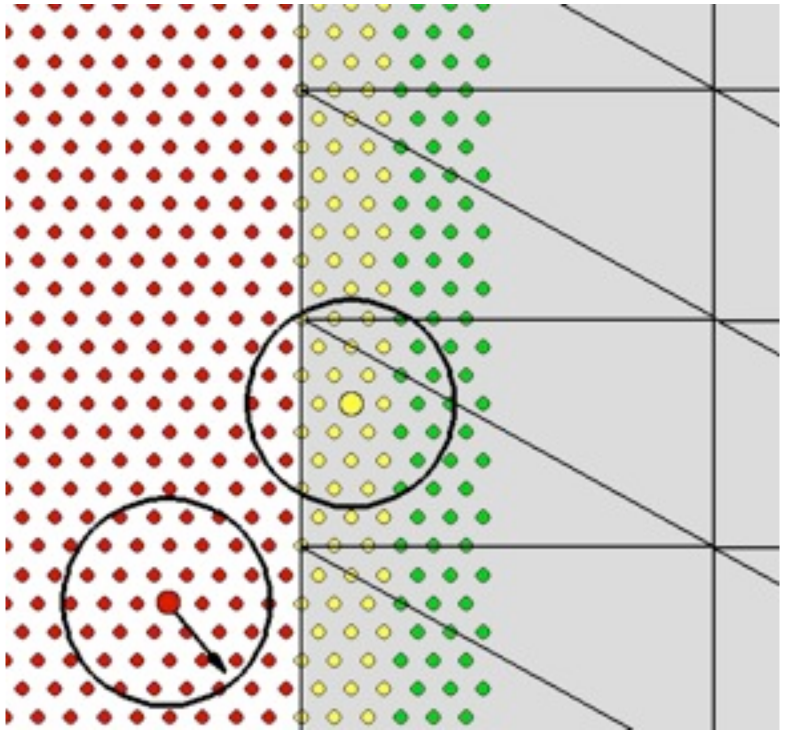

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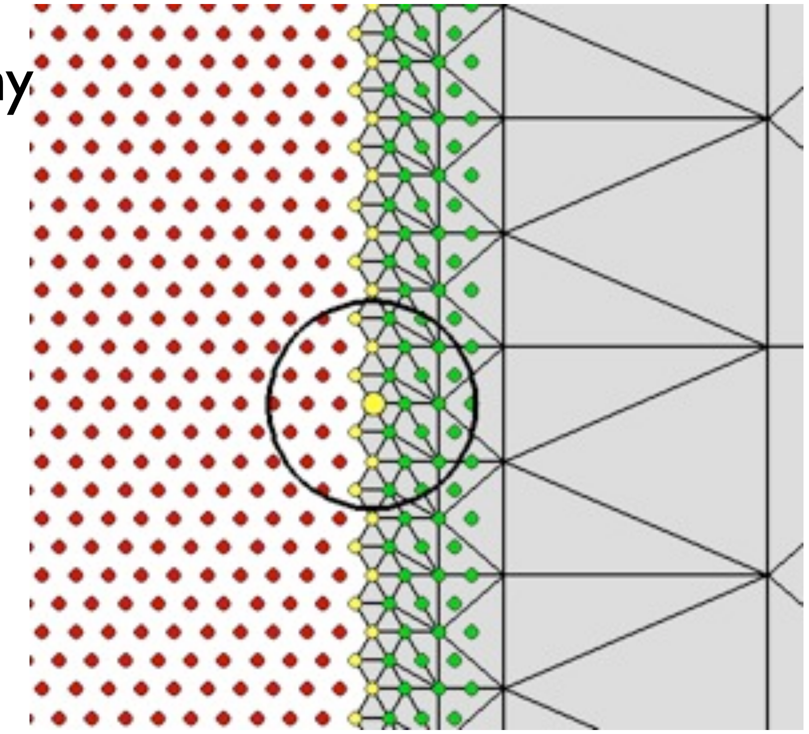

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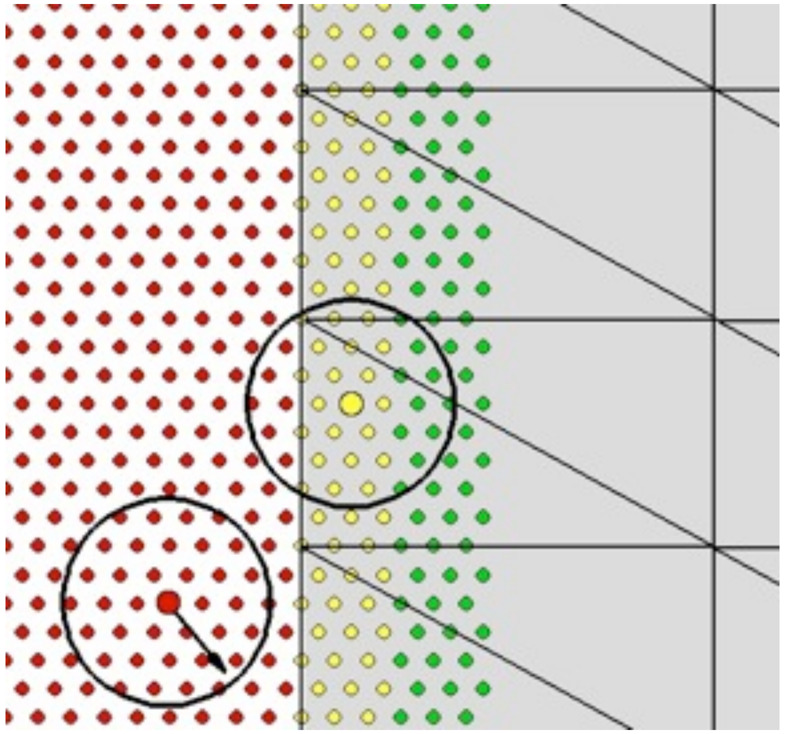

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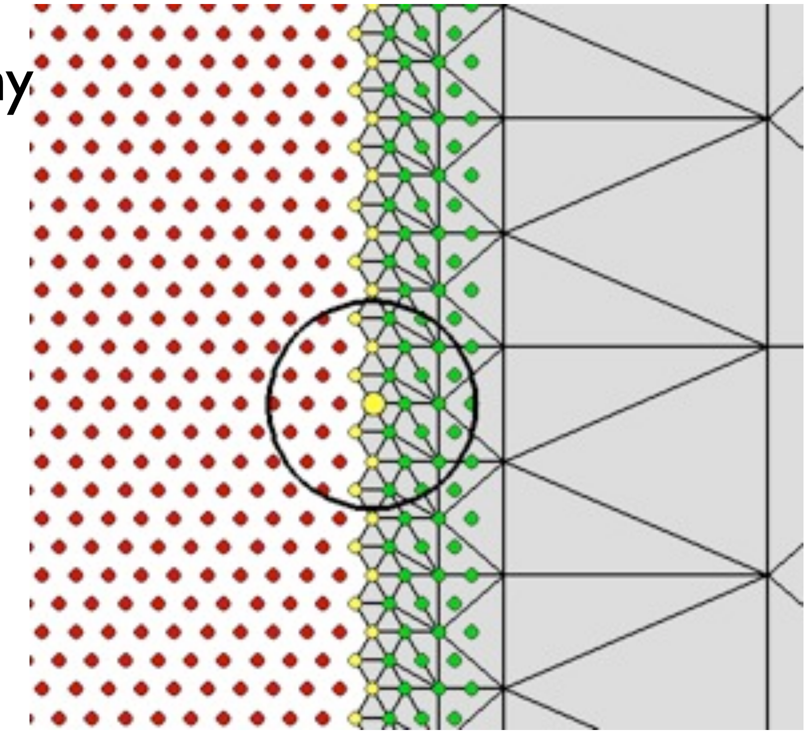
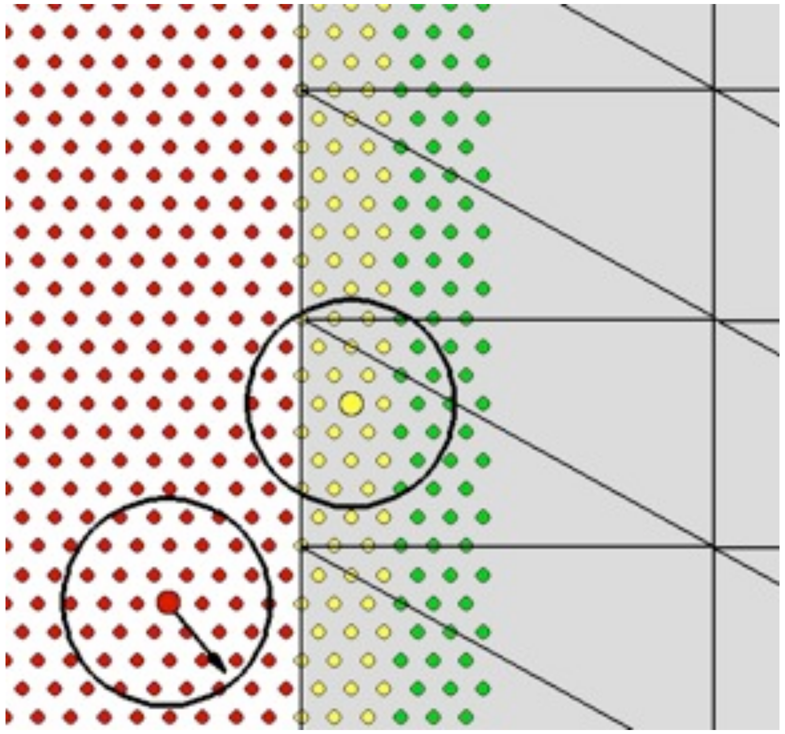
3. Interface compatibility is strong or weak
4. The choice of the finite element constitutive law





Comparison of 14 coupled methods (Miller and Tadmor, *MSMSE*, 2009)

8 Energy-based methods

Acronym	Key References	Continuum Model	Handshake	Coupling Boundary Condition
QC	[1, 2]	Cauchy-Born	None	Strong Compatibility
CLS	[3]	Linear Elasticity	None	Strong Compatibility
BD	[4]	Cauchy-Born	Linear mixing of energy	Weak Compatibility (penalty)
BSM	[5, 6]	Cauchy-Born	None	Weak/Stong Mix (least-squares fit)
CACM	[7]	Linear Elasticity	None	Weak Compatibility (average atomic positions)
CQC(m)-E	[8]	Averaging of atomic clusters	None	Strong Compatibility
QC-GFC	[9]	Cauchy-Born	None	Strong Compatibility
CQC(m)-GFC	[8]	Averaging of atomic clusters	None	Strong Compatibility

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6 Force-based methods

Acronym	Key References	Continuum Model	Handshake	Coupling Boundary Condition
FEAt	[10]	non-linear, nonlocal elasticity	None	Strong Compatibility
CADD	[11, 12]	Linear Elasticity	None	Strong Compatibility
HSM	[13]	Non-Linear Elasticity	atomic averaging for nodal B.C.	Weak Compatibility (average atomic positions)
AtC	[14, 15, 16, 17]	Linear Elasticity	Linear mixing of stress and atomic force	Strong Compatibility
AtC-GFC	unpublished	Linear Elasticity	Linear mixing of stress and atomic force	Strong Compatibility
CQC(m)-F	[18]	Averaging of atomic clusters	None	Strong Compatibility

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Coupled Atomistic/Continuum Models

[1] Tadmor, E. B., Ortiz, M., and Phillips, R. *Philos. Mag. A* **73**(6), 1529–1563 (1996).

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[16] Badia, S., Parks, M., Bochev, P., Gunzburger, M., and Lehoucq, R. *Multiscale Model. Simul.* **7**(1), 381–406 (2008).

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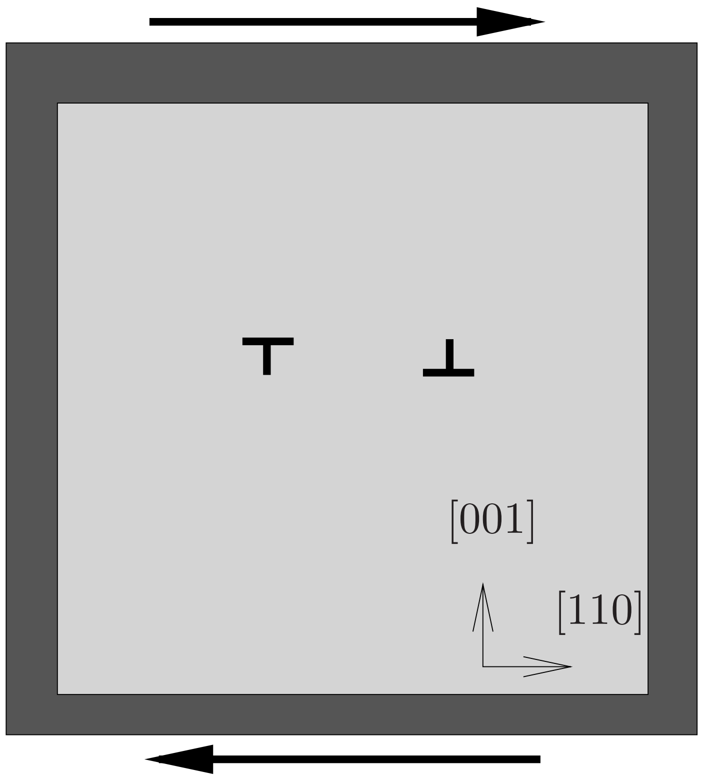
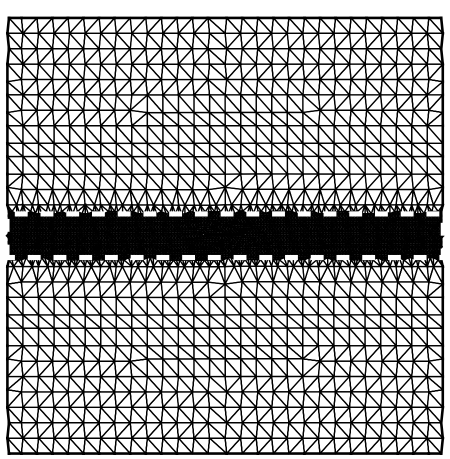
Comparison of Accuracy: Force-based methods

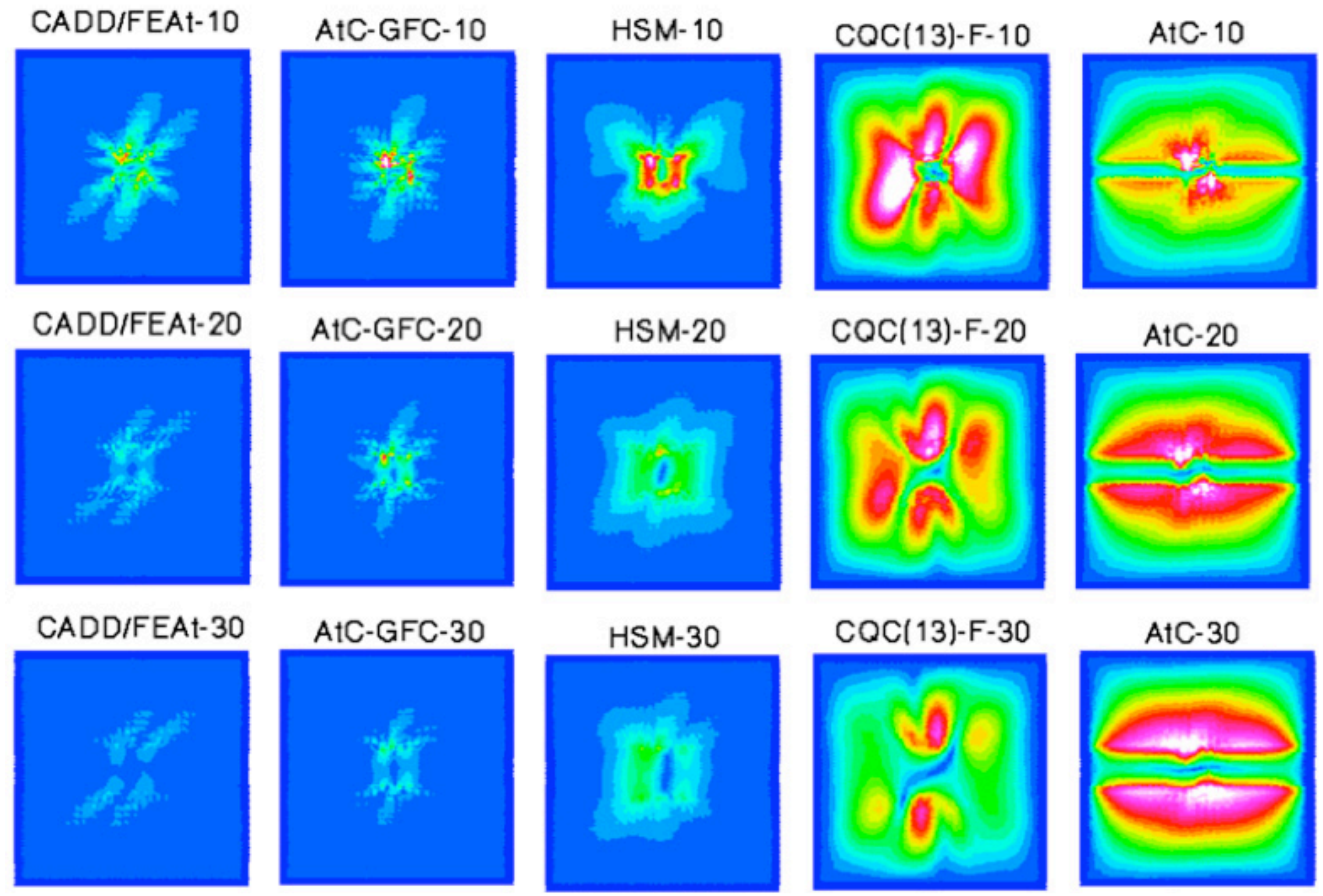


About 28,000 Aluminum atoms
400Å × 400Å × 3Å



"Multibench" code at www.qcmethod.org

$$\epsilon^{\alpha} = \left| \boldsymbol{u}^{\alpha} - \boldsymbol{u}^{\alpha}_{\mathrm{exact}} \right|$$



Comparison of Accuracy: Energy-based methods

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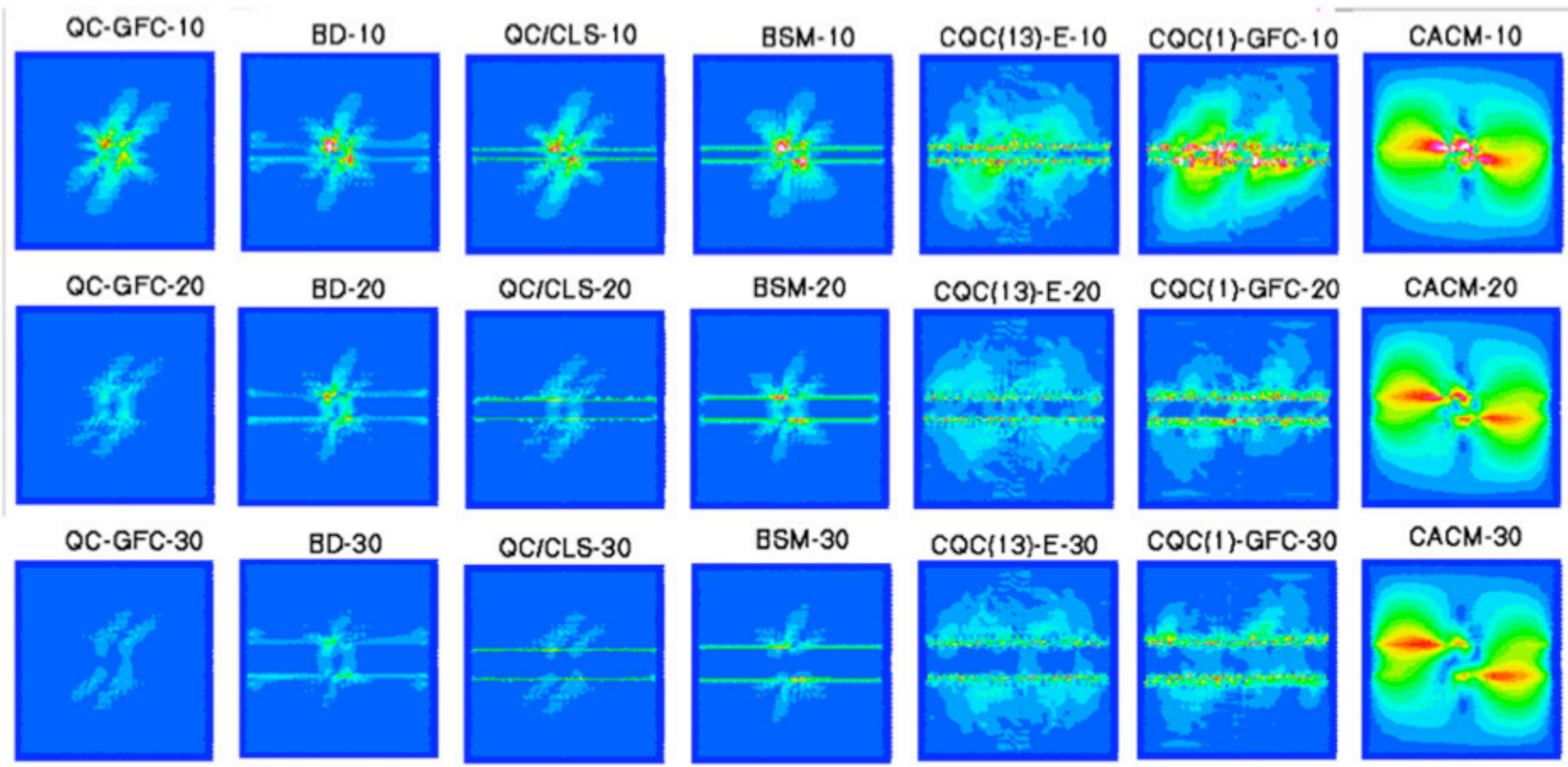
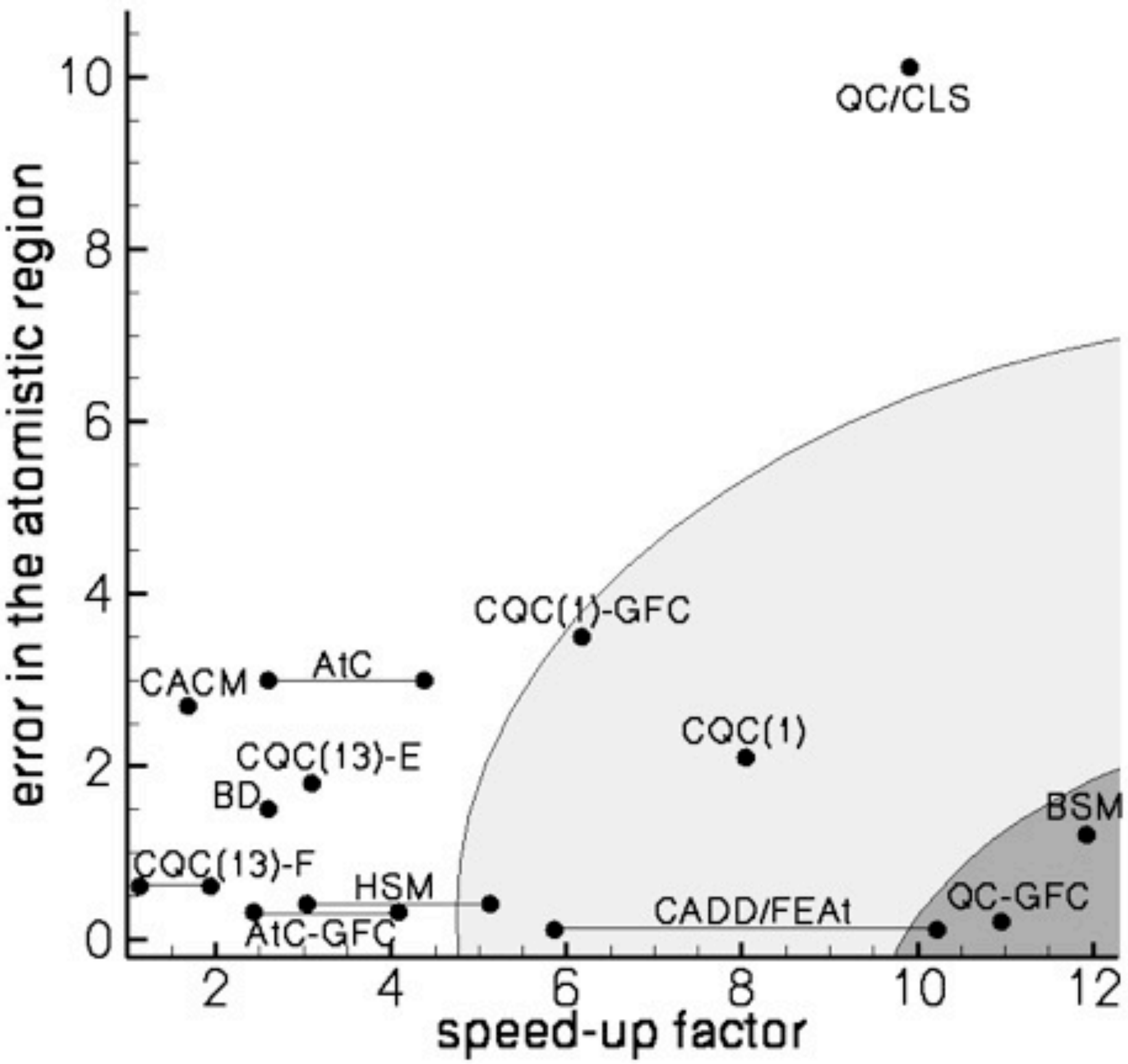


Comparison of Speed and Accuracy of Coupling Methods



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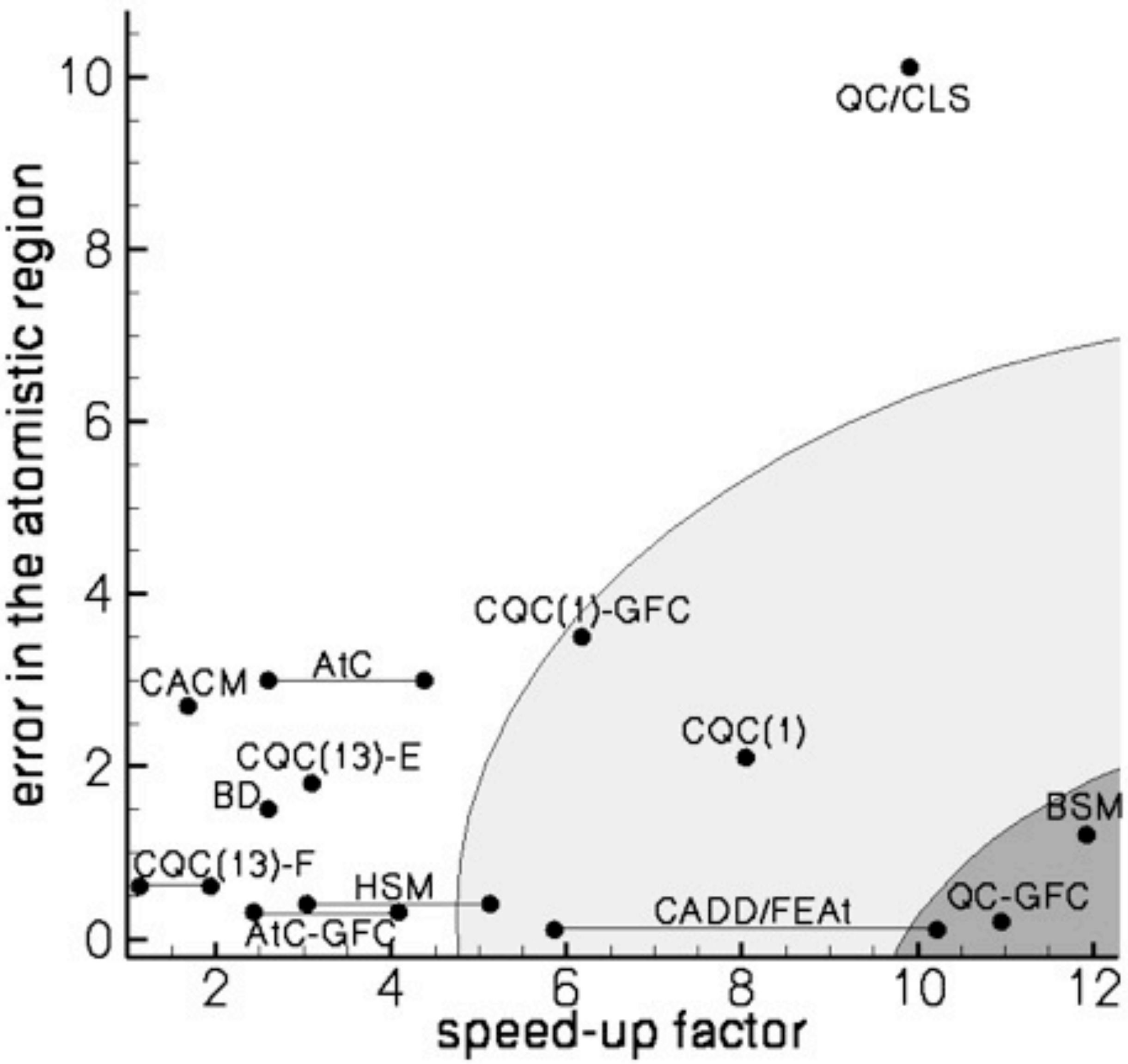

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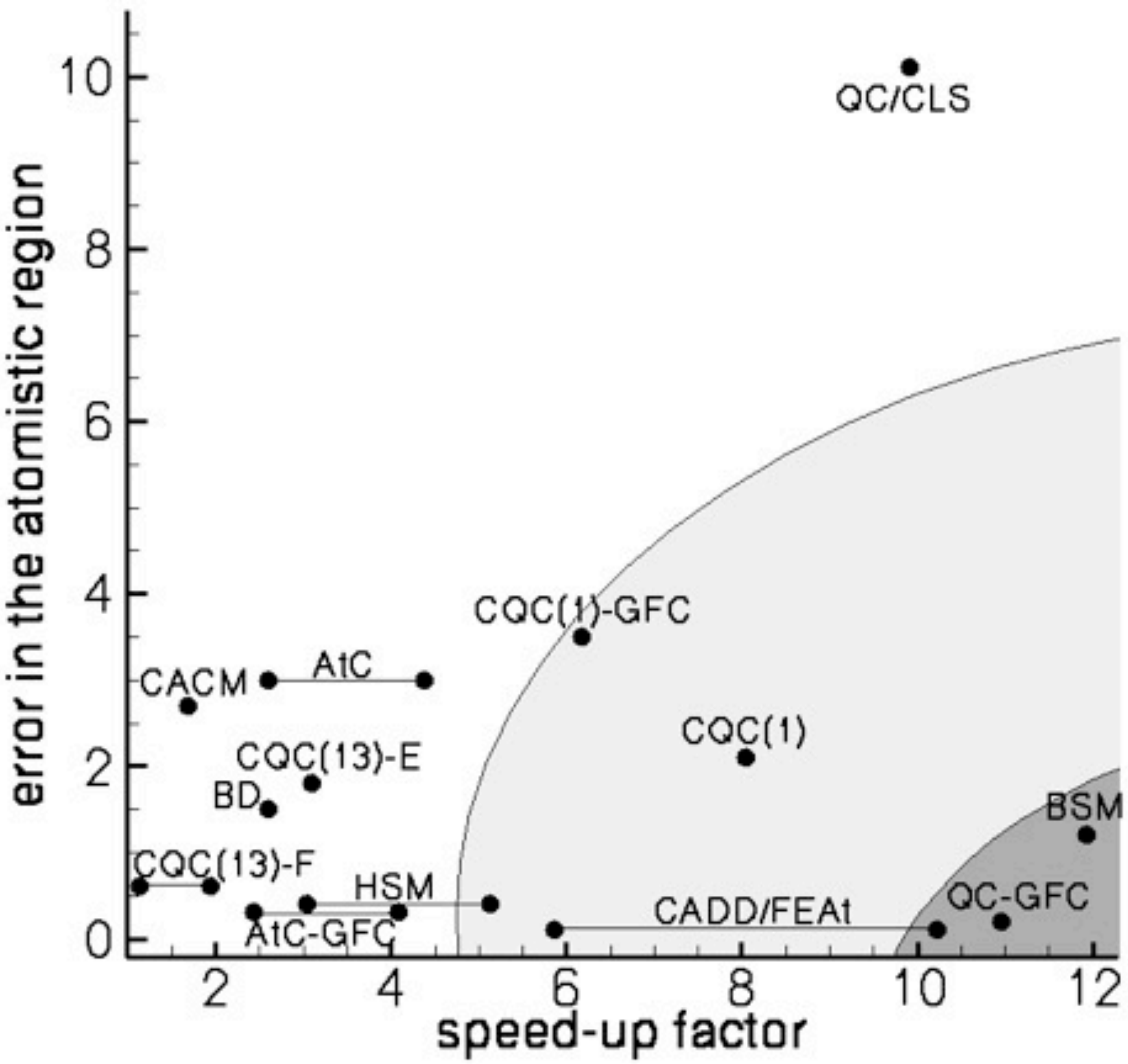

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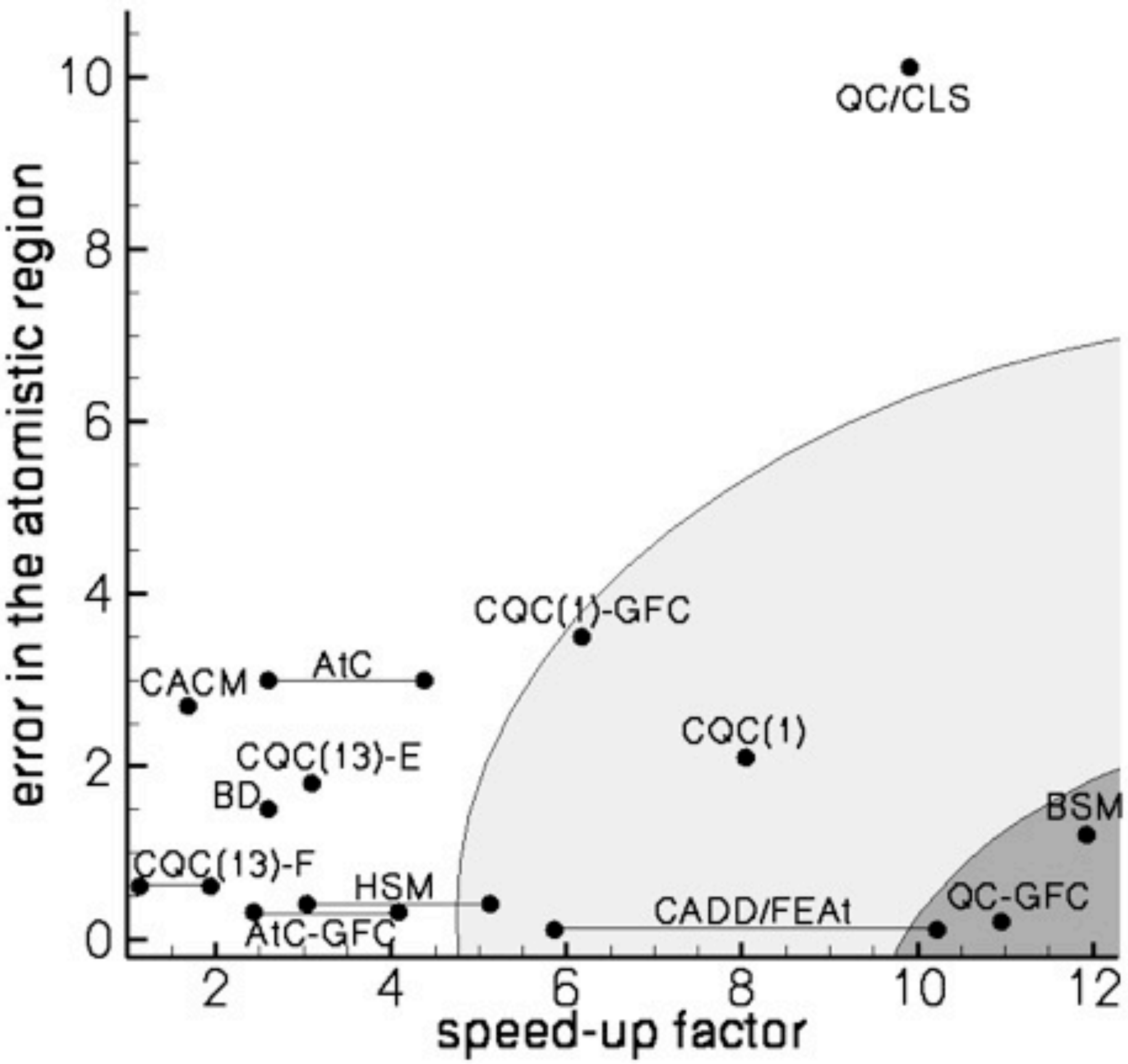

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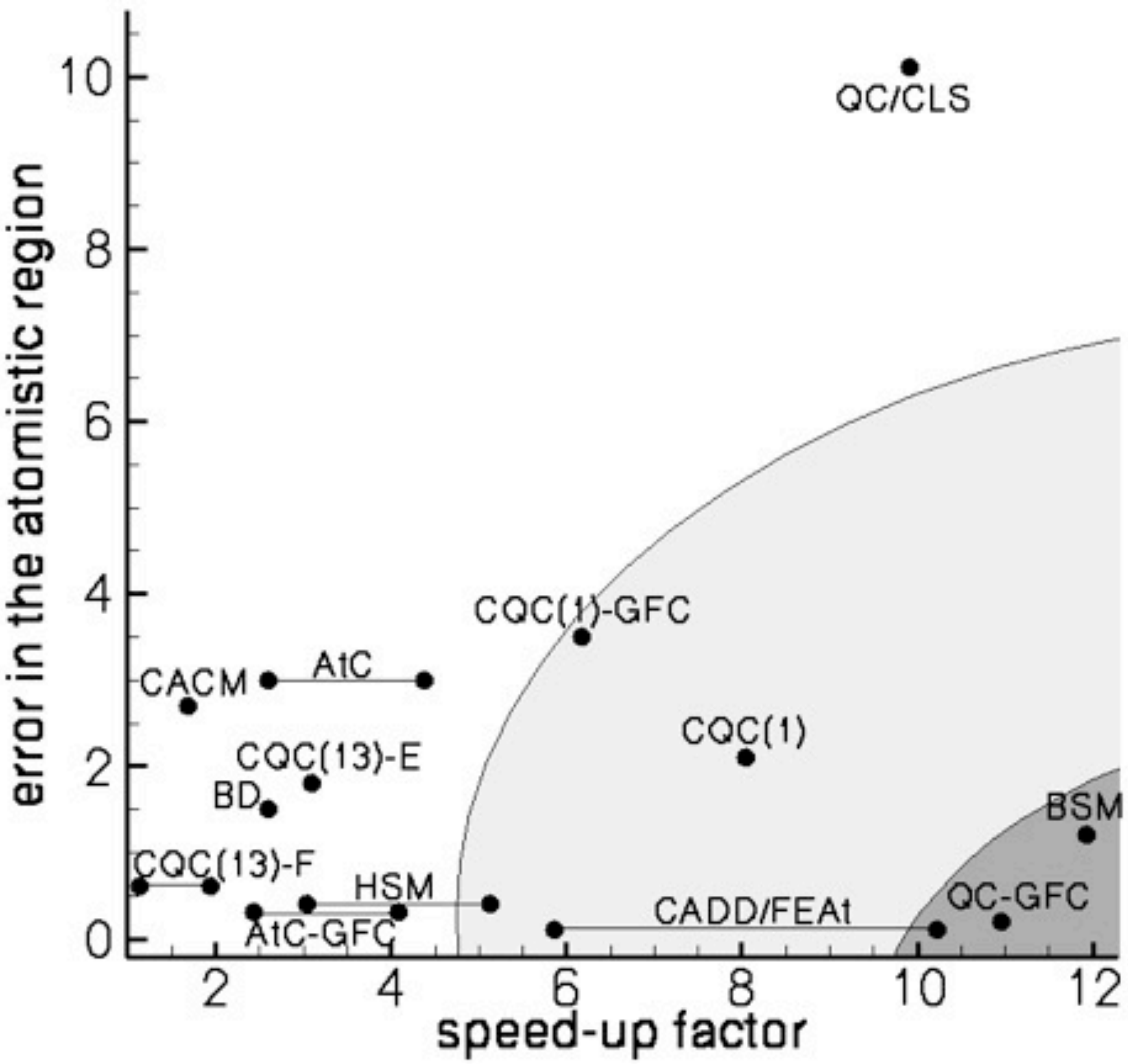

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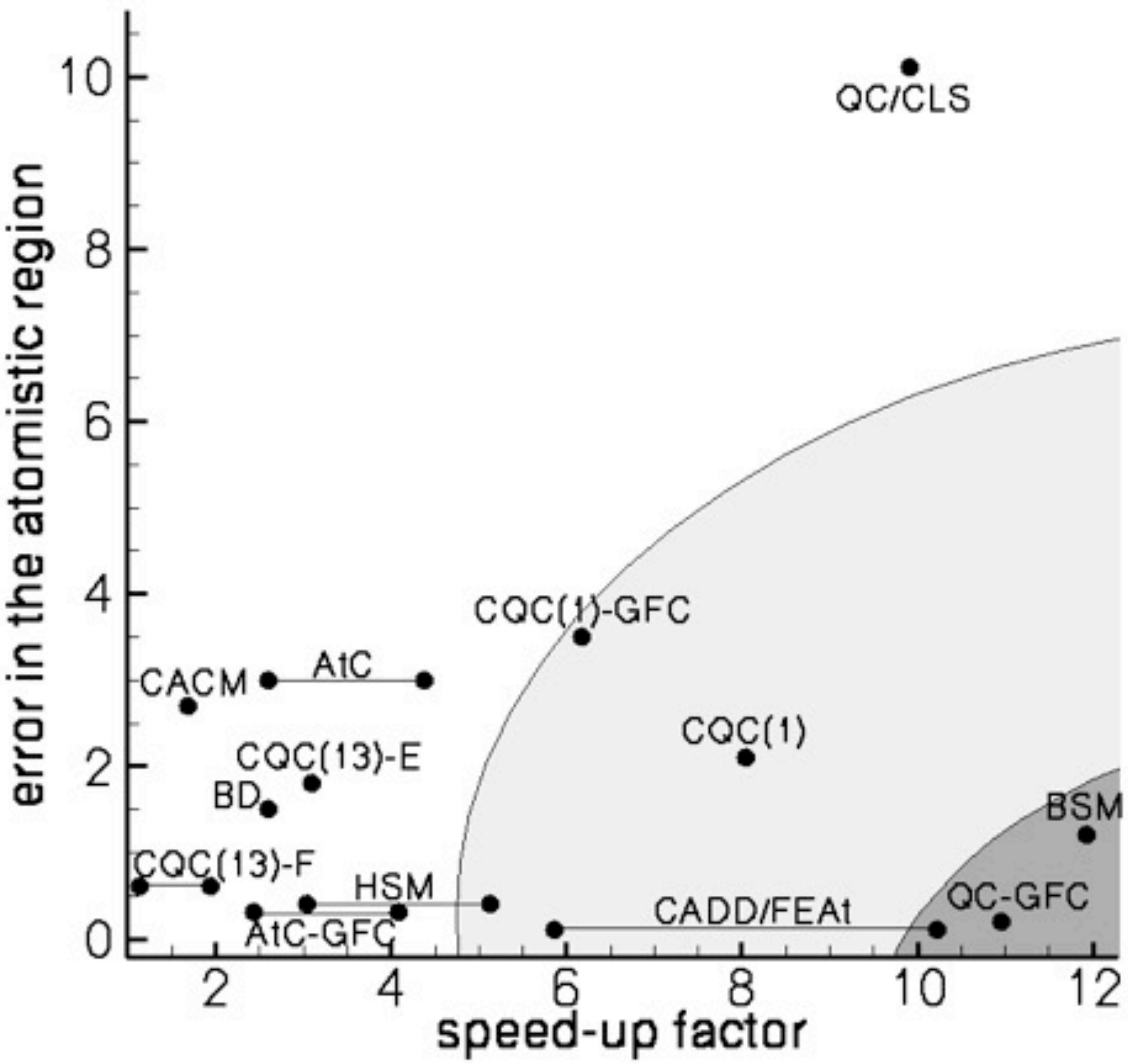

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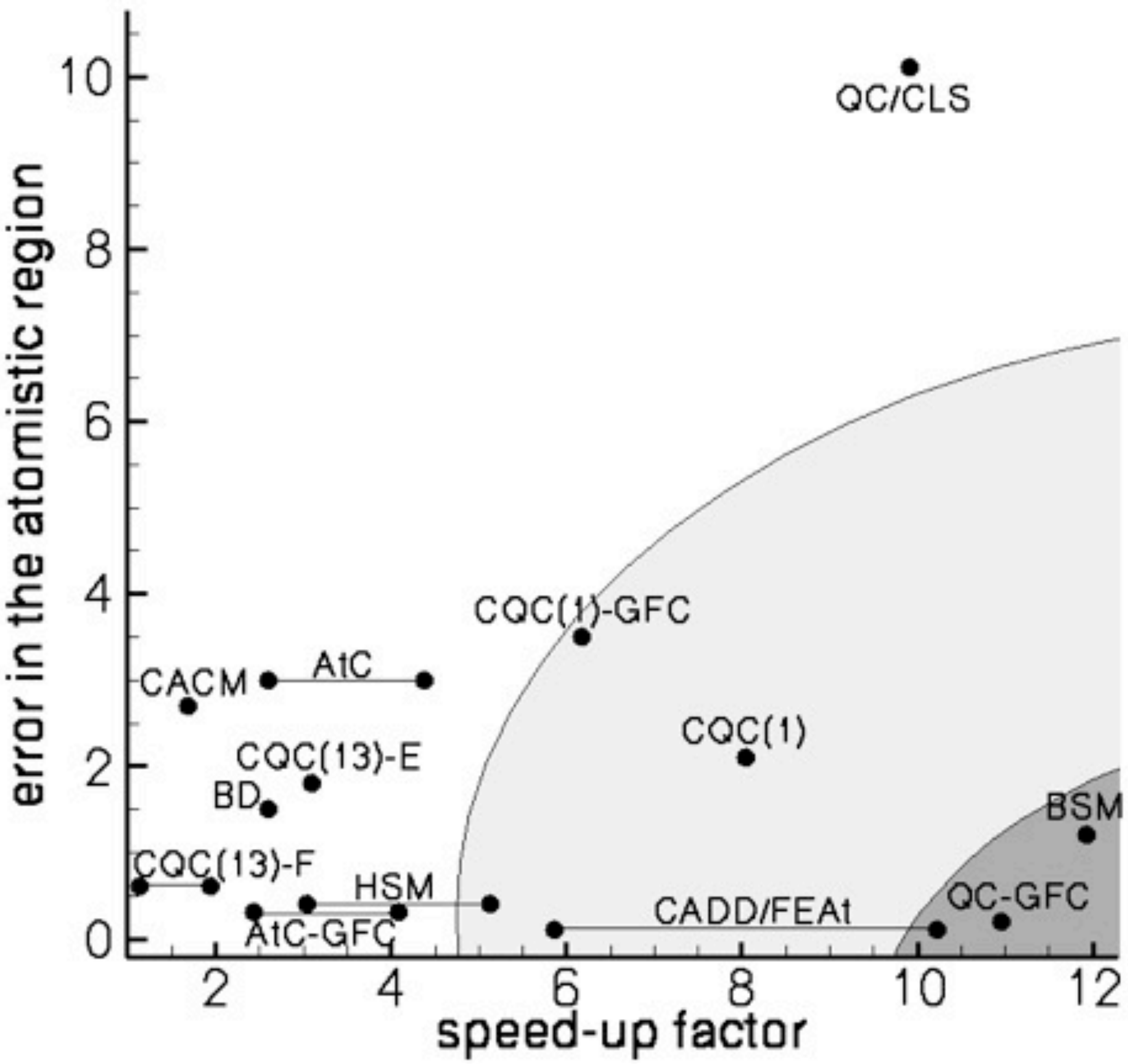

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- Ghost force correction in many methods may be a good idea.

What are the challenges at finite temperature?

1. Small atomistic region: thermostats are more intrusive
2. How do we correctly account for the missing entropy coarsened degrees of freedom?
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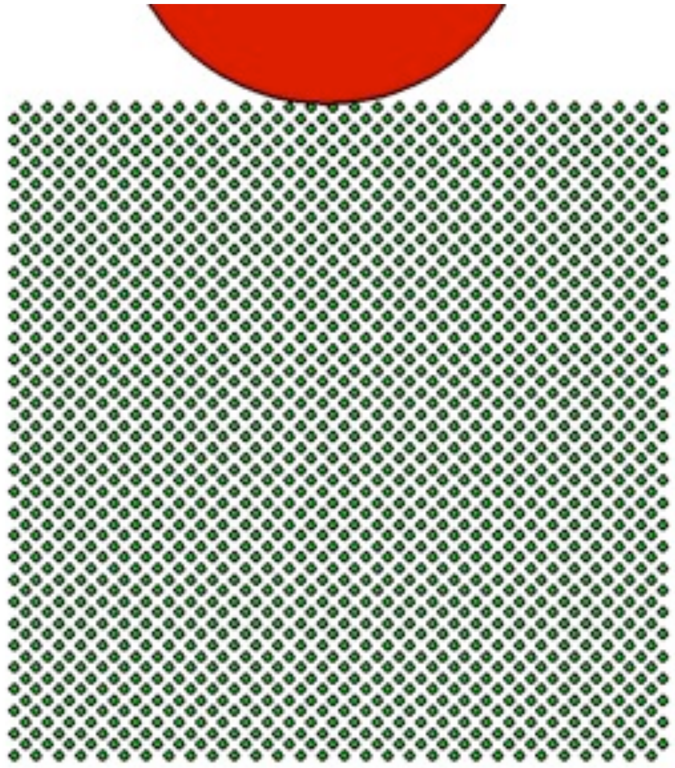

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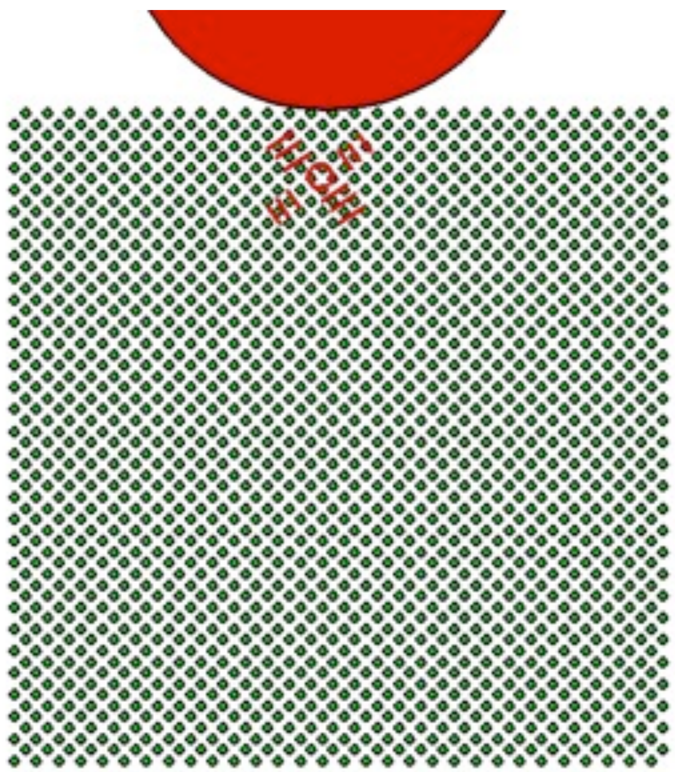

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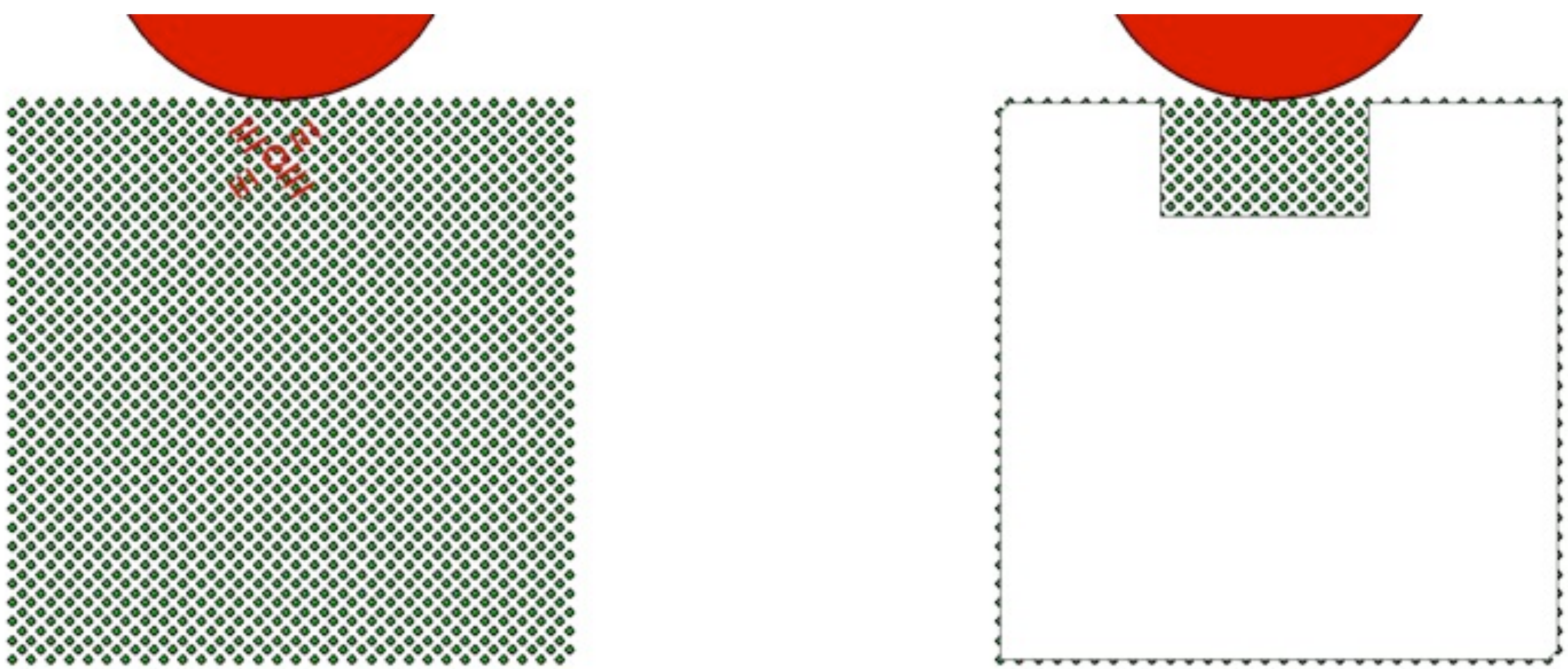

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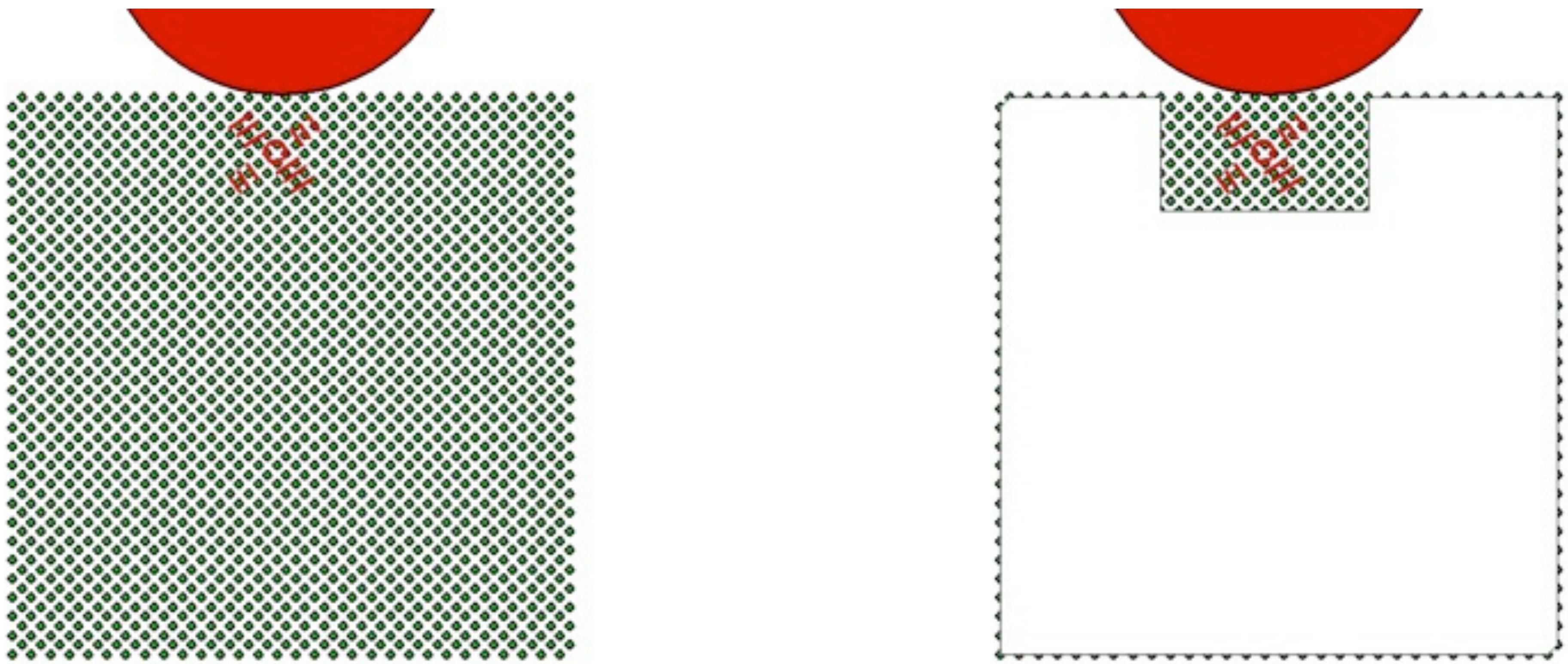

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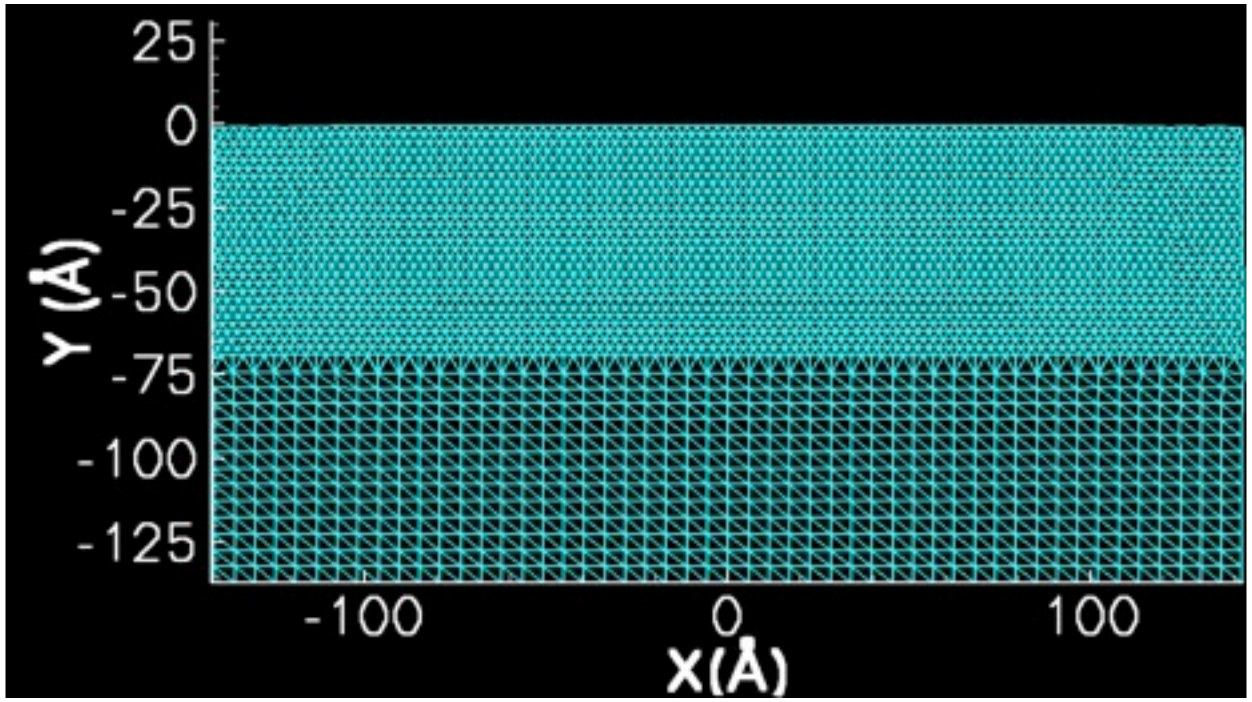

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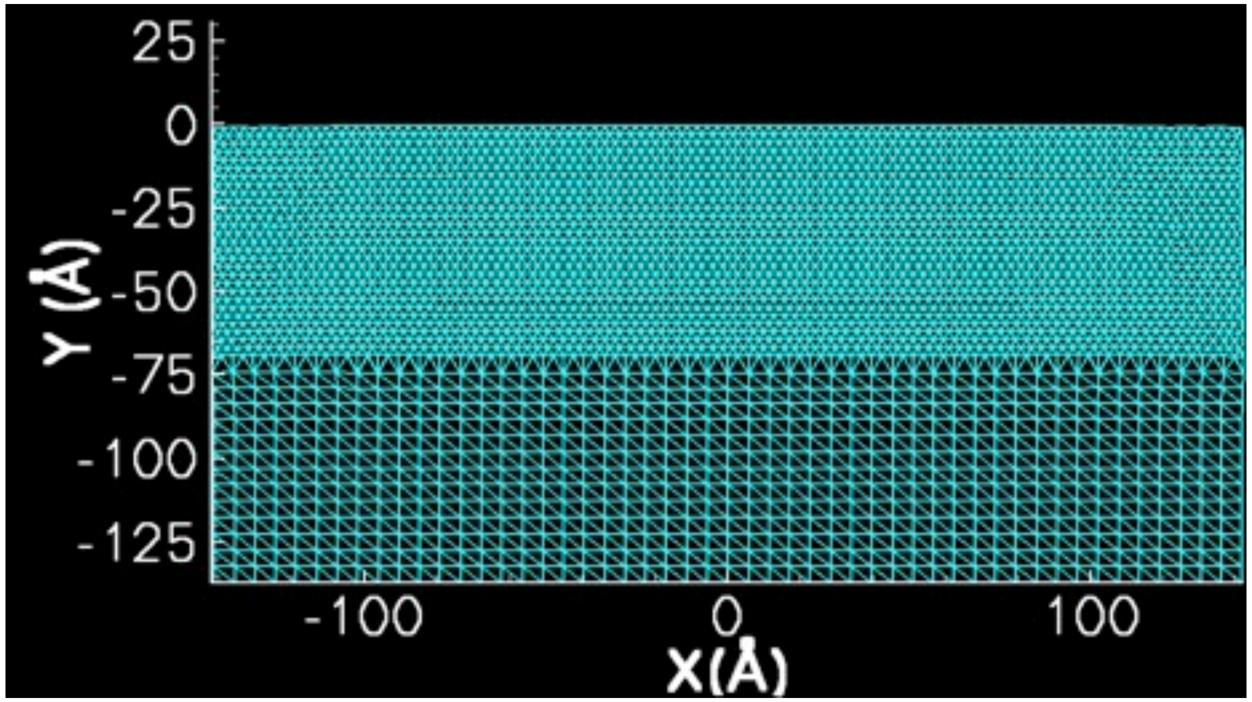

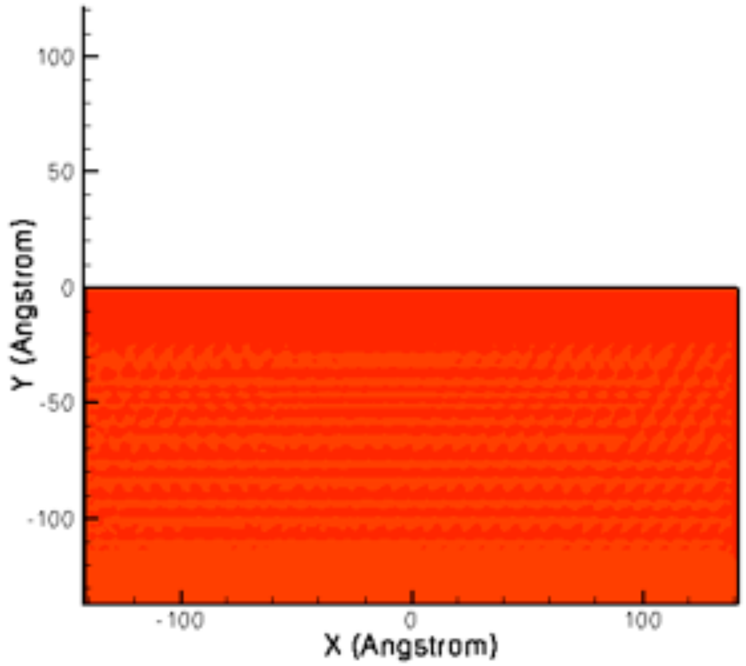

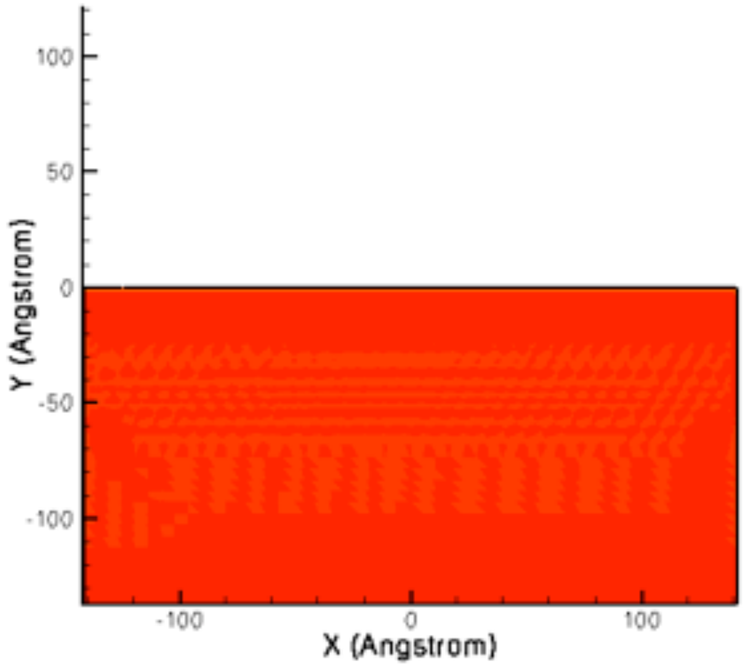

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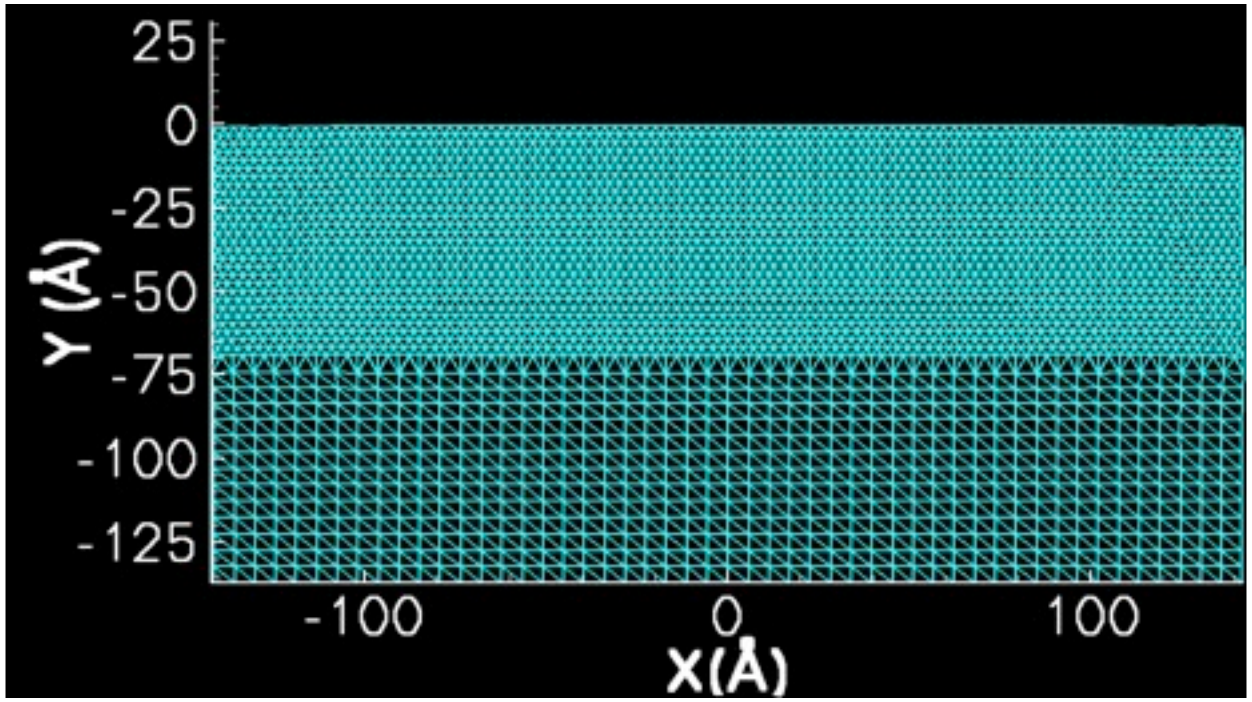

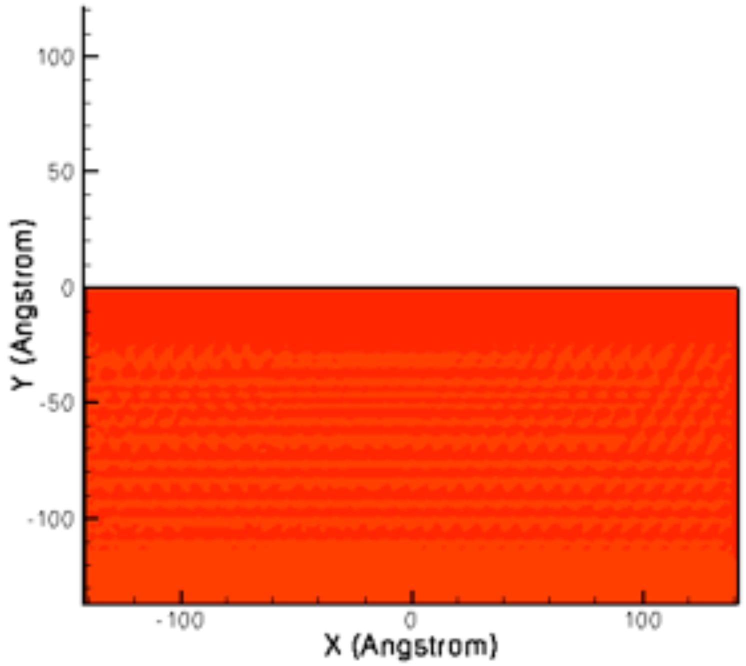

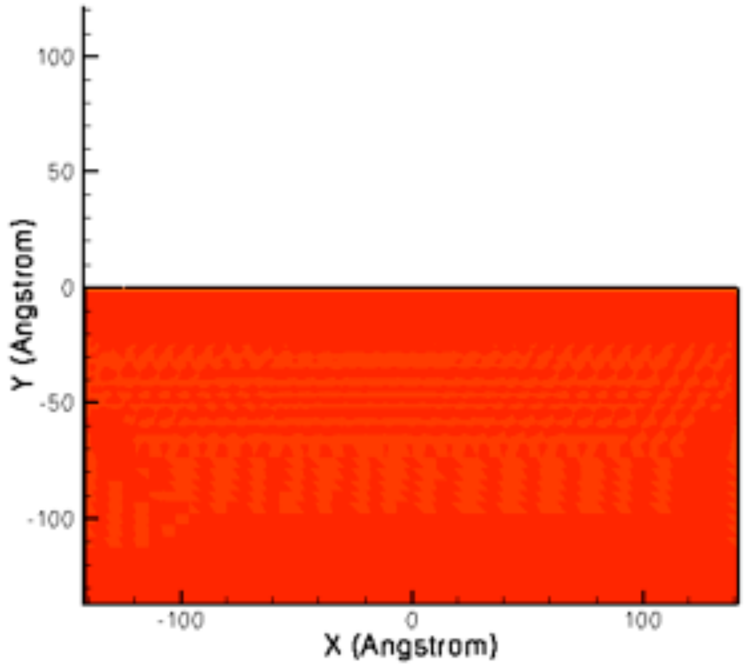

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1. Absorbing boundary conditions (ABC)
   i) mitigates the wave reflection problem
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2. Coarse-Grained Canonical Ensemble
   i) full temperature control
   ii) correct (or at least approximate) treatment of missing entropy
   iii) no direct control of wave reflections
   iv) not suitable for NEMD problems

The QC method at finite temperature: "Hot QC"

Dupuy et al, PRL, 2005,
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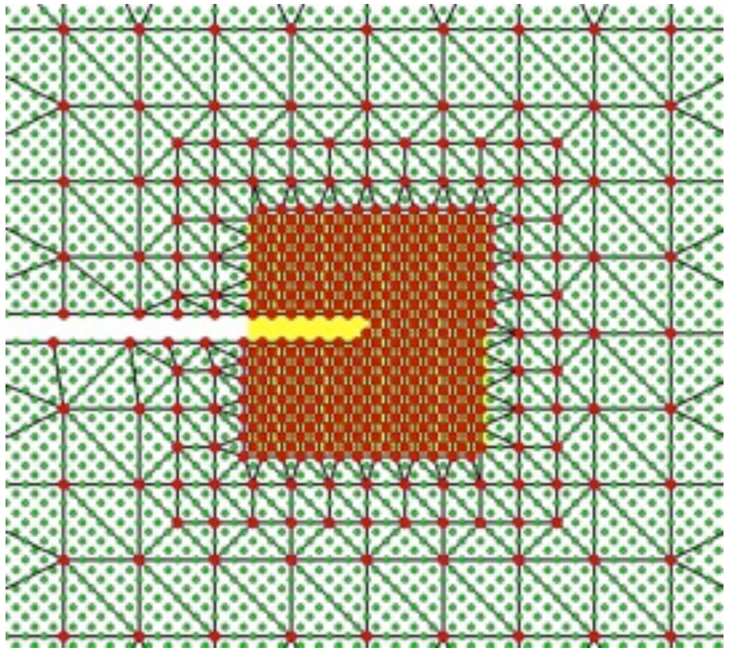

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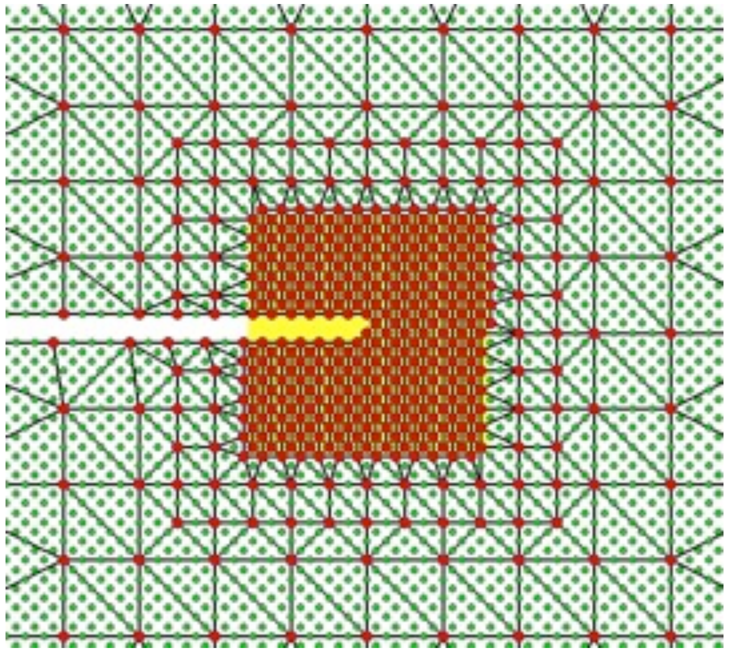

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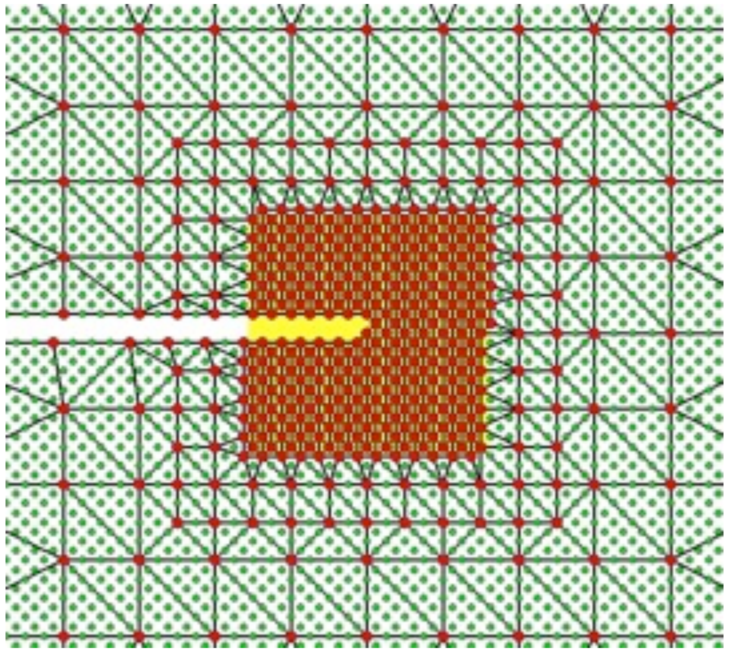

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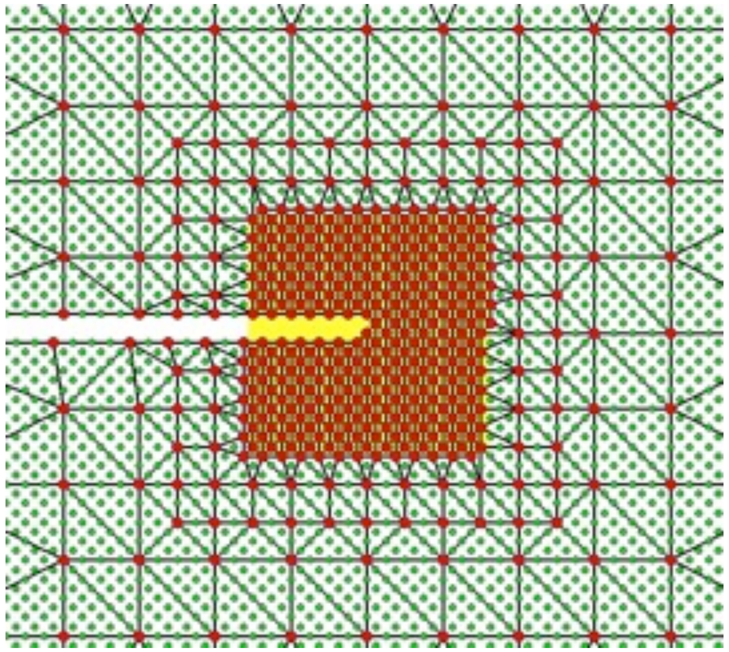

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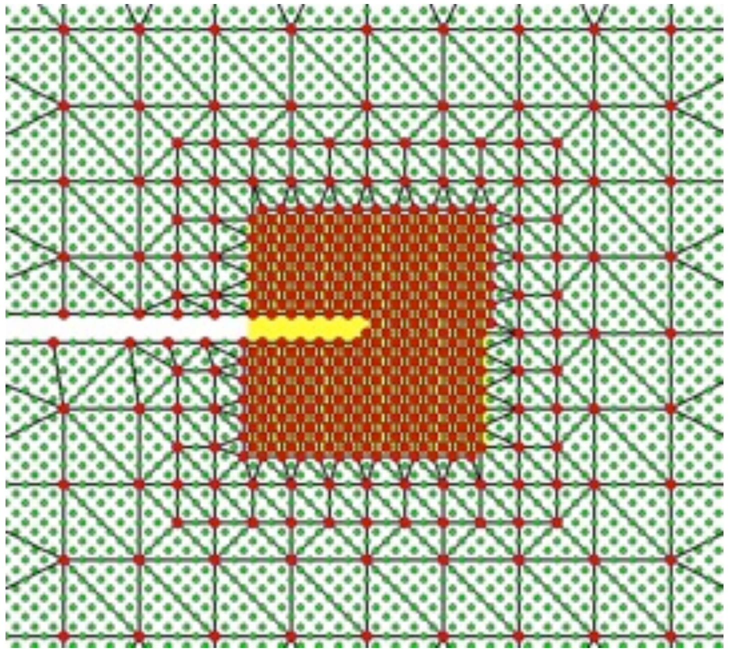

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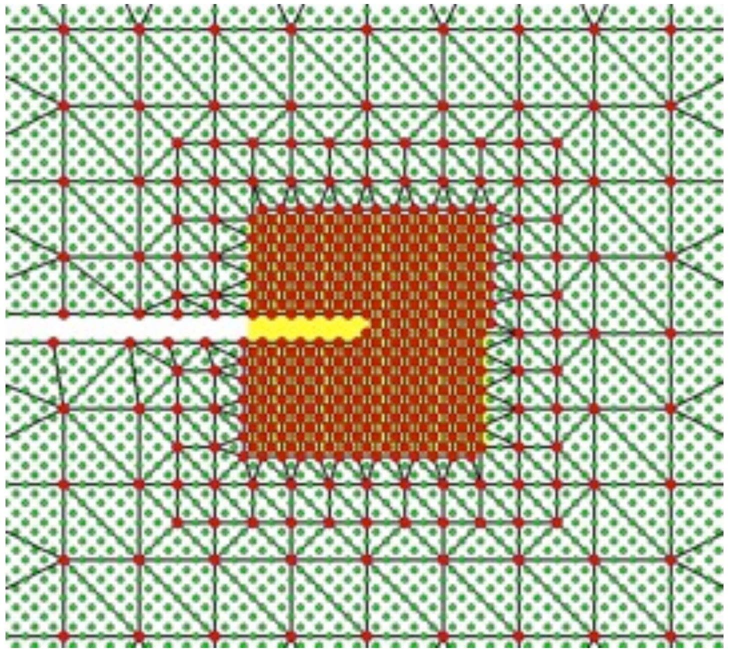

Write the potential energy in terms of the repatom positions only (PMF)

$$\mathcal{V}_{\mathrm{CG}}(\boldsymbol{q}^{\mathrm{r}}, T) = -k_{\mathrm{B}} T \ln \int d\boldsymbol{q}^{\mathrm{c}} \exp \frac{-\mathcal{V}(\boldsymbol{q}^{\mathrm{r}}, \boldsymbol{q}^{\mathrm{c}})}{k_{\mathrm{B}} T}$$

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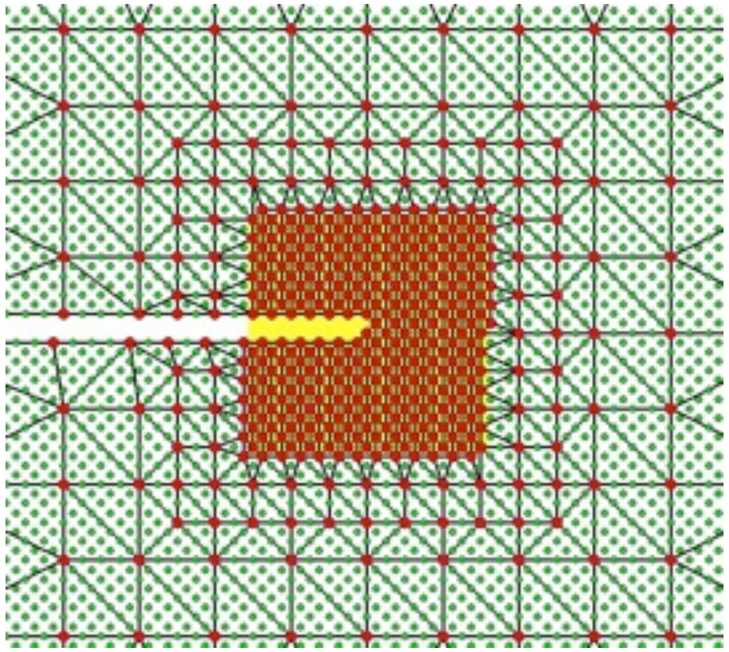

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exact but intractable

The Cauchy-Born Rule and the Local Harmonic Approximation

Write the potential energy as the sum of two parts:

1. The zero temperature contribution (use Cauchy-Born Rule)

2. A contribution due to the thermal fluctuations of the coarsened atoms about their mean positions (use Local Harmonic Approximation (LeSar et al., PRL, 1989) AND the Cauchy-Born Rule)

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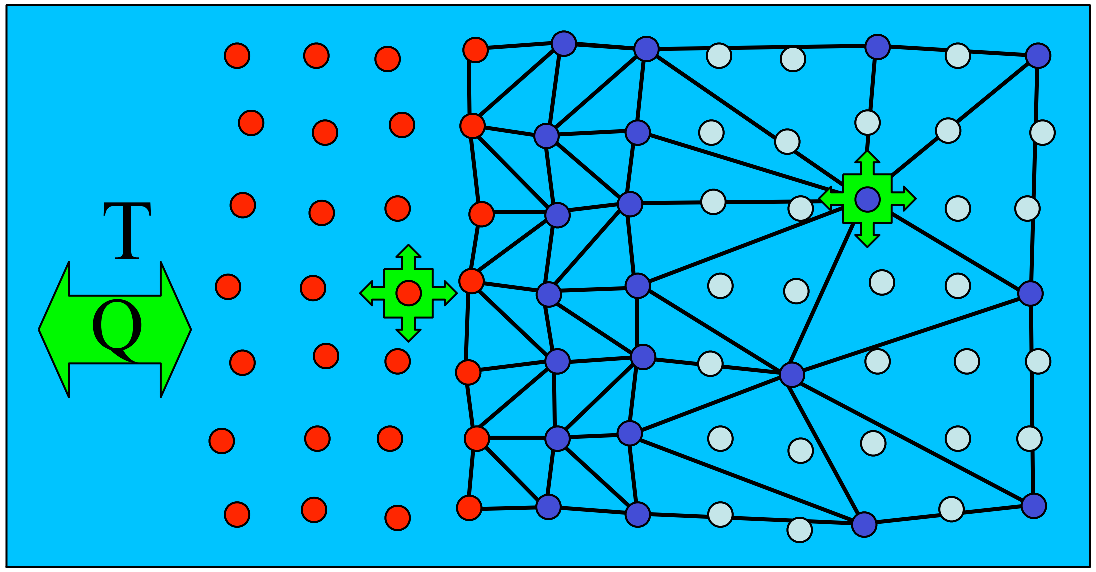
This Doesn't Work: Mesh size and shape dependent properties!

The Culprit: “Mesh entropy”

Problem:

- the motion of the nodes is really the change of the mean positions of the atoms over time
- this carries an unphysical vibrational entropy
- this extra entropy is a negligible contribution if the elements are very big... but not all of them are big.



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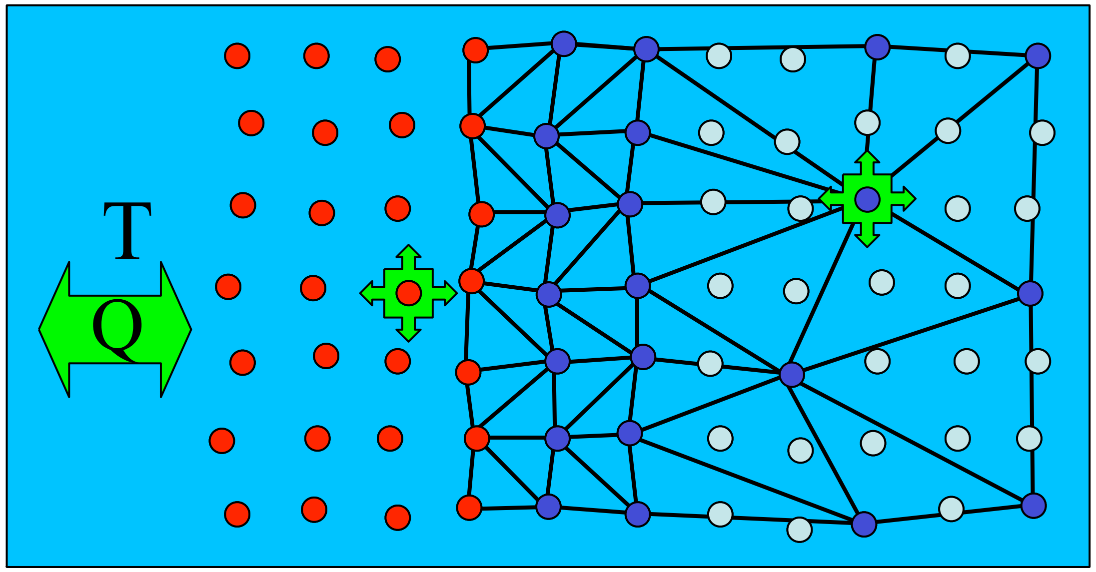

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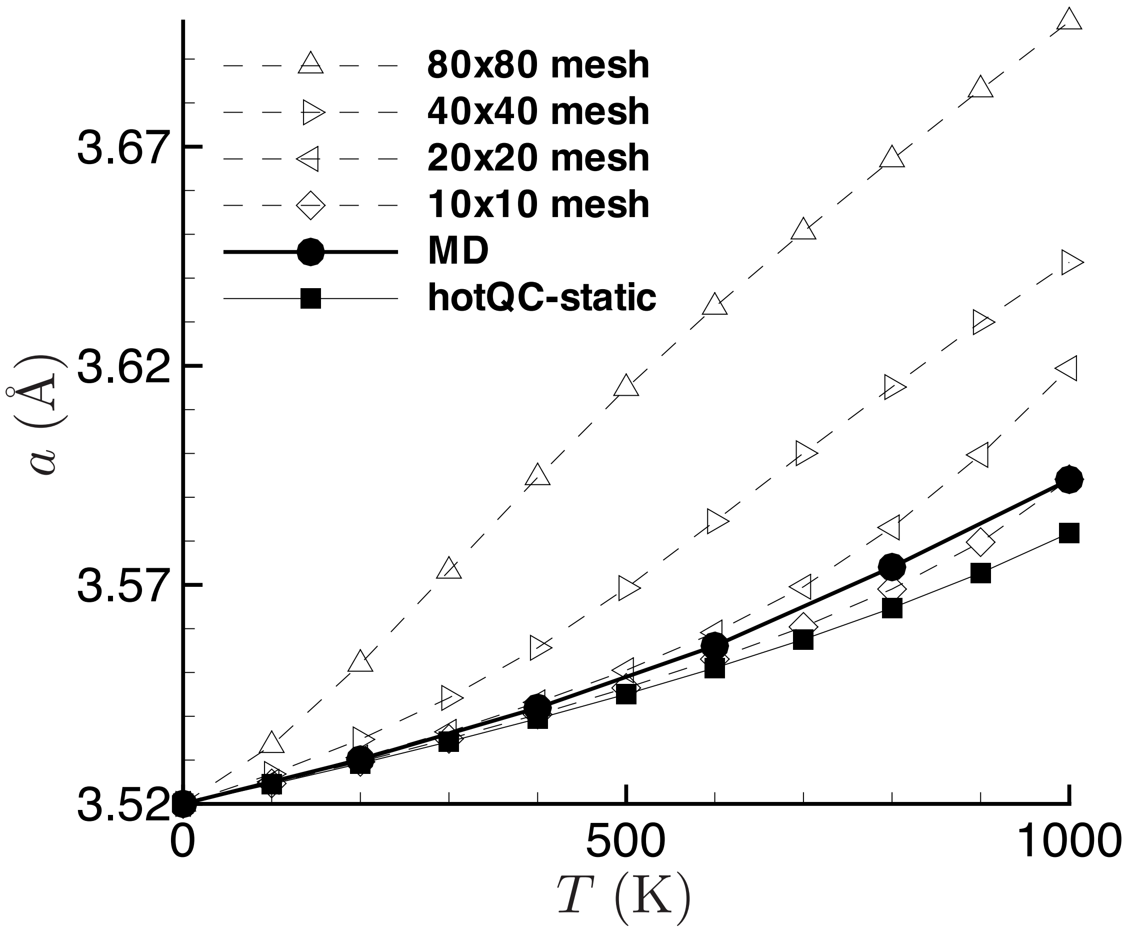
Solution:

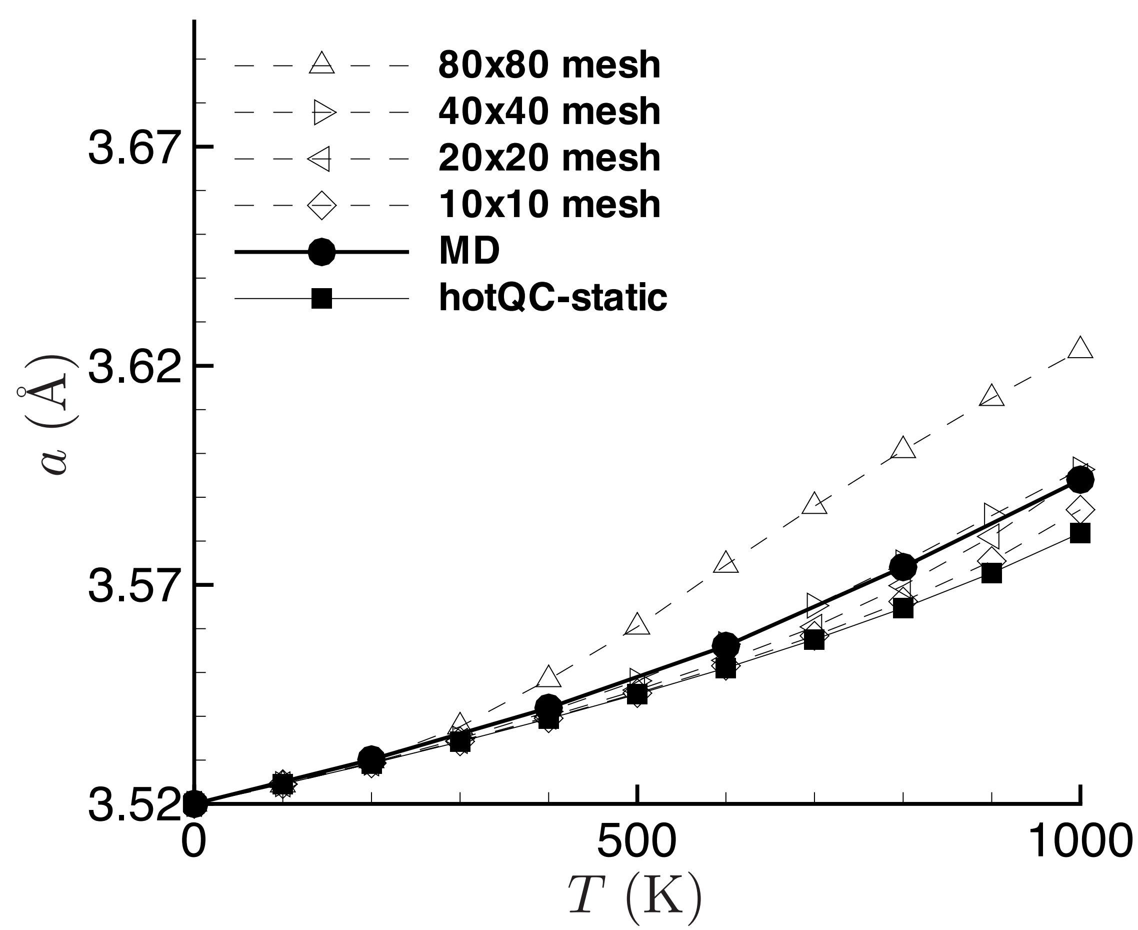
- Subtract an approximate mesh entropy correction from the potential energy:

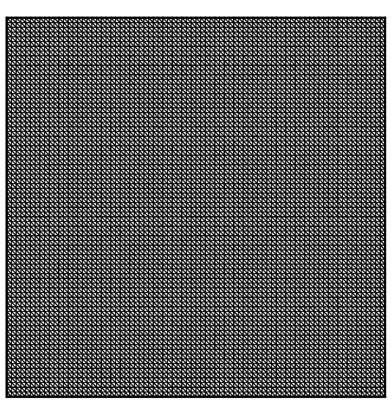
$$\widehat{\mathcal{V}} = \mathcal{V} - TS_{\mathrm{mesh}}$$

$$S_{\mathrm{mesh}} \approx -\frac{k_{\mathrm{B}}}{2} \ln \frac{\det \boldsymbol{K}}{(2\pi k_{\mathrm{B}} T)^{3N_{\mathrm{loc.}}}}$$

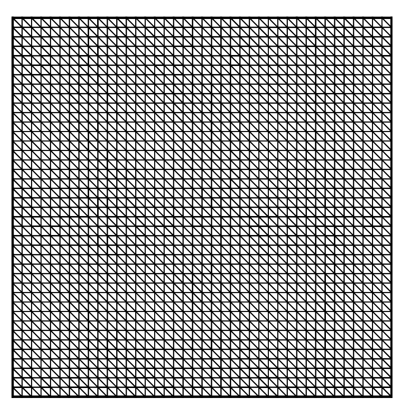
Test: Thermal Expansion of Ni (Angelo et al., *MSMSE*, 1995)



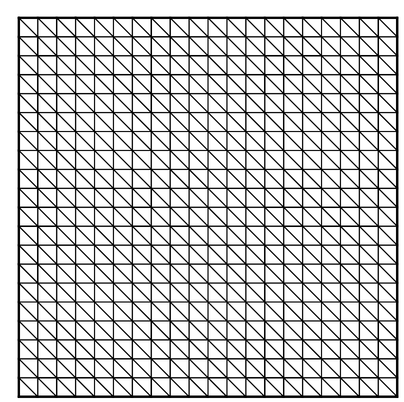




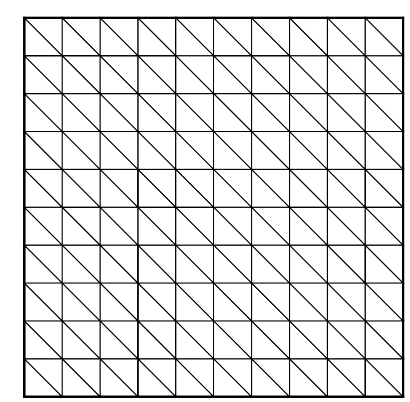
1 atom per element



2 atoms per element

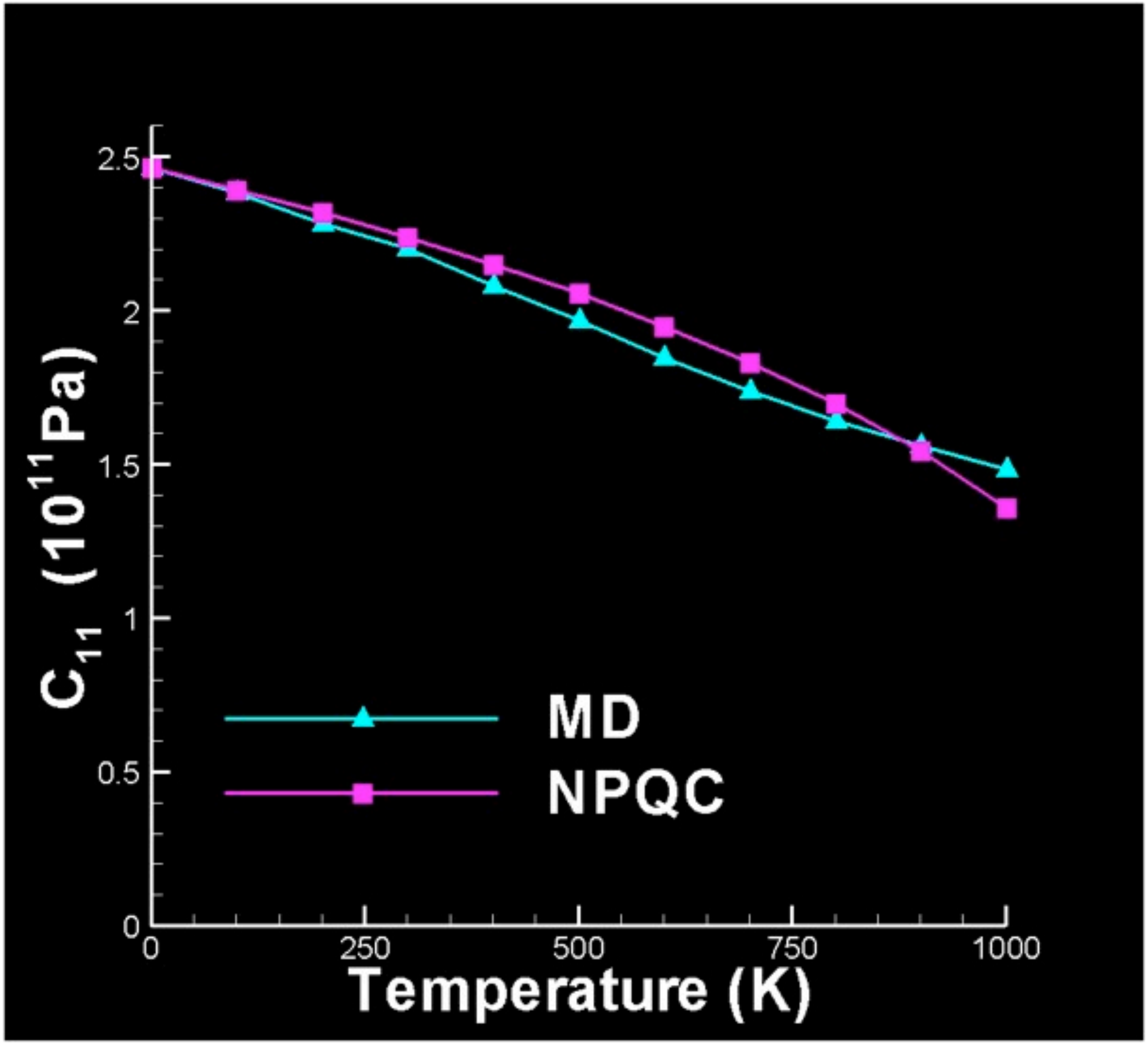


8 atoms per element



32 atoms per element

Another Test: Elastic Constants of Ni



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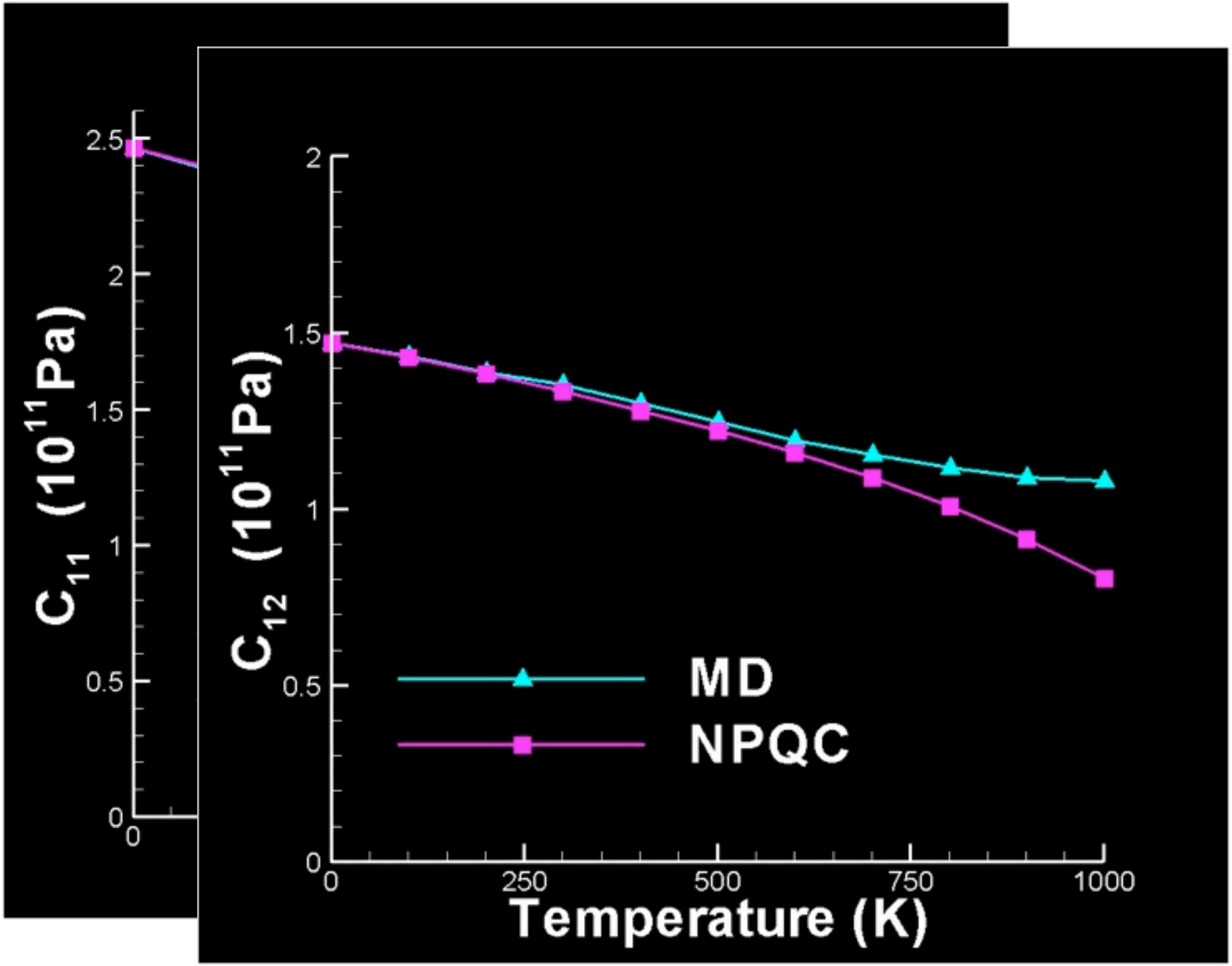

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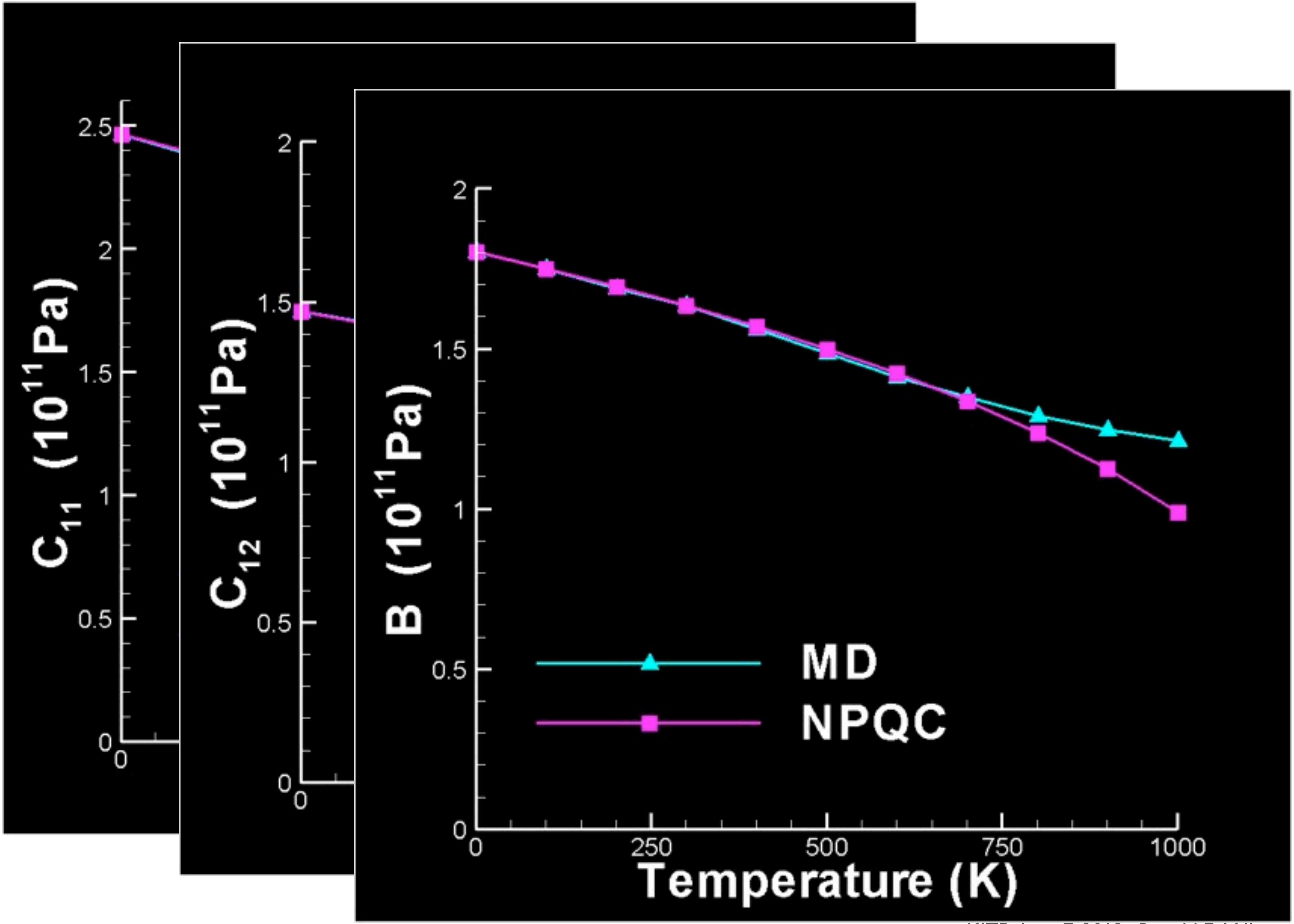
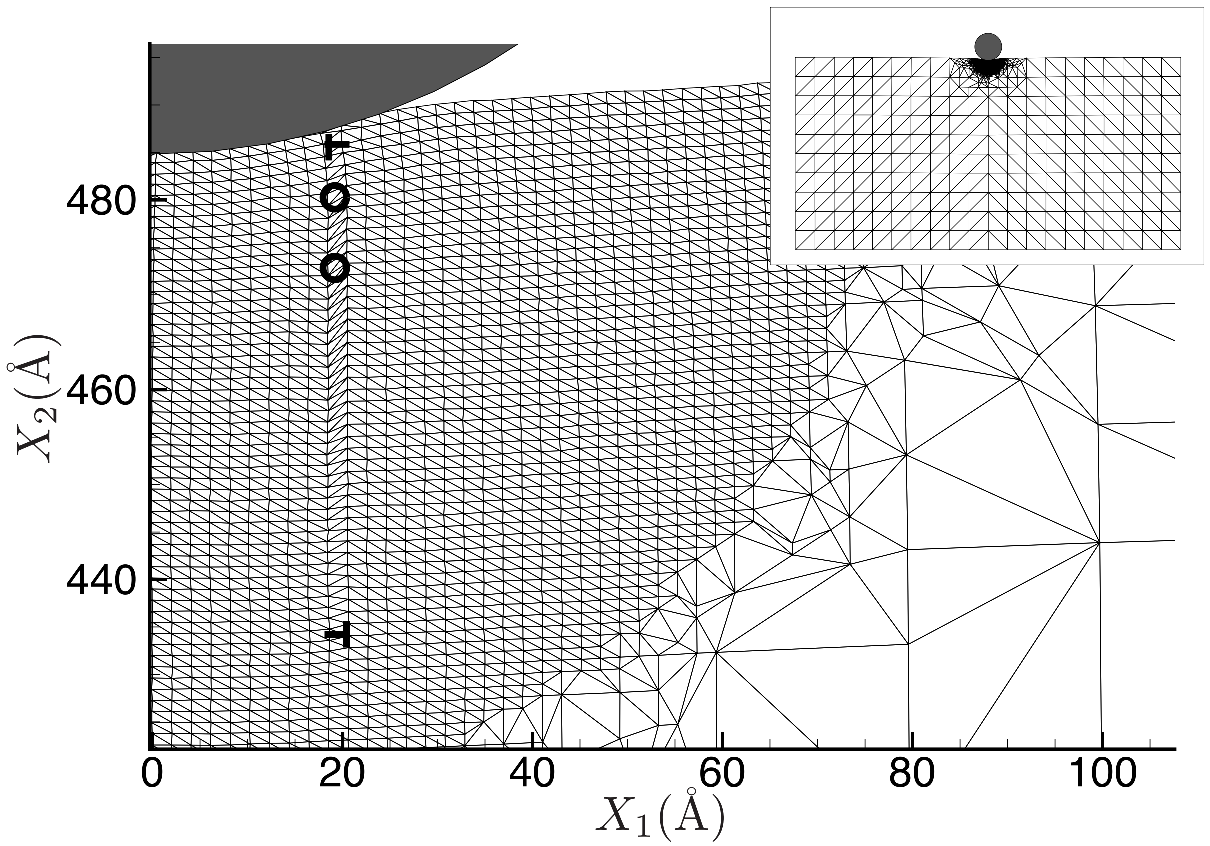
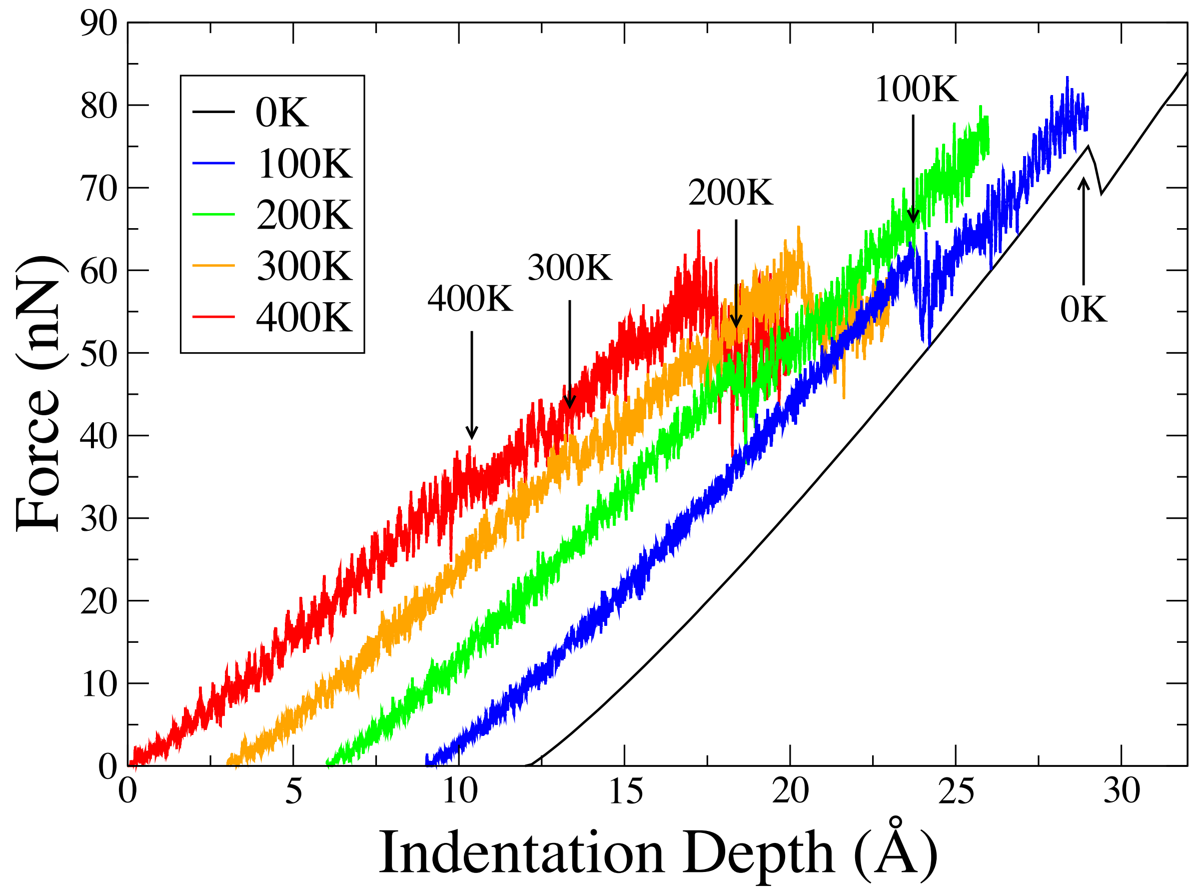
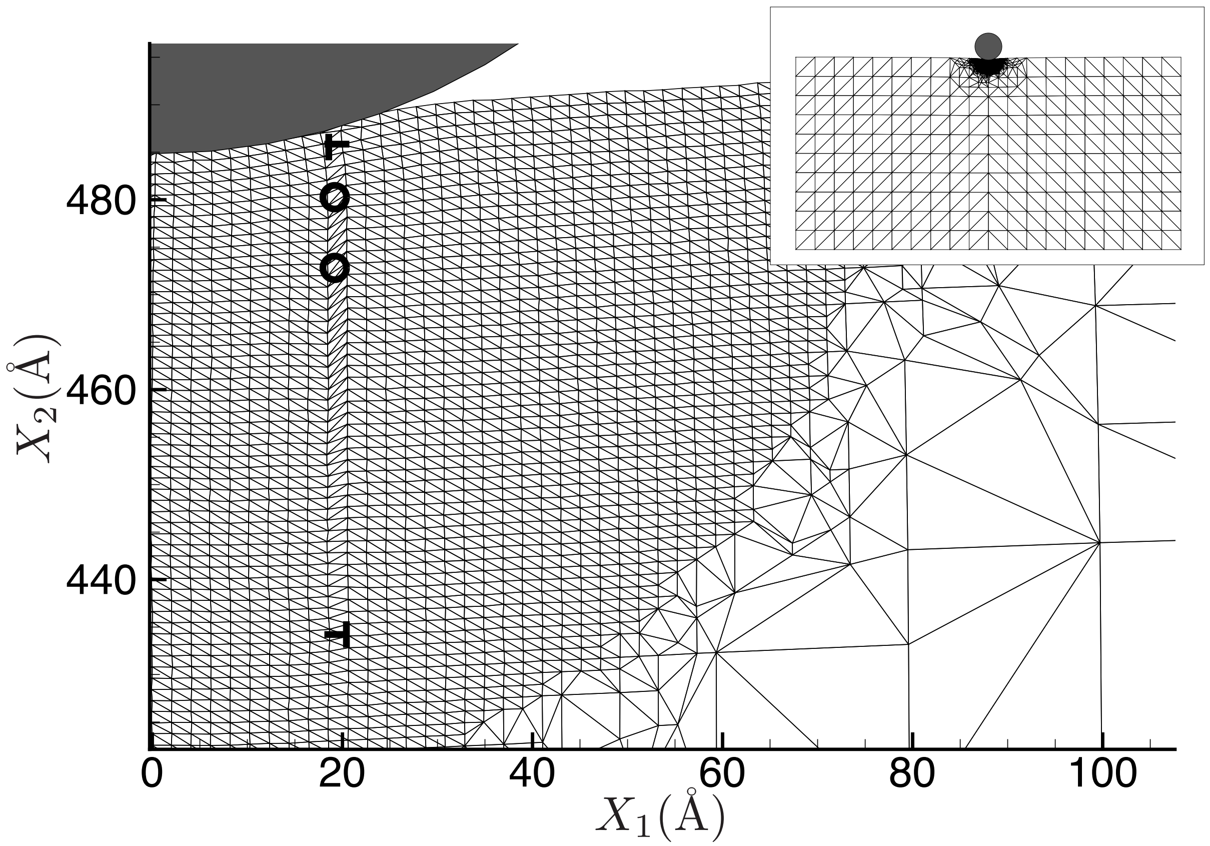


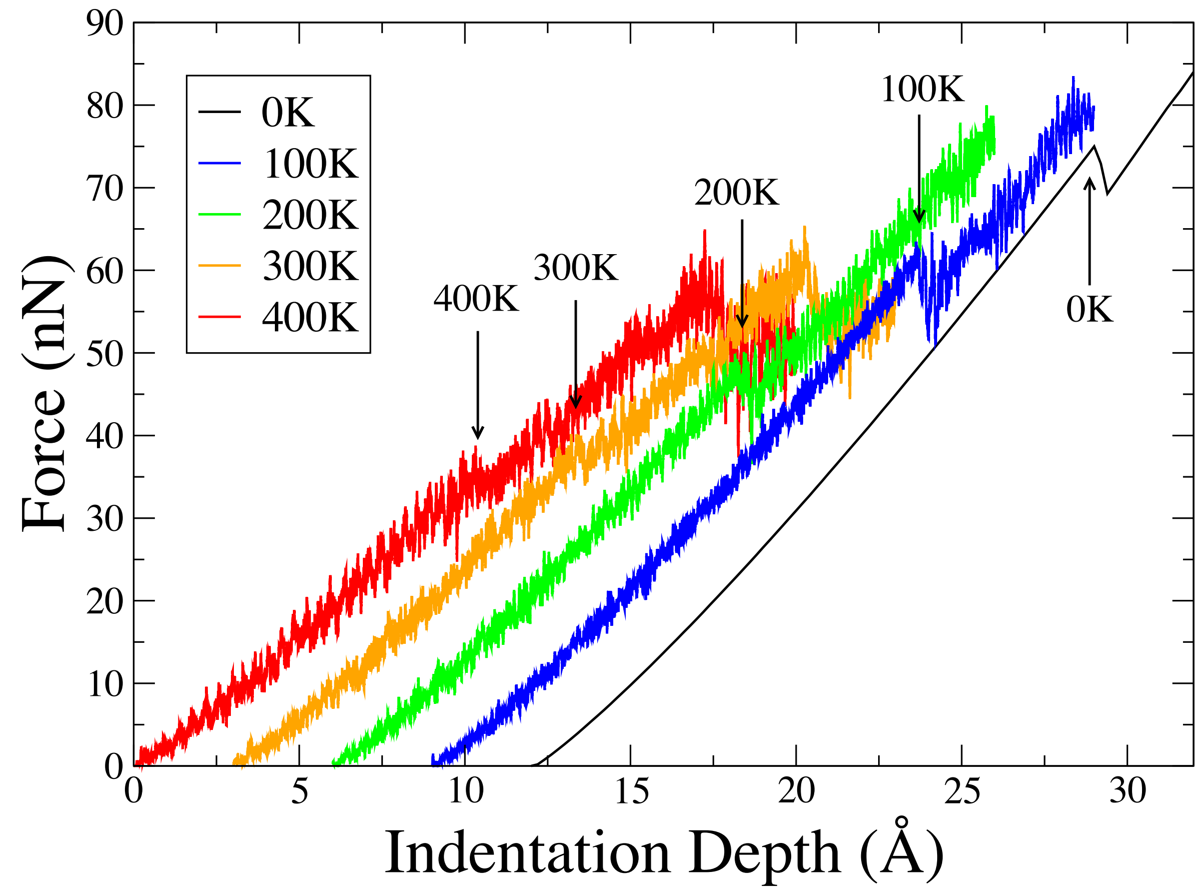
Nano-indentation at finite temperature

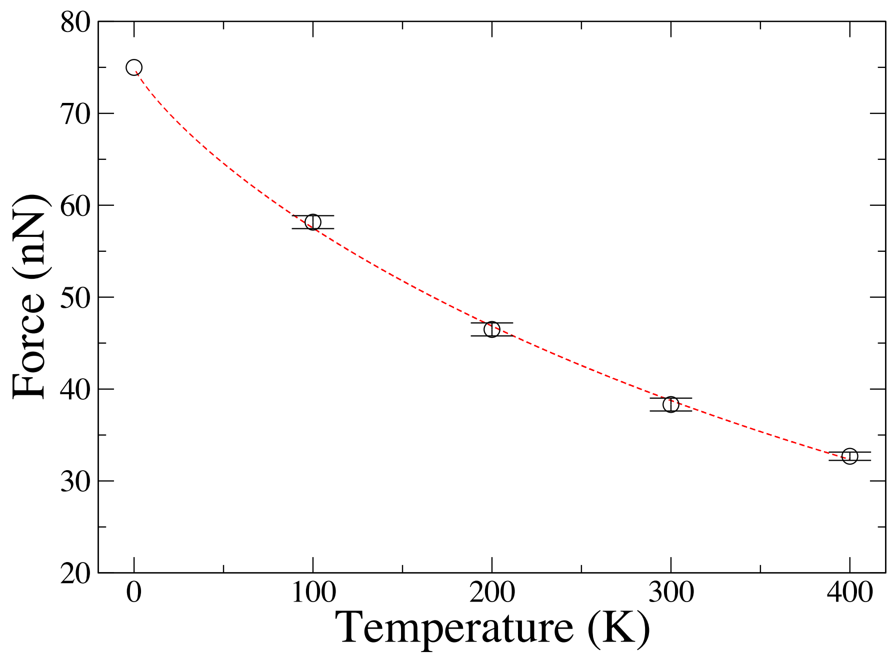




Nano-indentation at finite temperature







Excellent fit to a modified Tomlinson model proposed for thermally-activated friction of an AFM on NaCl (Gnecco et al, *PRL*, 2000)

$$f_{\text{indent}} = f^0_{\text{indent}} + \lambda_1 T \ln \frac{\lambda_2}{T}.$$

Credits

Lead Actors

Collaborator on many things (QC, hot QC, comparisons):
Ellad Tadmor, U. Minnesota

Post-Docs:
Denis Saraev (PDF, currently at large)
Behrouz Shiari (PDF, now at NNIN Michigan)

Collaborators on CADD:
Leo Shilkrot (currently at large)
Bill Curtin (Brown and EPFL)

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Supporting Cast

Help with all the comparisons of methods:
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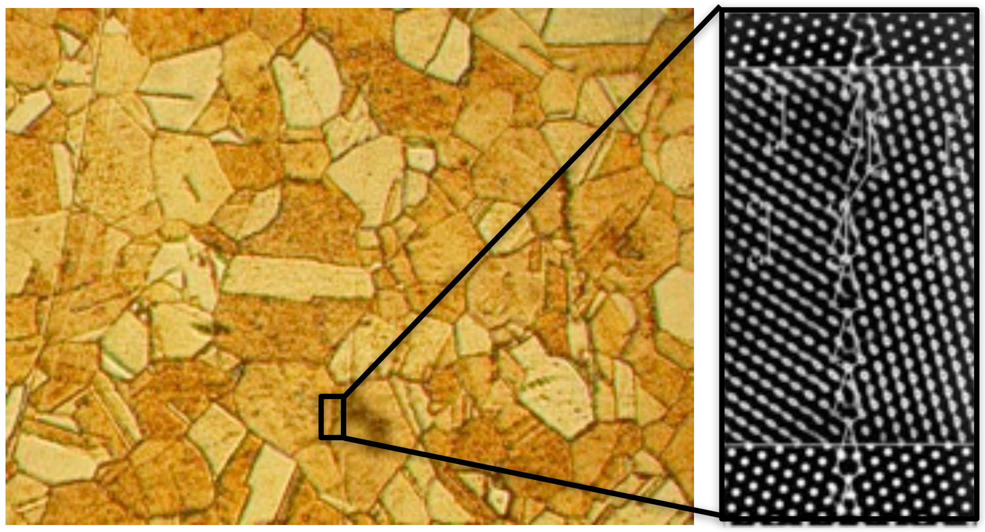
Producers

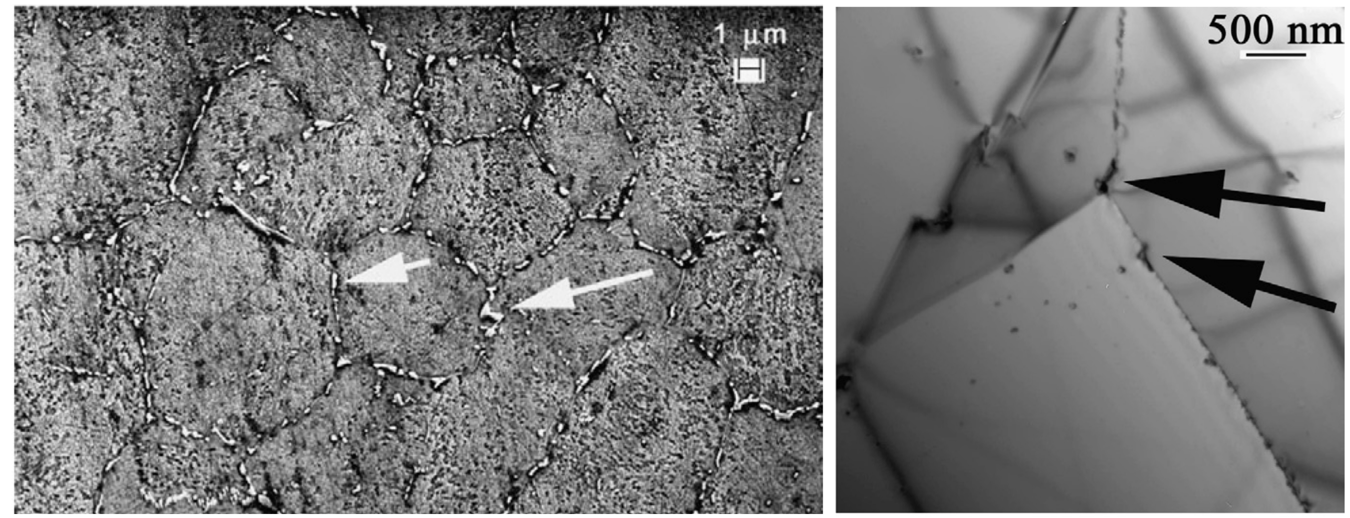
NSERC CRSNG

Ontario Premier's Research Excellence Awards (PREA)

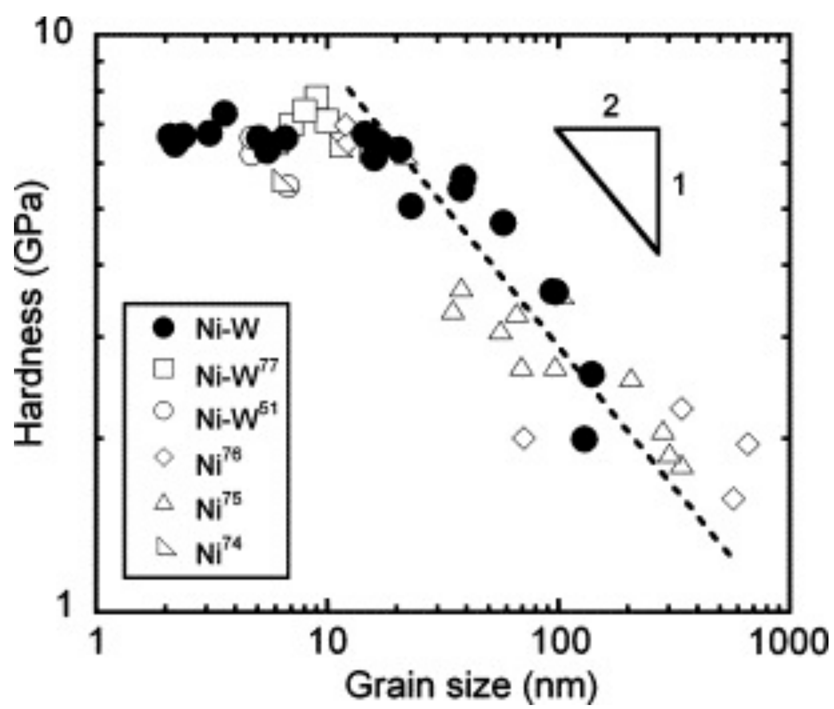
Dislocations, Grain Boundaries and Strength



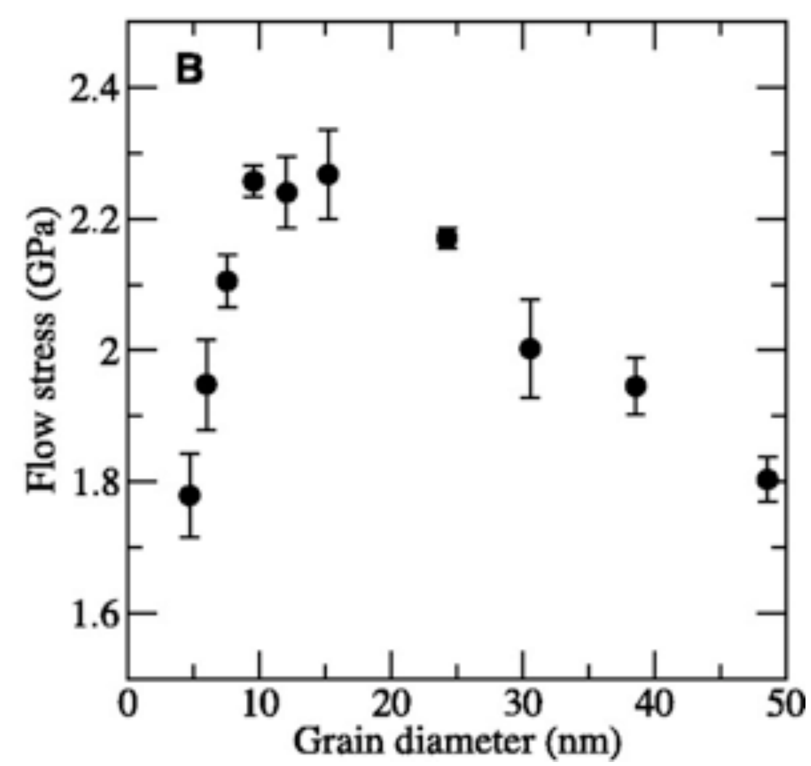
Hu et al., *Mater. Chem. Phys.*, 2002.



Han et al., *Mater. Sci. Eng. A*, 2009



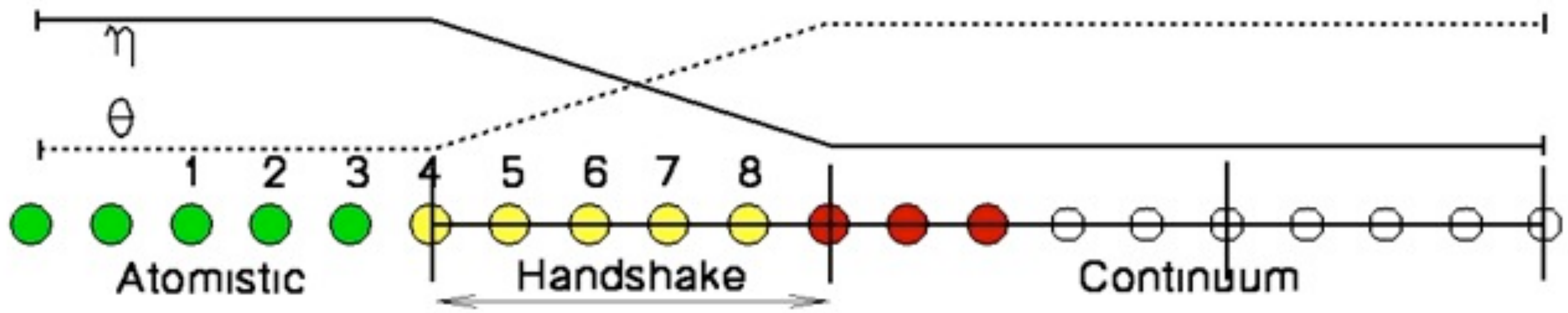
Detor and Schuh, *Acta Mat.*, 2007



Schiotz and Jacobsen, *Science*, 2003

Example 2: The AtC Method

Badia, S., Bochev, P., Lehoucq, R., Parks, M. L., Fish, J., Nuggehally, M., and Gunzburger, M. *Int. J. Multiscale Comput. Eng.* **5**(5), 387–406 (2007).



1. Introduce blending functions
2. Compute atomic forces
3. Find force on each atom using blending:

$$\boldsymbol{f}^{\alpha} = \sum_{\beta \neq \alpha} \eta^{\alpha,\beta} \boldsymbol{f}^{\alpha\beta} \qquad \eta^{\alpha,\beta} = \frac{\eta^{\alpha} + \eta^{\beta}}{2}$$

4. Find nodal forces using complementary blending function:

$$\mathbf{f}^{I} = -\sum_{e=1}^{n_{\text{elem}}} \int_{B_e} \Theta(\boldsymbol{X}) \boldsymbol{P}(\widetilde{\boldsymbol{F}}(\mathbf{u})) \frac{\partial S^{I}}{\partial \boldsymbol{X}} \, dV,$$

5. Impose positions of handshake atoms from interpolated displacements (strong compatibility)
6. Linear elasticity in the continuum

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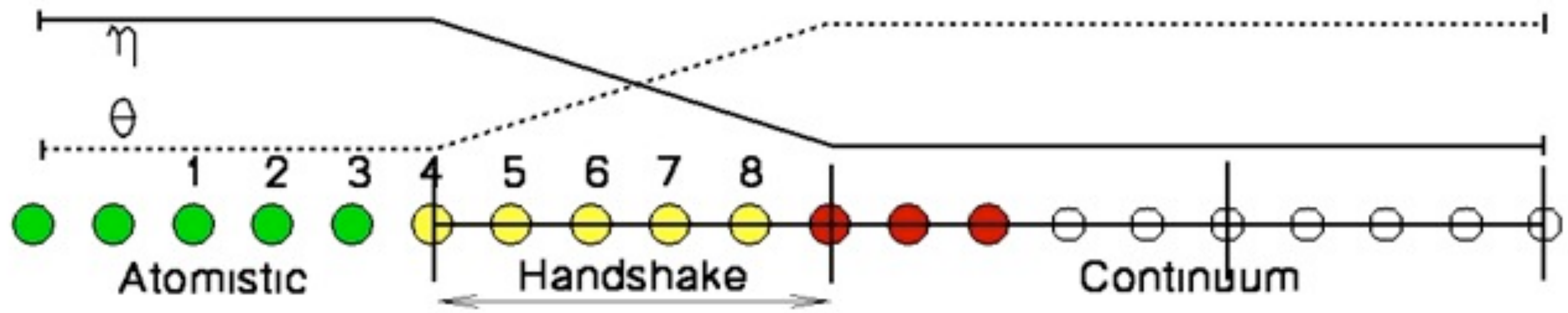

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AtC summary:

- force-based
- overlap (handshake)
- strong compatibility
- Linear Elasticity

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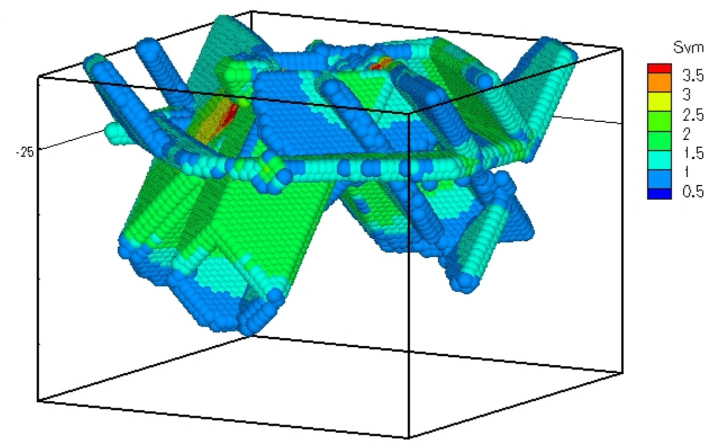
  - NEMD: non-equilibrium MD (constant energy)

Example: Nano-Indentation using the CADD method

Goal: To replace this...



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Miller et al, *Acta Mat.*, 2003

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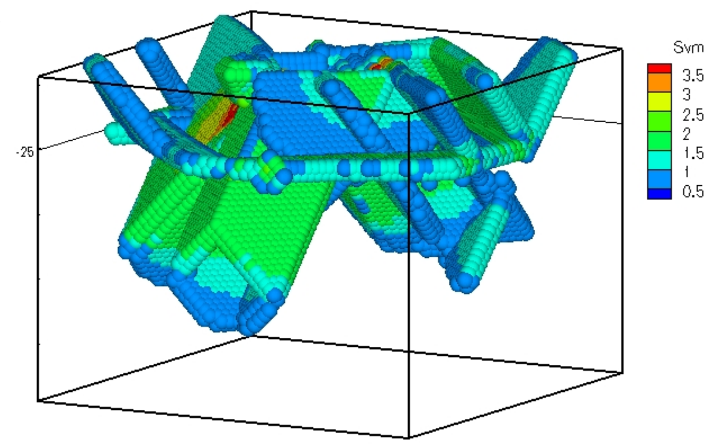

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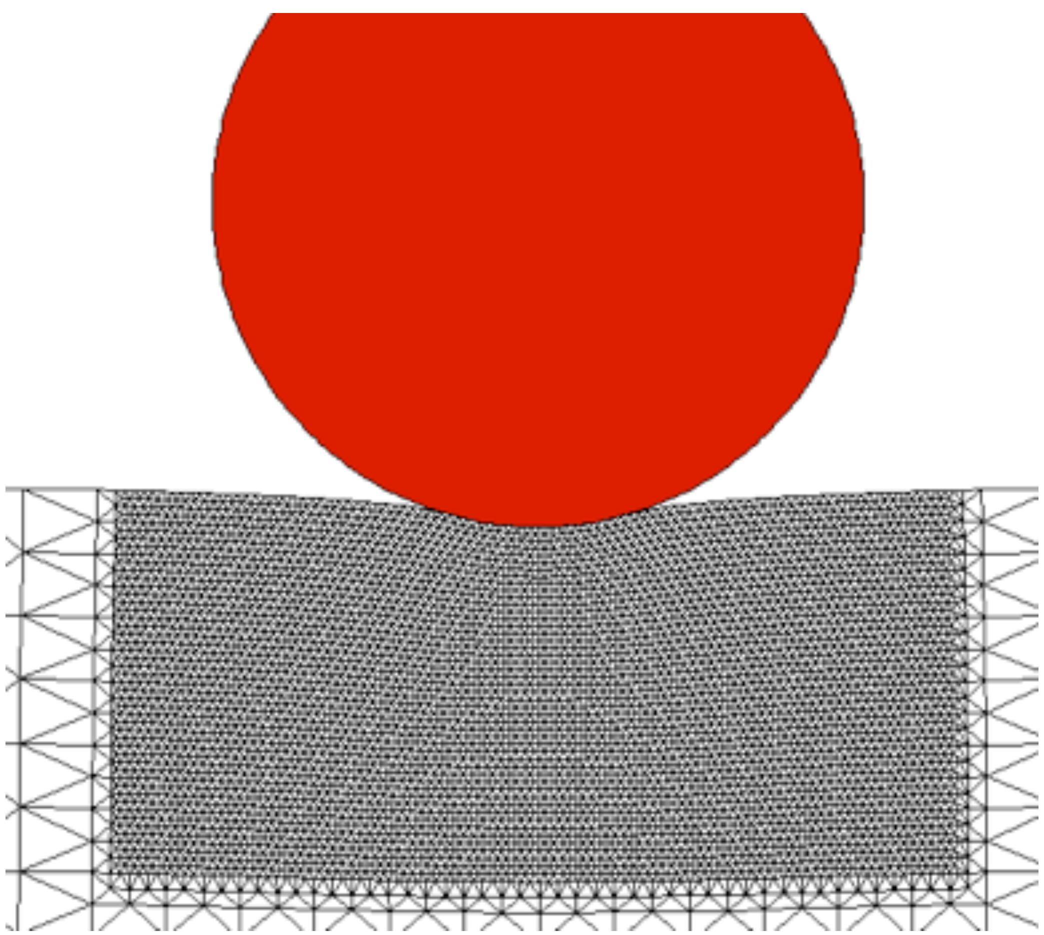

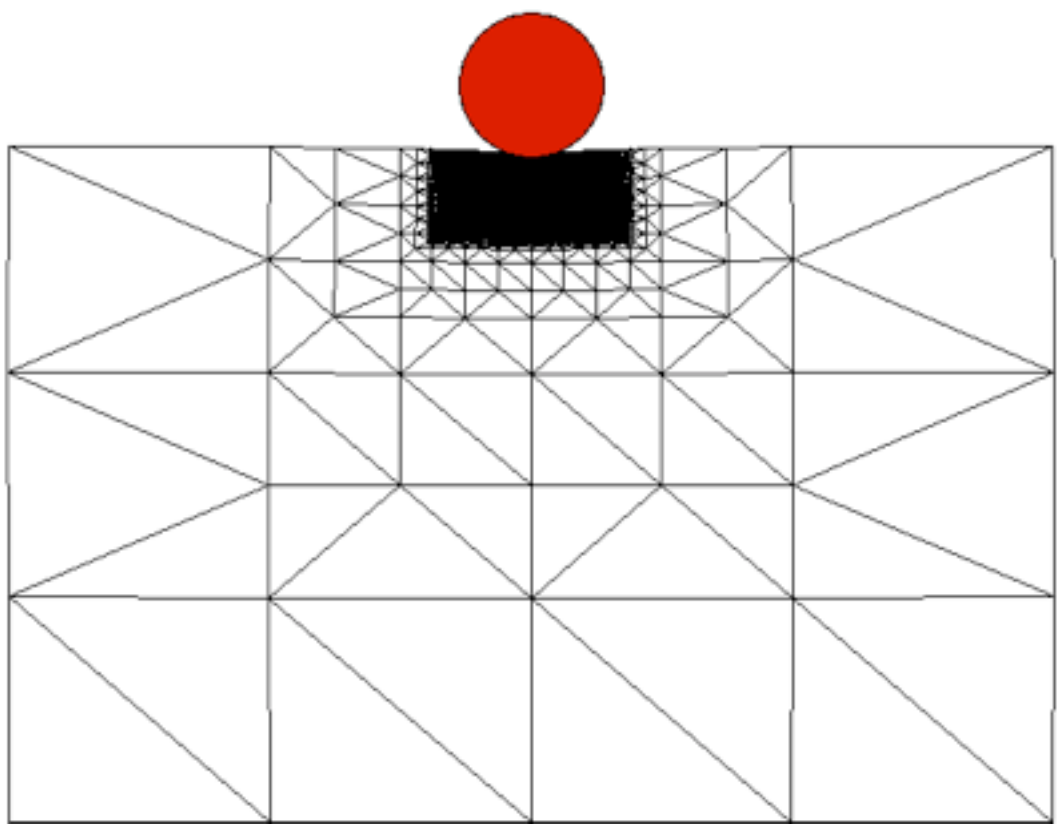

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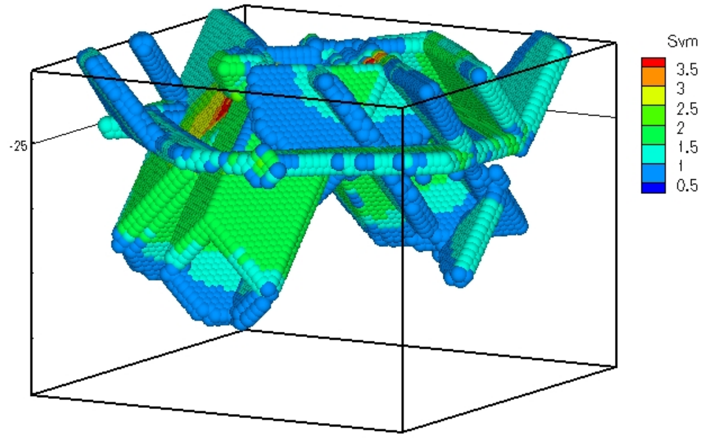

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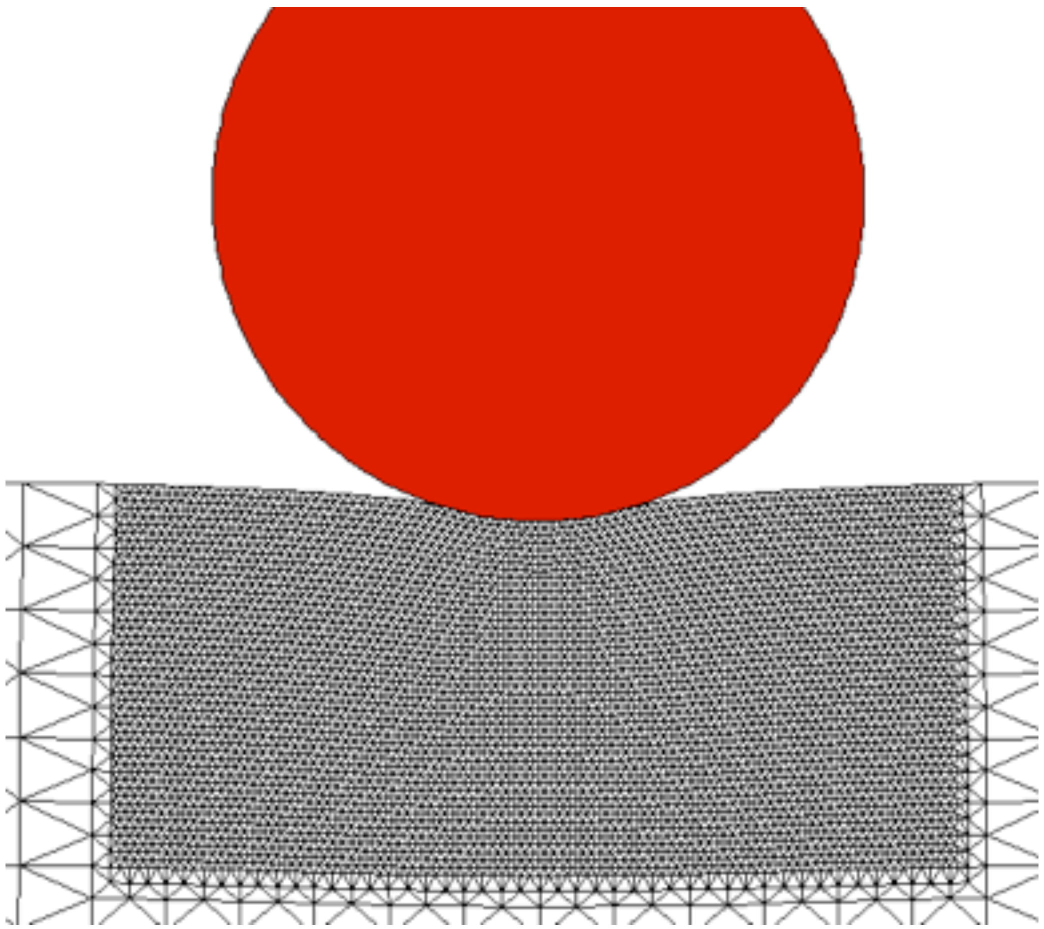

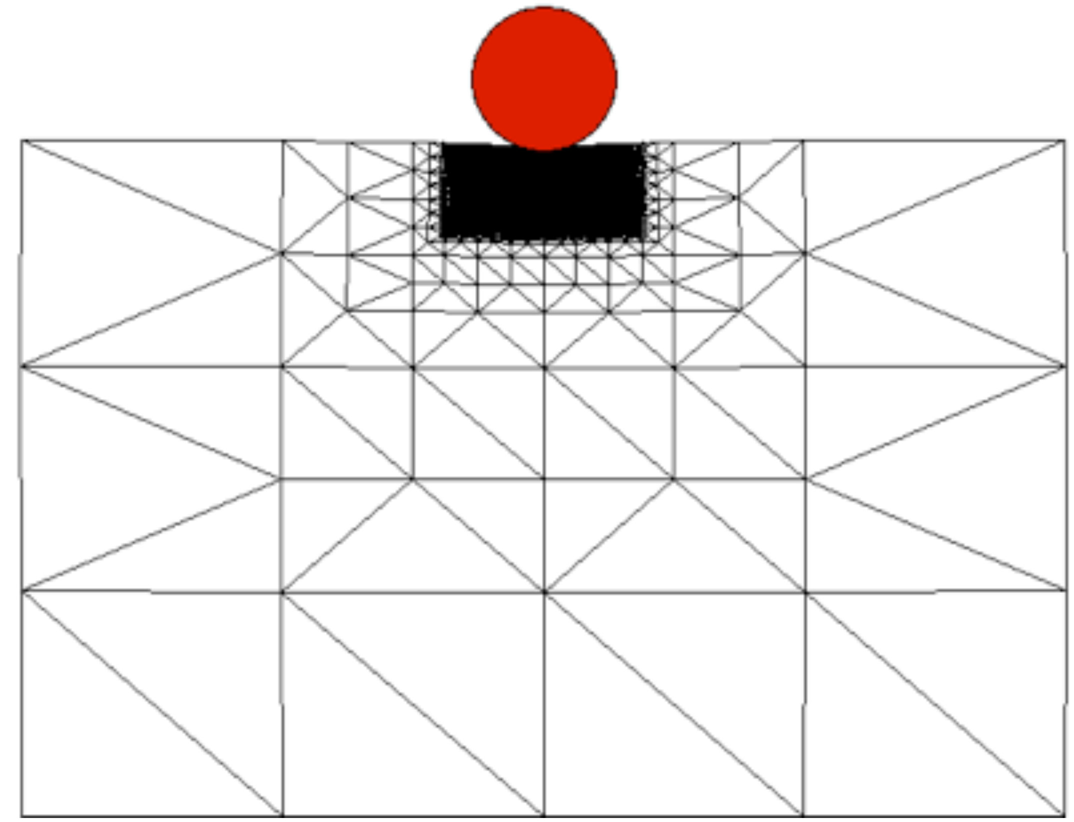

Miller et al, *Acta Mat.*, 2003

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de la fuente is gold.

Stress-induced dislocation motion

Dislocations move long distances due to high local stresses and low lattice resistance

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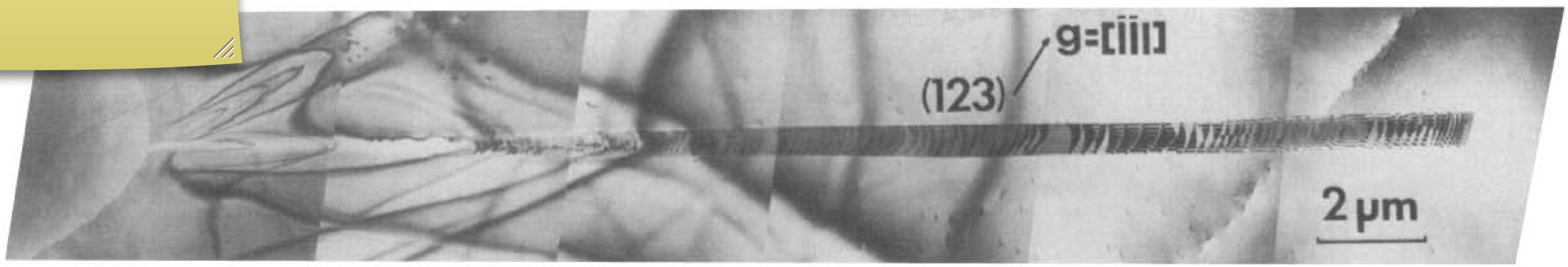

Ohr, *Mater. Sci. Eng.*, *1985*

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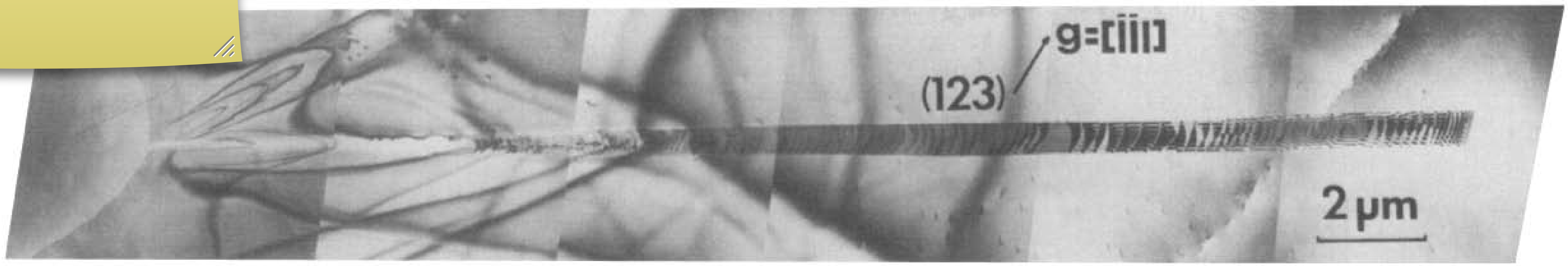


Ohr, *Mater. Sci. Eng.*, 1985

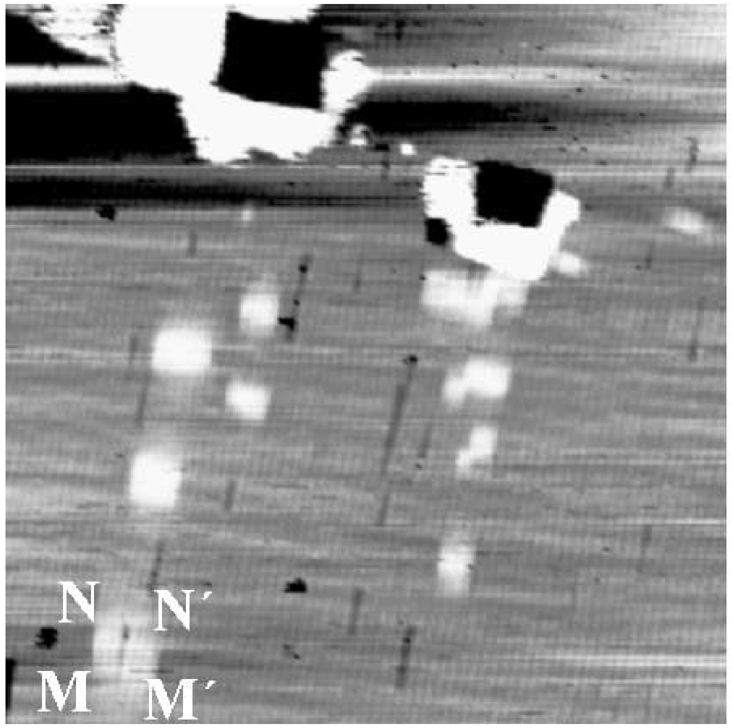
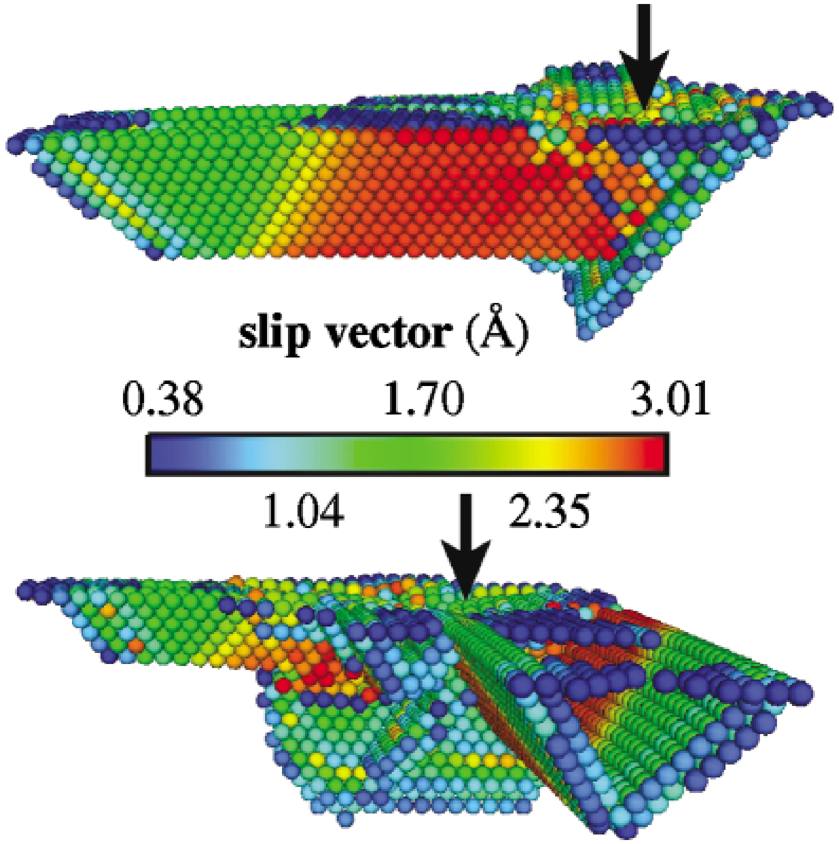


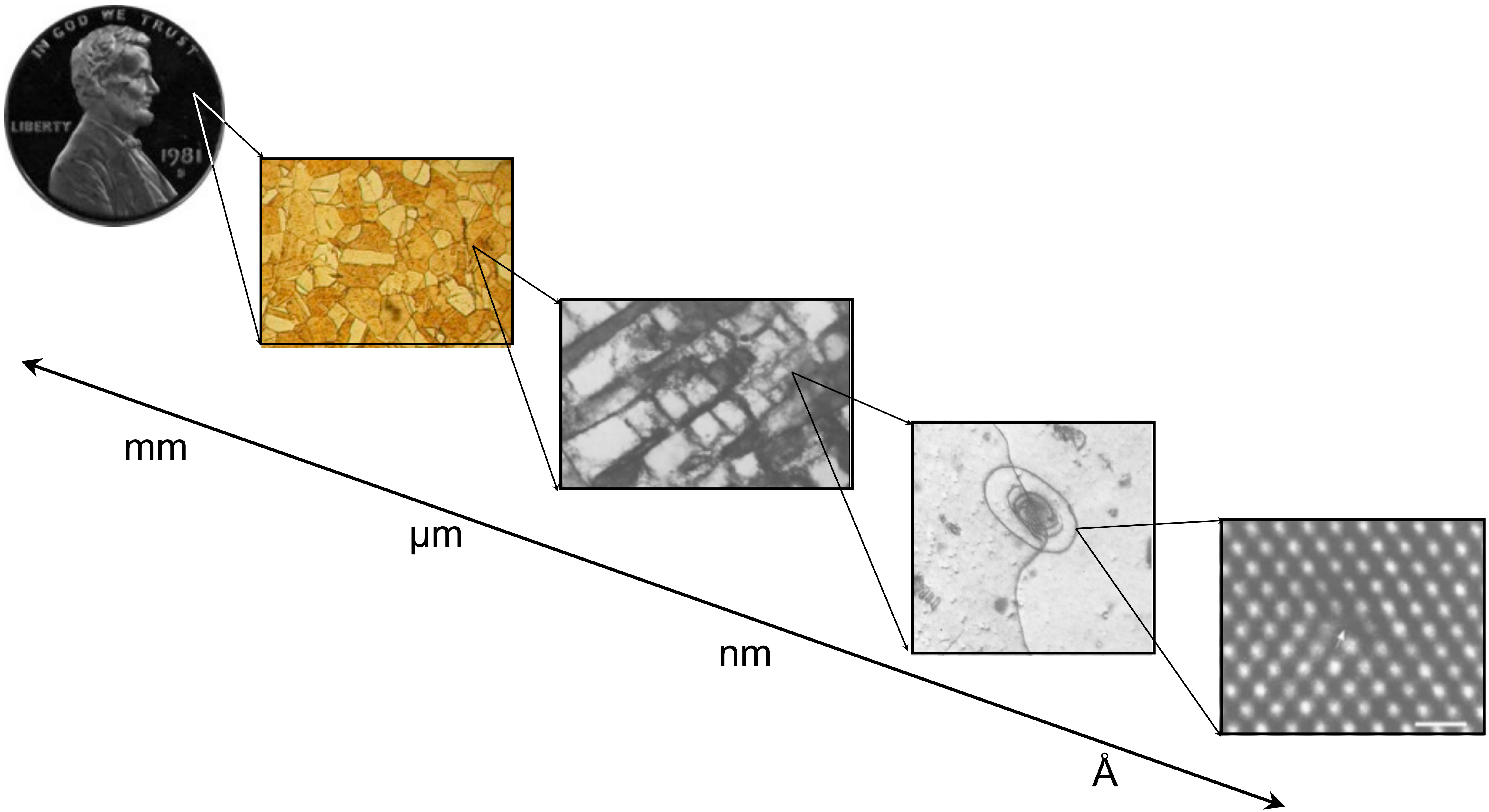
FIG. 1. (98 × 98 nm^2) STM image of two nanoindentations

de la Fuente et al., *PRL*, 2002



de la Fuente et al., *PRL*, 2002

Length Scales in Crystalline Copper



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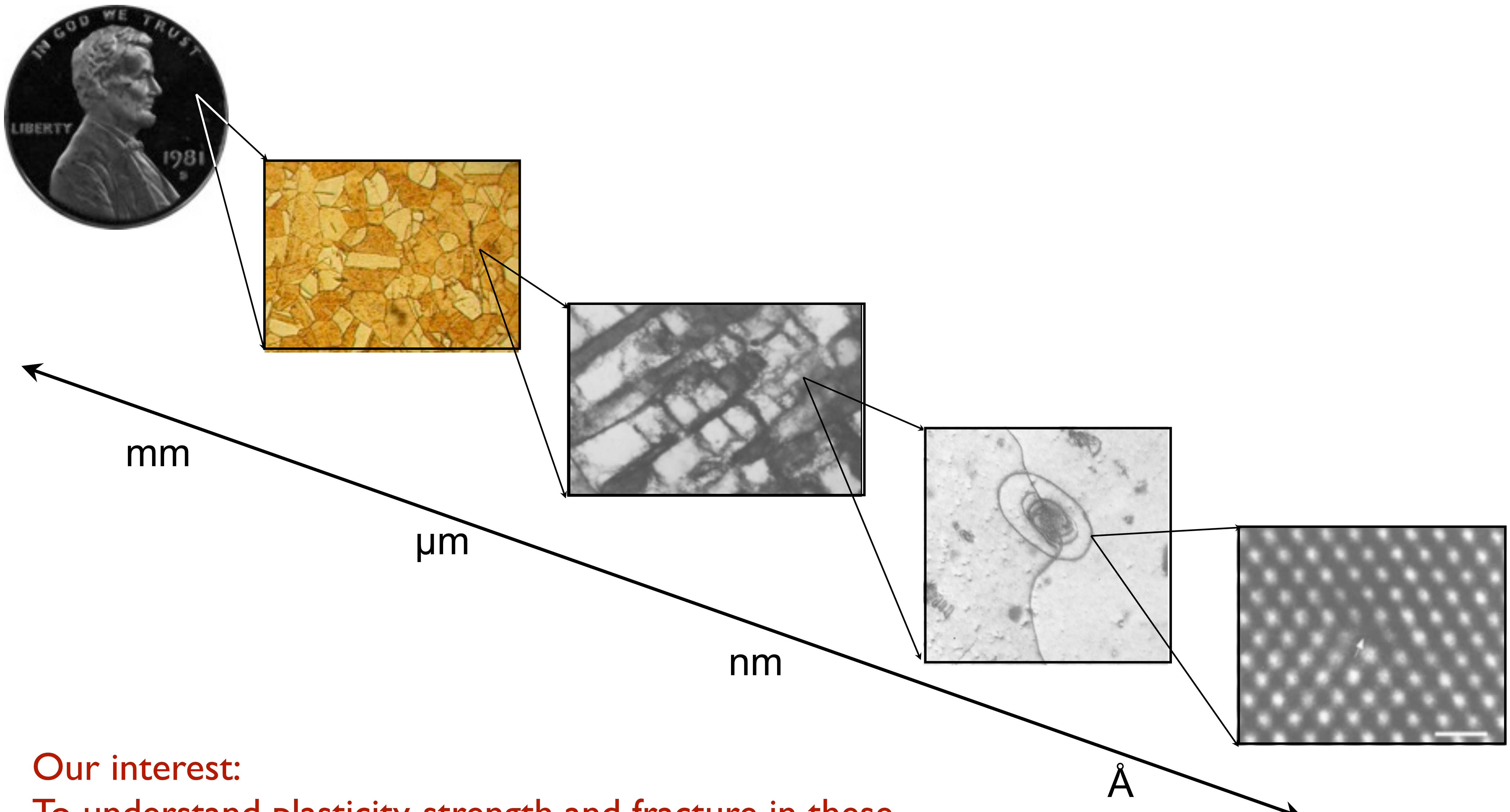
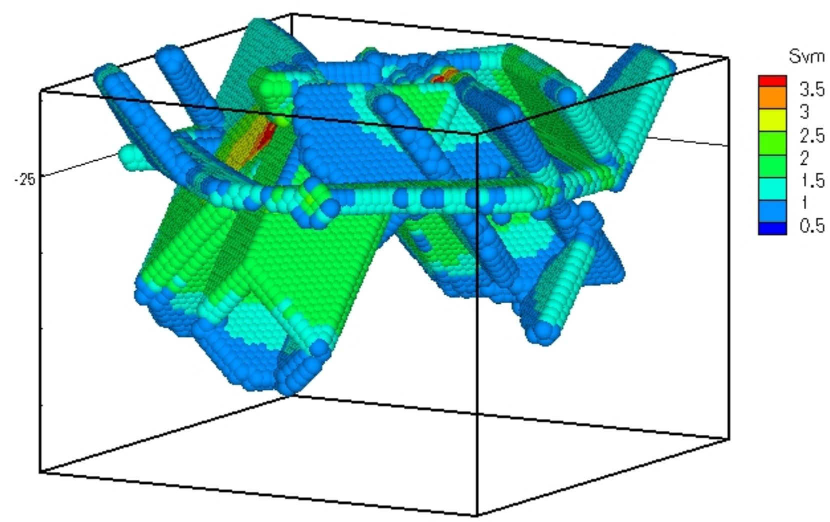


Our interest:
To understand plasticity, strength and fracture in these materials from the point of view of atomic interactions

Example: Multiscale Nano-Indentation

The goal is to replace this...



Miller et al., *Acta Mat.*, 2004

Miller and Tadmor, *MRS Bulletin*, 2007

Knap and Ortiz, *PRL*, 2003

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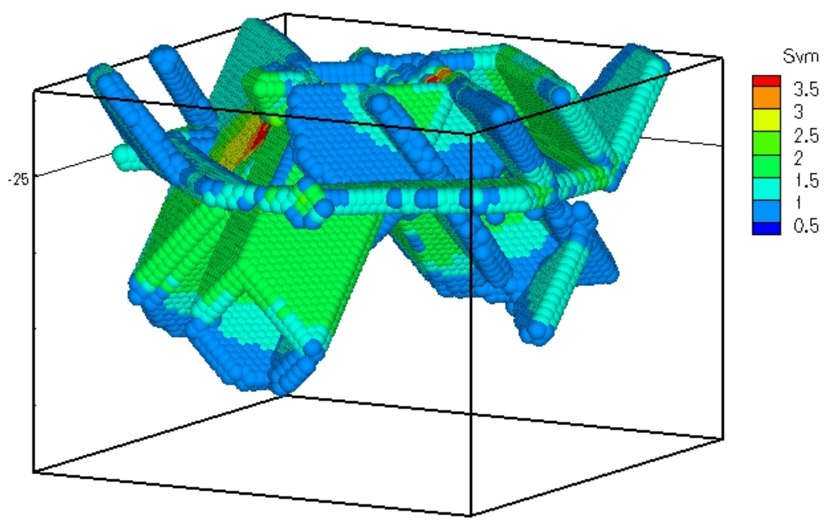

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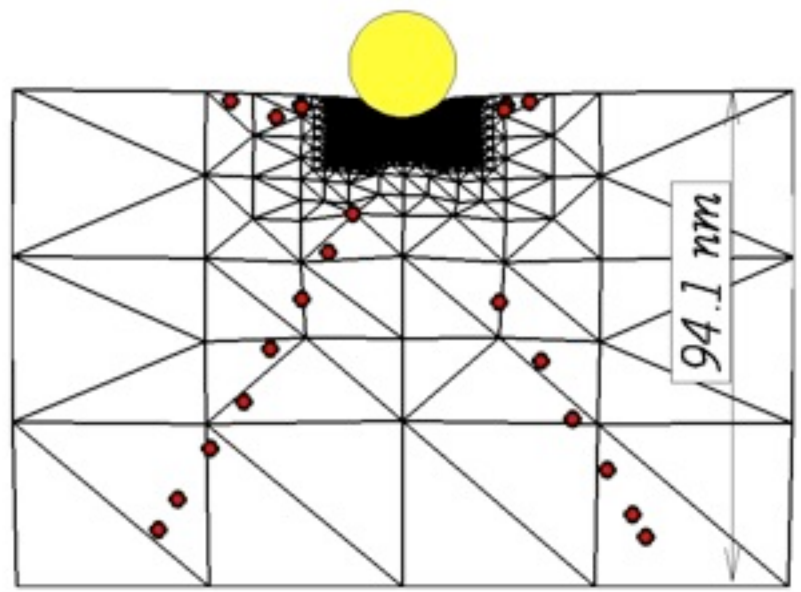
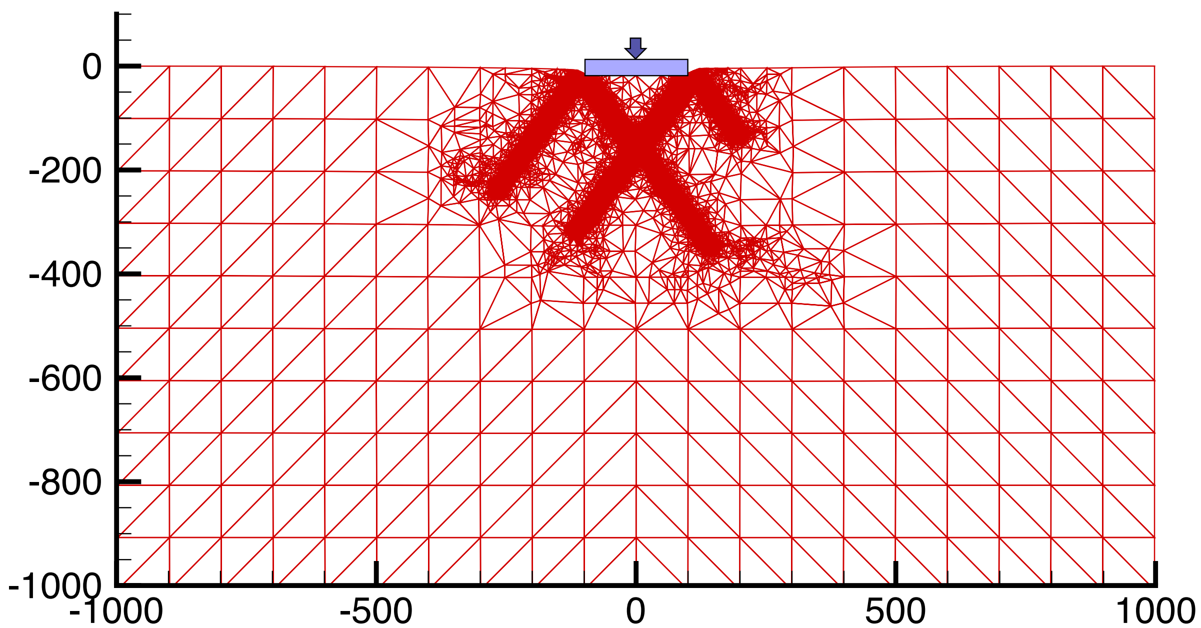


Miller et al., *Acta Mat.*, 2004



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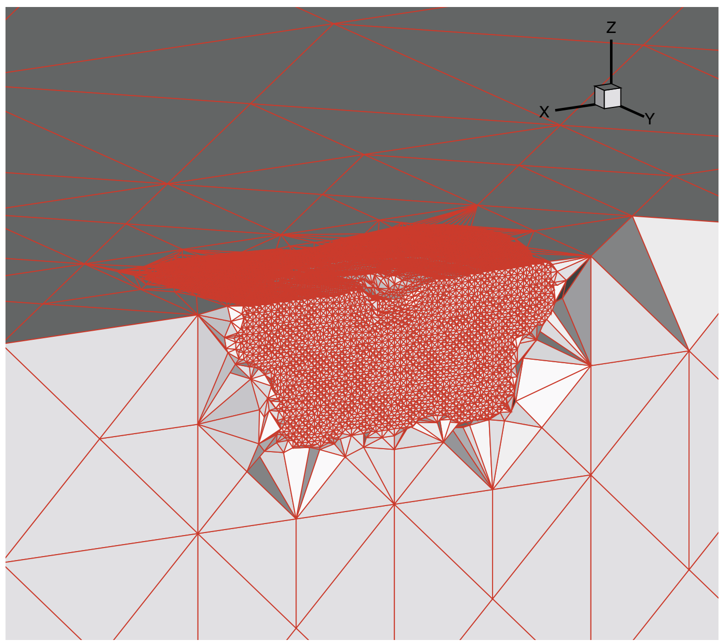

Knap and Ortiz, *PRL*, 2003

Test: Thermal Expansion of Ni (Angelo et al., *MSMSE*, 1995)