

Quasistatic Coupled Atomistic-Continuum Simulation using Arbitrary Overlapping Domains

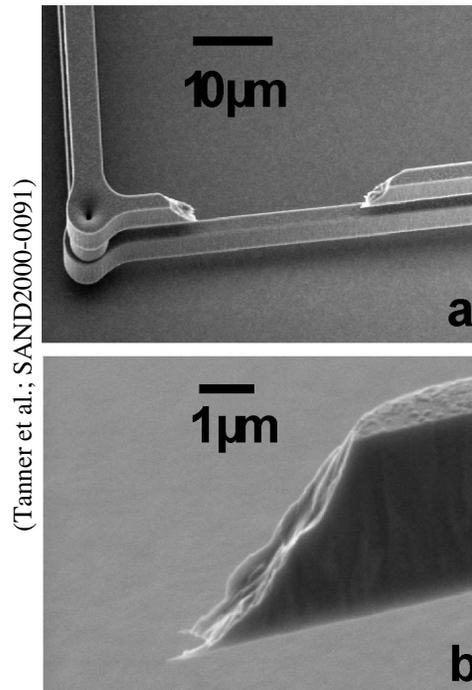
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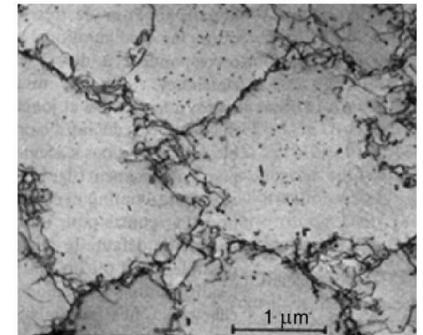
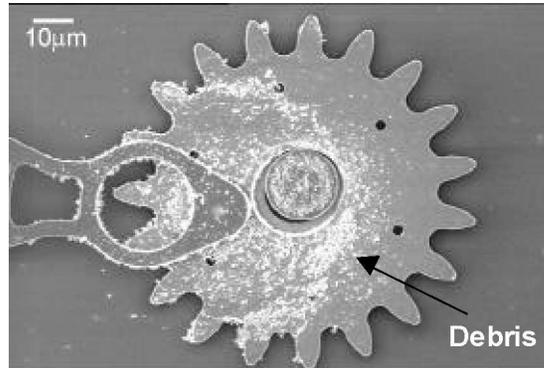
Motivation

Sandia has numerous efforts centered on the design and manufacture of microdevices. Multiple modes of material failure at various length scales need to be modeled for accurate predictions.

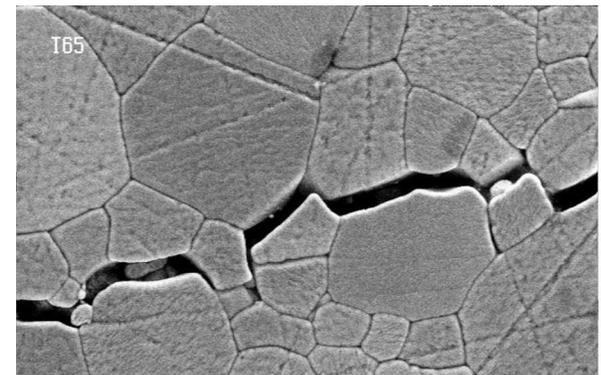


- **Fracture**
- **Dislocation activity**
- **Grain boundary fracture/sliding**
- **Stiction, friction and wear**

(Tanner et al.; SAND2000-0091)



(Bulatov, Tang and Zbib; 2001)



(Pferner; 1999)

Simulation techniques

Continuum Mechanics

Can only display anticipated failure modes.

Does not show the detailed physics occurring at the nano-scale.

Exhibits mesh-dependent behavior.

Atomistic Simulation

Computational cost is too large for micro-scale systems

Method is not efficient for modeling a majority of the system where deformation is elastic and well treated by continuum theory.

Small size of simulation region introduces fictitious boundary effects.

Coupled Atomistic-Continuum Simulation

We are developing a simulation methodology that contains atomistics to model the defect-related mechanisms operating at the nano-scale while using continuum mechanics to simulate a micro-scale geometry.

Issues with coupled methods

Material description differs between methods:

Atomistics (MS): position, force

Continuum (FE): displacement, stress

Nevertheless, previous approaches have been “one-to-one”.
Nodes and elements do not have a physical meaning, whereas atoms do.

Interface conditions are not easily defined.

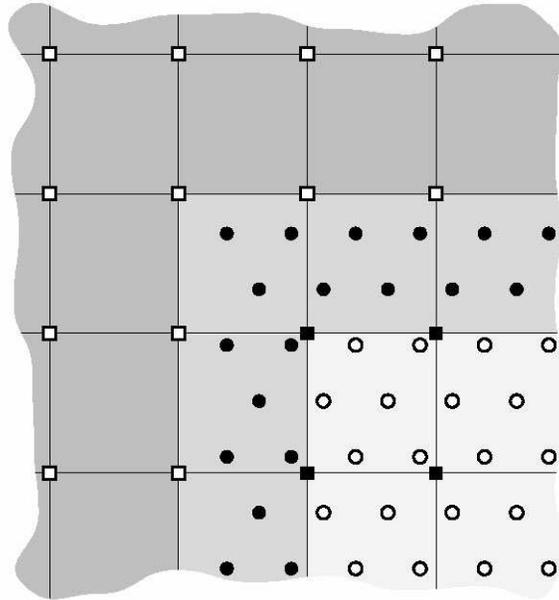
Boundary conditions versus system constraints:

Continuum: traction is prescribed at the boundaries.

Atomistics: extra variables are used to enforce isobaric conditions.

Our goal is to develop an approach that maintains the integrity of the **atomistic and continuum** views of material deformation.

Arbitrary overlapping domain formulation



Finite element mesh exists throughout the simulation region:

- — U free nodes
- — \hat{U} nodes with displacement prescribed via **projection** from atomistics

Atoms are present in limited regions:

- — Q free atoms
- — \hat{Q} ghost atoms with displacement prescribed via **interpolation** from the continuum

Wagner and Liu (2003)

Datta, Picu and Shephard (USNCCM7 - 2003)

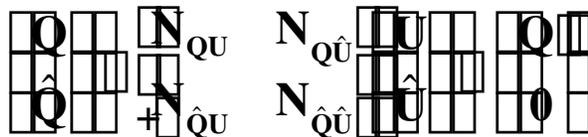
System potential energy is the sum of energy in the atomic regions and energy in the continuum elements:

$$\sum_q [Q, \hat{Q}] + \sum_u [U, \hat{U}] + \sum_q (F_Q^T Q) + \sum_u (F_U^T U)$$

Kinematic coupling

Projection

Atomistic displacements (\mathbf{Q}) are separated into the coarse scale projection and a fine scale remainder.



$$\mathbf{N}_{\hat{Q}U} \mathbf{Q} = \mathbf{0}$$

For quasi-statics, \mathbf{Q}' is used as an error estimator and can be used to:

- guide mesh refinement
- track material defects
- activate adaptive lattice extension or removal

Interpolation

The continuum impacts the atomistic region(s) through the use of ghost atoms. Their displacements ($\hat{\mathbf{Q}}$), and other properties are determined through interpolation of continuum fields at ghost atom positions.

To minimize \mathbf{Q}' :
$$\hat{\mathbf{U}} = \mathbf{M}_{\hat{U}U}^{-1} \mathbf{N}_{\hat{Q}U}^T \mathbf{Q} \quad \mathbf{M}_{\hat{U}U} = \mathbf{N}_{\hat{Q}U}^T \mathbf{N}_{\hat{Q}U}$$

$$\hat{\mathbf{Q}} = \mathbf{N}_{\hat{Q}U} \mathbf{U} = \mathbf{N}_{\hat{Q}U} \mathbf{M}_{\hat{U}U}^{-1} \mathbf{N}_{\hat{Q}U}^T \mathbf{Q}$$

Coupled equilibrium equations

System potential energy:

$$\Pi(\mathbf{Q}, \mathbf{U}) = \frac{1}{2} \mathbf{Q}^T \hat{\mathbf{K}} \mathbf{Q} + \mathbf{U}^T \hat{\mathbf{K}} \mathbf{U} - \mathbf{F}_Q^T \mathbf{Q} - \mathbf{F}_U^T \mathbf{U}$$

The equations of static equilibrium are:

$$\mathbf{R}_U = \frac{\partial \Pi}{\partial \mathbf{U}} = \frac{\partial \Pi}{\partial \hat{\mathbf{Q}}} \mathbf{N}_{\hat{\mathbf{Q}}\mathbf{U}} - \mathbf{F}_U = 0$$

$$\mathbf{R}_Q = \frac{\partial \Pi}{\partial \mathbf{Q}} = \mathbf{R}_U^T \mathbf{N}_{\hat{\mathbf{Q}}\mathbf{Q}} - \mathbf{F}_Q = 0$$

where

$$\mathbf{R}_U = \mathbf{M}_{\hat{\mathbf{Q}}\mathbf{U}}^{\mathbf{U}} = \mathbf{N}_{\hat{\mathbf{Q}}\mathbf{U}}^T \frac{\partial \Pi}{\partial \hat{\mathbf{Q}}}$$

Projection using moving least squares functions

The use of a L_2 projection makes the matrix $M_{\hat{U}\hat{U}}^{[1]}$ expensive to calculate. However, a diagonal approximation affects the accuracy of the solution.

An alternative approach is local moving least squares (MLS) method:

$$\hat{U} = M_{\hat{U}\hat{U}}^{[1]} N_{\hat{Q}\hat{U}}^T Q \quad \rightarrow \quad \hat{U} = \tilde{N}_{\hat{U}\hat{Q}} Q \quad \hat{Q} = N_{\hat{Q}\hat{U}} U = N_{\hat{Q}\hat{U}} \tilde{N}_{\hat{U}\hat{Q}} Q$$

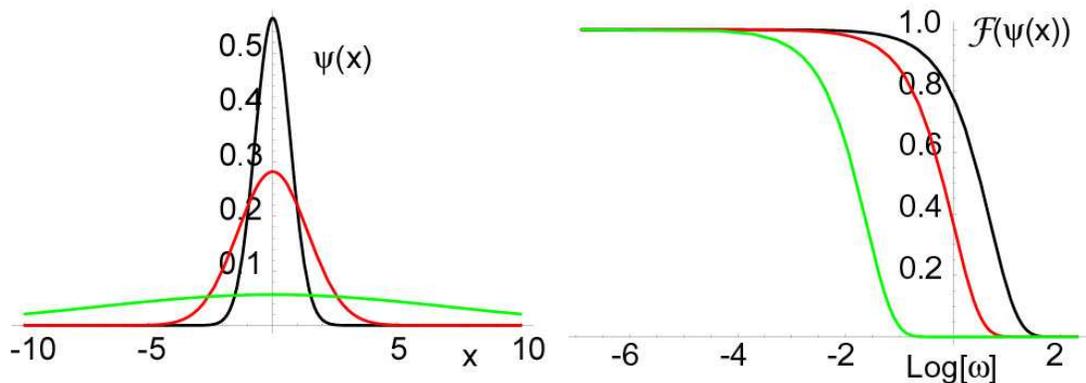
The equilibrium equations can be expressed as

$$\mathbf{R}_Q = \frac{\partial \Pi_Q}{\partial Q} = \mathbf{R}_{\hat{U}} \tilde{N}_{\hat{U}\hat{Q}} = \mathbf{F}_Q = 0 \quad \mathbf{R}_{\hat{U}} = \frac{\partial \Pi_U}{\partial \hat{U}} = \frac{\partial \Pi_Q}{\partial Q} N_{\hat{Q}\hat{U}} \quad \mathbf{R}_U = \frac{\partial \Pi_U}{\partial U} = \frac{\partial \Pi_Q}{\partial Q} N_{\hat{Q}\hat{U}} = \mathbf{F}_U = 0$$

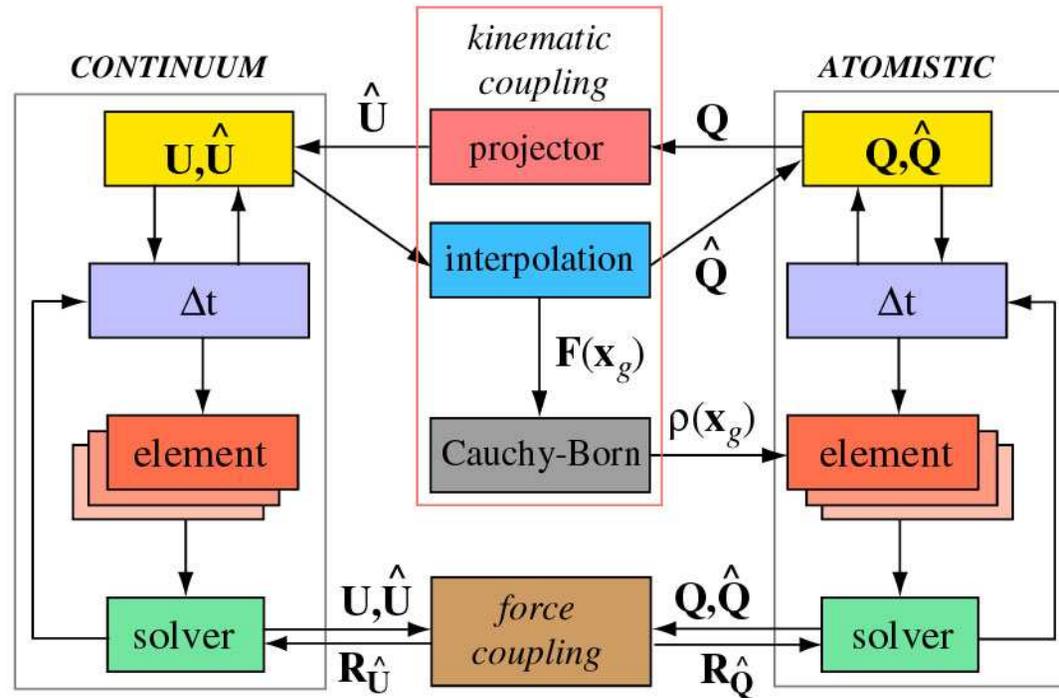
MLS has 2 advantages over global projection methods:

1. Specific types of deformation, such as homogeneous (linear), can be represented exactly.
2. Window functions act as low pass filters and can be used to obtain frequency information on the displacements.

Liu and Chen (1996)
E and Huang (2001)



Multi-module approach

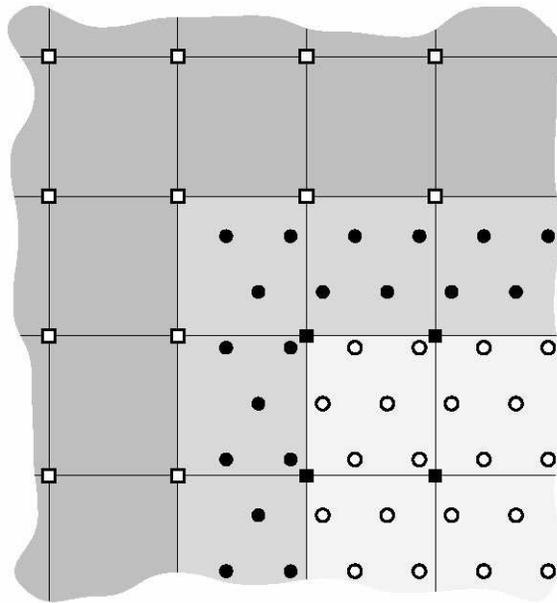


Cauchy-Born

Additional properties of ghost atoms can be obtained from the Cauchy-Born rule by using the continuum deformation field evaluated at the ghost atom position ($F(x_g)$), *e.g.* for EAM the electron density of ghost atoms ($\rho(x_g)$).

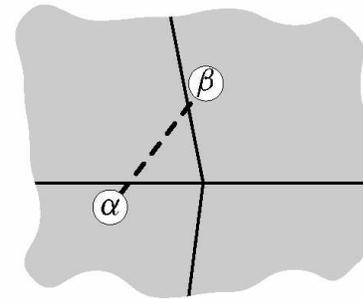
This calculation eliminates the need for ghost-ghost atoms.

“double-counting” of bond energy



“double-counted,, bonds

Heuristic approach: “bond fraction,,



Direct approach: consider internal force

- — **U** free nodes
- — **Q** free atoms

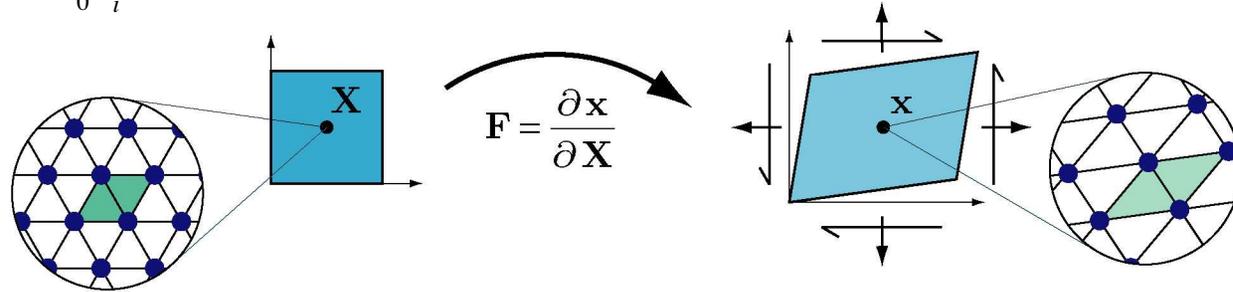
- introduce weighting on bonds and elements
- enforce balanced internal force
- for consistency, find bond weights = 1

Cauchy-Born correction for overlap elements

Atomistic potential energy is determined from a sum of bond energies in the crystal.

Continuum strain energy is computed using the Cauchy-Born rule:

$$\rho = \frac{1}{V_0} \sum_i U(\mathbf{l}^{(i)}) = \frac{1}{V_0} \sum_i \tilde{U}(\mathbf{l}_o^{(i)}, \mathbf{F})$$



For overlap elements, the energy from real atom - ghost atom bonds is present.

A density term must be introduced so that the Cauchy-Born rule used for these elements only accounts for the bonds that are not explicitly represented:

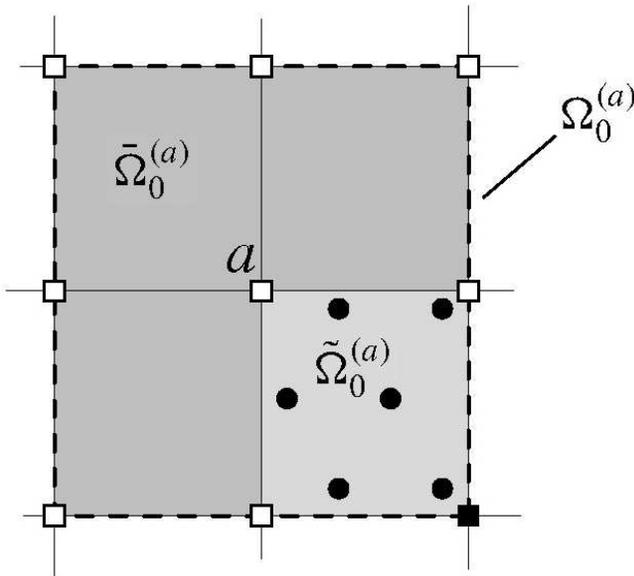
$$\rho = \frac{1}{V_0} \left(\sum_{\mathbf{l} \in \mathbf{X}} U(\mathbf{l}^{(i)}) + \sum_{\mathbf{l} \in \tilde{\mathbf{X}}} \tilde{U}(\mathbf{l}_o^{(i)}, \mathbf{F}) \right) \chi(\mathbf{X})$$

Cauchy-Born correction

Total force on boundary node a under homogeneous deformation:

$$\mathbf{f}^{(a)} = -\mathbf{F} \sum_i^{n_b} \left[\frac{\varphi'(r)}{r} \right]_{(i)} \mathbf{f}_{(i)}^{(a)}$$

$$\mathbf{f}_{(i)}^{(a)} = \mathbf{R}_{(i)} \sum_{\substack{\beta: \mathbf{X}^{(\beta)} \in \tilde{\Omega}_0^{(a)}, \\ \mathbf{R}^{(\alpha\beta)} = \mathbf{R}_{(i)}}} N^{(a)}(\mathbf{X}^{(\beta)}) + \frac{1}{V_0} [\mathbf{R} \otimes \mathbf{R}]_{(i)} \left[\int_{\tilde{\Omega}_0^{(a)}} \frac{\partial N^{(a)}}{\partial \mathbf{X}} d\Omega + \int_{\tilde{\Omega}_0^{(a)}} \rho_{(i)} \frac{\partial N^{(a)}}{\partial \mathbf{X}} d\Omega \right]$$



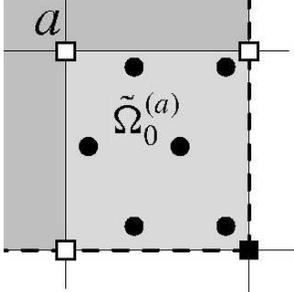
Regularized objective function:

$$\tilde{P}^* = \frac{1}{2} \sum_{a \in \mathcal{N}_{\tilde{\Omega}_0}} \sum_i^{n_b} \mathbf{f}_{(i)}^{(a)} \cdot \mathbf{f}_{(i)}^{(a)} + \frac{1}{2} \kappa \sum_i^{n_b} \int_{\tilde{\Omega}_0} \nabla_{\mathbf{X}} \rho_{(i)} \cdot \nabla_{\mathbf{X}} \rho_{(i)} d\Omega$$

$\square_{(i)}(\mathbf{X})$ are determined by enforcing a consistency condition of homogeneous deformation given the appropriate boundary conditions. Ideally, $\square_{(i)}$ are **independent** of the deformation.

Decoupling for homogeneous deformation

The ideal way to eliminate the forces on nodes bounding overlap elements is to have:



The diagram shows a square element with side length \$a\$. The top-left corner is labeled \$a\$. Inside the square, there are several black dots representing atoms. A dashed line outlines a region \$\tilde{\Omega}_0^{(a)}\$ which is a square of side \$a\$ shifted towards the top-right corner. This region contains some of the atoms. The region outside the dashed line but within the square is shaded gray. The force on the node at the top-left corner is denoted as \$\mathbf{f}_{(i)}^{(a)}\$.

$$\mathbf{f}_{(i)}^{(a)} = \mathbf{R}_{(i)} \sum_{\substack{\beta: \mathbf{X}^{(\beta)} \in \tilde{\Omega}_0^{(a)}, \\ \mathbf{R}^{(\alpha\beta)} = \mathbf{R}_{(i)}}} N^{(a)}(\mathbf{X}^{(\beta)}) - \frac{1}{V_0} [\mathbf{R} \otimes \mathbf{R}]_{(i)} \int_{\tilde{\Omega}_0^{(a)}} (1 - \rho_{(i)}) \frac{\partial N^{(a)}}{\partial \mathbf{X}} d\Omega = 0$$

using:

$$\int_{\Omega_0^{(a)} = \bar{\Omega}_0^{(a)} \cup \tilde{\Omega}_0^{(a)}} \frac{\partial N^{(a)}}{\partial \mathbf{X}} d\Omega = \oint_{\partial \Omega_0^{(a)}} N^{(a)} \mathbf{N} d\Gamma = 0$$

This end result can be obtained naively by omitting force cross-terms between real nodes and ghost atoms:

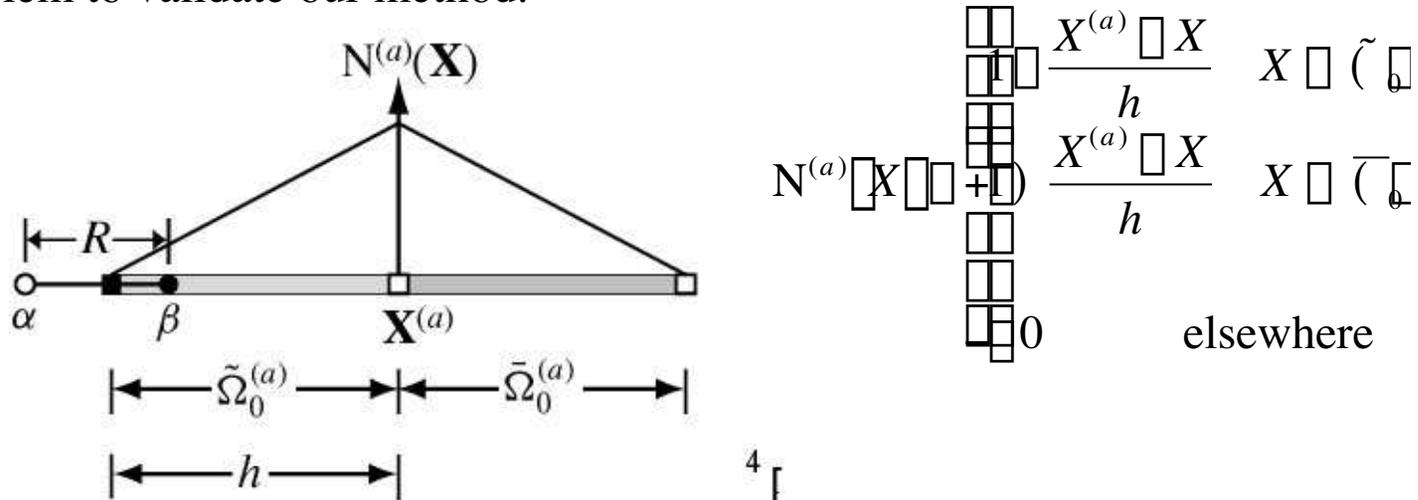
$$\mathbf{R}_{(i)} \sum_{\substack{\beta: \mathbf{X}^{(\beta)} \in \tilde{\Omega}_0^{(a)}, \\ \mathbf{R}^{(\alpha\beta)} = \mathbf{R}_{(i)}}} N^{(a)}(\mathbf{X}^{(\beta)}) \rightarrow 0$$

and by using the uncorrected Cauchy-Born rule within the overlap elements:

$$\rho_{(i)} = 1 \quad \text{implies} \quad \frac{1}{V_0} [\mathbf{R} \otimes \mathbf{R}]_{(i)} \int_{\tilde{\Omega}_0^{(a)}} (1 - \rho_{(i)}) \frac{\partial N^{(a)}}{\partial \mathbf{X}} d\Omega \rightarrow 0$$

Coupling of a 1-Dimensional System

The homogeneous deformation of a 1-D coupled atomistic-continuum chain is an ideal test problem to validate our method.



The energy is corrected by choosing a den such that:

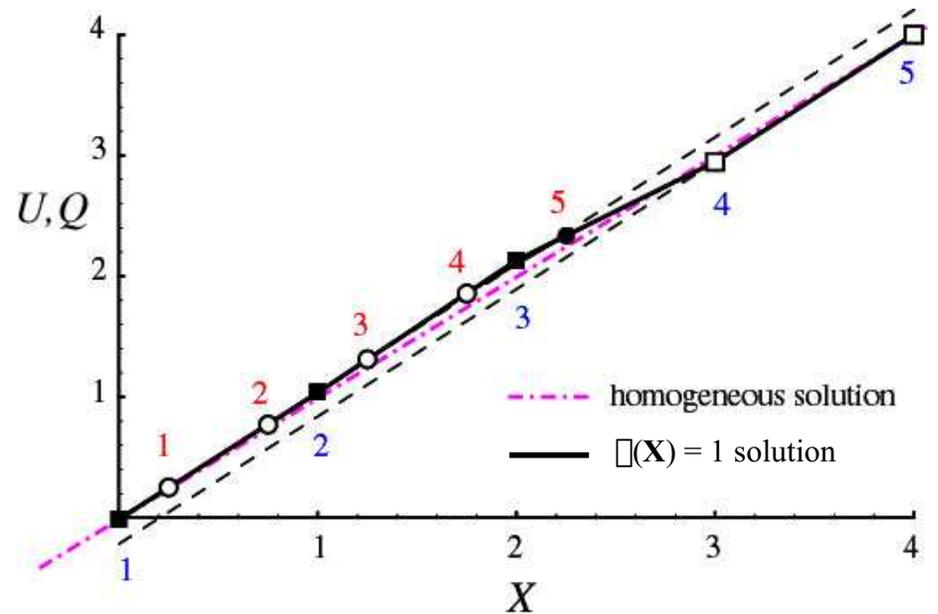
$$\int_{\tilde{\Omega}} dX \int_{\bar{\Omega}} dX \int_{\tilde{\Omega}} dX \int_{\bar{\Omega}} dX \dots$$

In this case, the density function does not have a unique solution.

The simplest solution is:

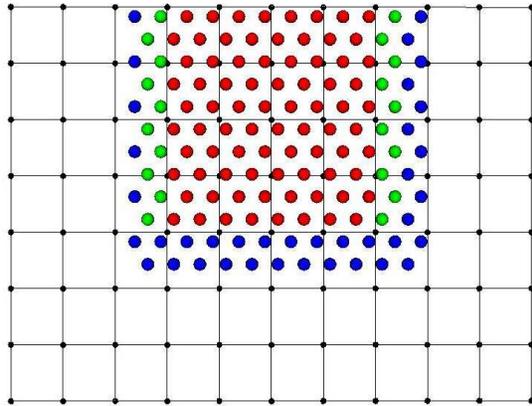
$$\rho = 1 - N^{(a)} \chi^{(\tilde{\Omega})}$$

“bond overlap”

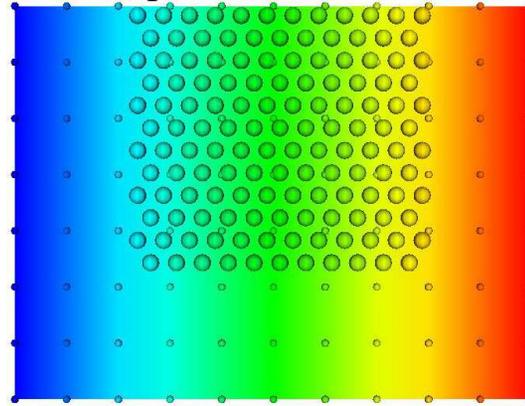


2D Lennard-Jones 6/12 (w/o force cross terms)

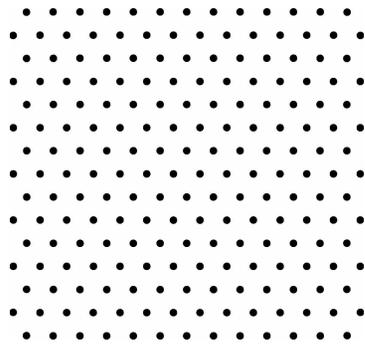
uniform stretching: nearest neighbor



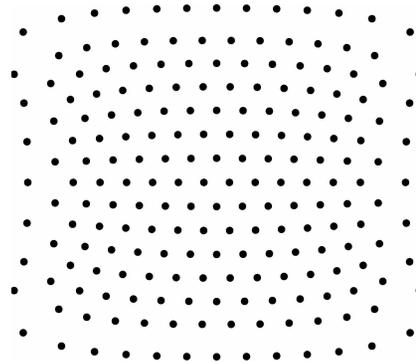
x -displacement contours



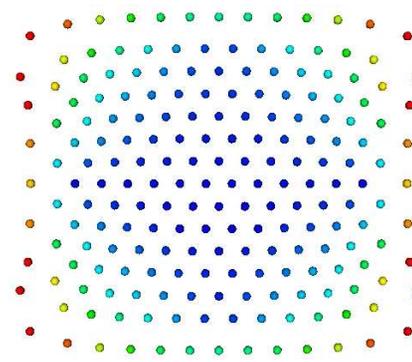
surface relaxation: 5th neighbor



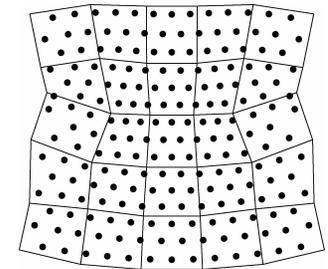
initial configuration



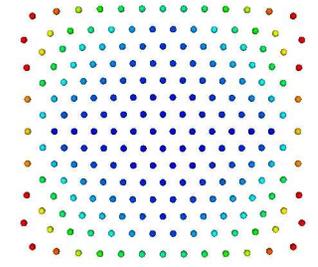
atomistic solution
displacements at 128x mag



coupled solution
MLS projection

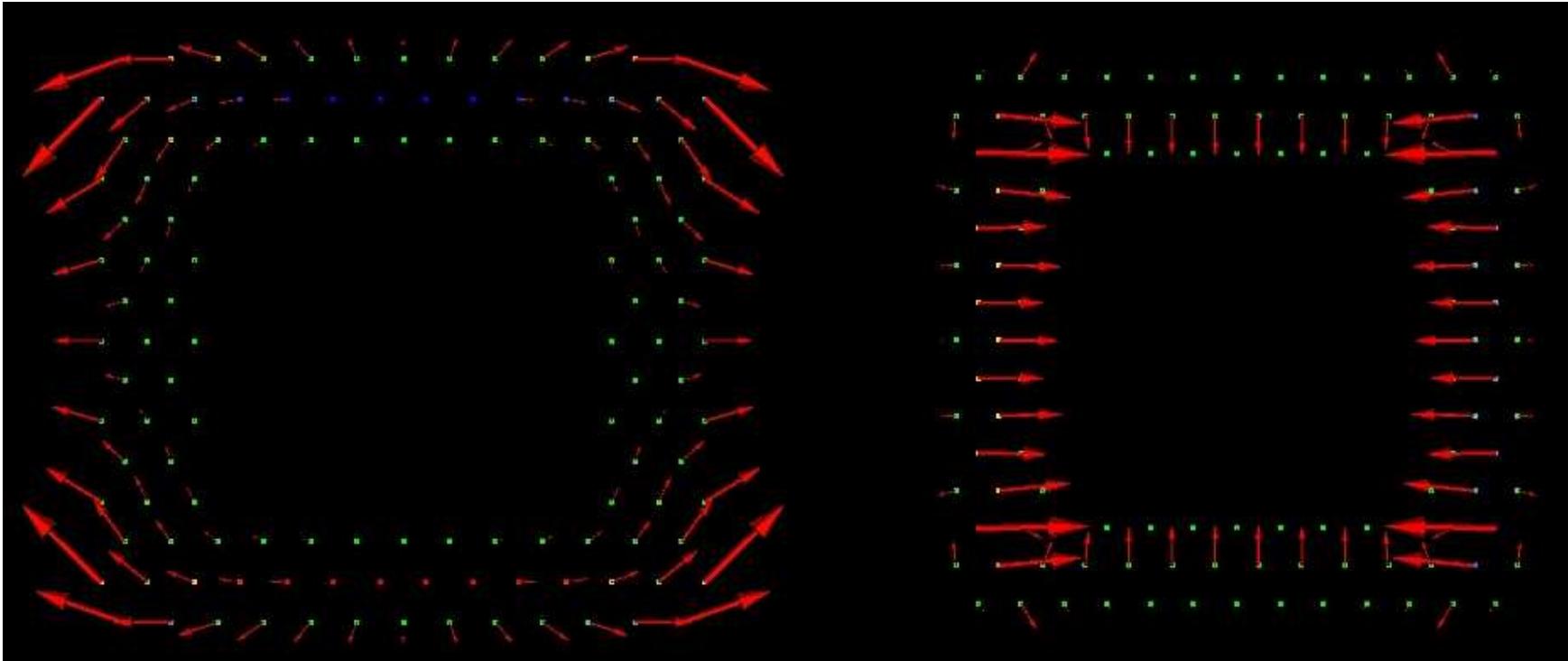


L_2 projection (64x)



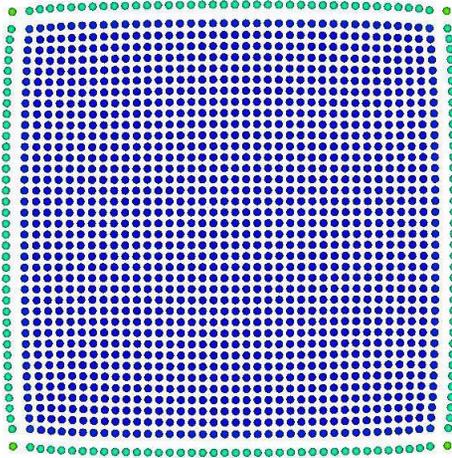
MLS projection (64x)

Coarse and fine scale displacements of atoms



While the coarse scale portions of the atomic displacements capture most of the deformation, information on the location of large displacement gradients is obtained with the fine scale components.

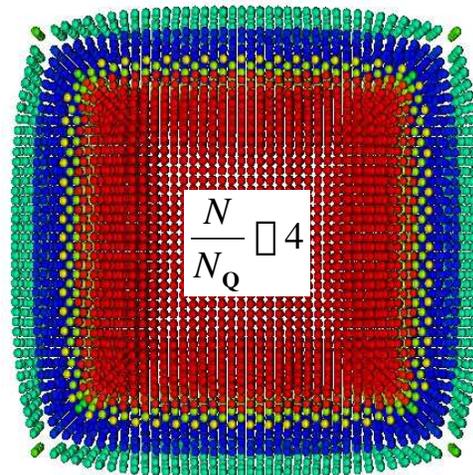
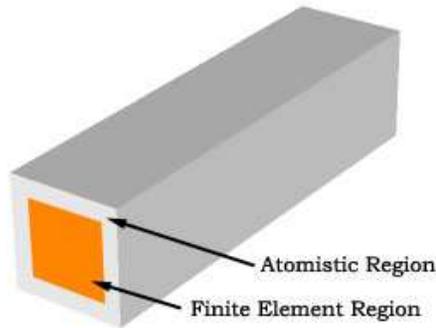
3D nanowire relaxation (w/o force cross terms)



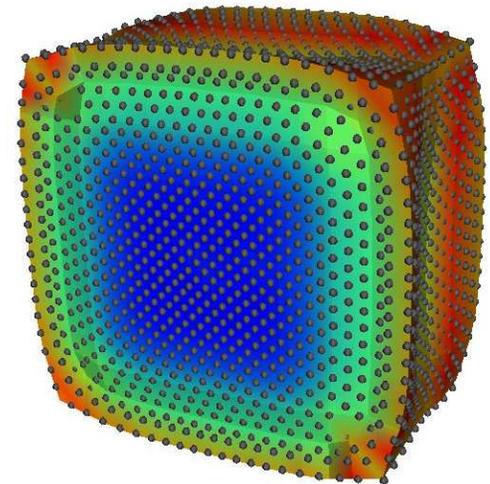
- 5th neighbor Lennard-Jones 6/12
- periodic boundary conditions along axis

*displacements
magnified
by a factor
of 40*

deformed configuration



potential energy



pressure

Conclusions

We have presented a formulation for atomistic-continuum coupling comprised of three components:

- kinematics - transferal of displacements between nodes and atoms
- coupled equilibrium equations - system energy + kinematics
- generalized Cauchy-Born rule - alter bond density to compensate for real atom-ghost atom bonds

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