Banff International Research Station
for Mathematical Innovation and Discovery

A Multiscale Micromorphic Molecular Dynamics (MMMD) and Its Applications

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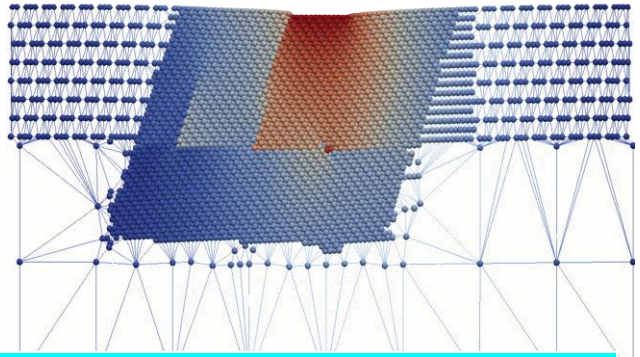
Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications, Banff, Alberta, Canada, September 1th , 2016

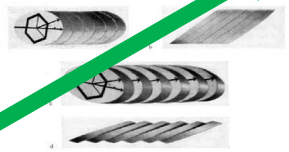
I. Introduction



- Quasi-continuum method
- Bridging scale method

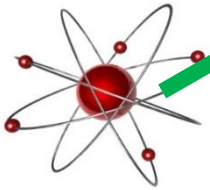
Multiscale Methods

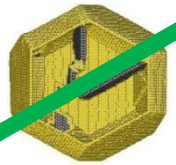
Continuum mechanics &
Mechanics of materials



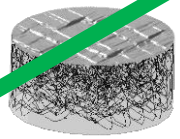
Crystal Plasticity

DFT

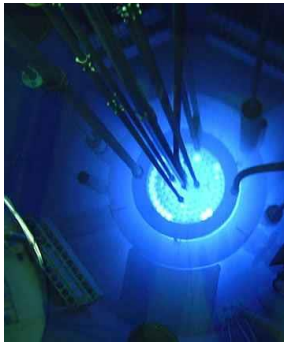


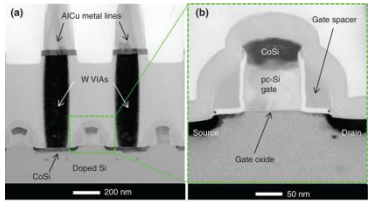


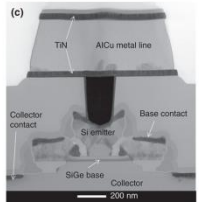
MD



DDD

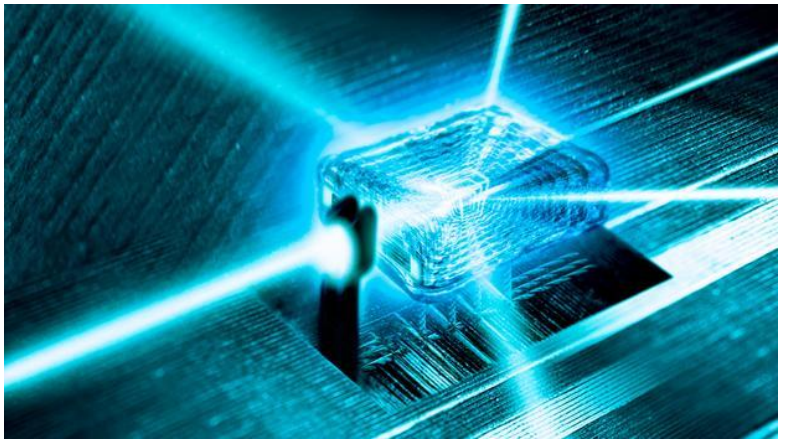






I. Is Multiscale simulation is a science ? or it is an ad hoc numerical method aiming at saving computational cost.

One day we shall have the Quantum Computer ….

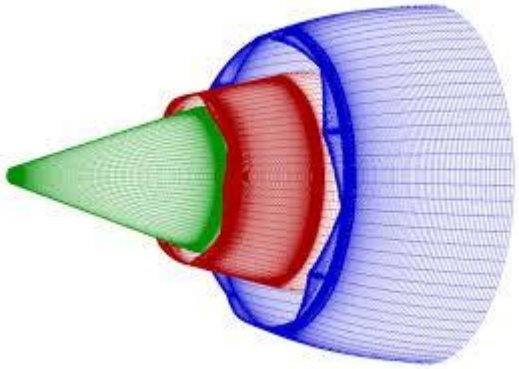


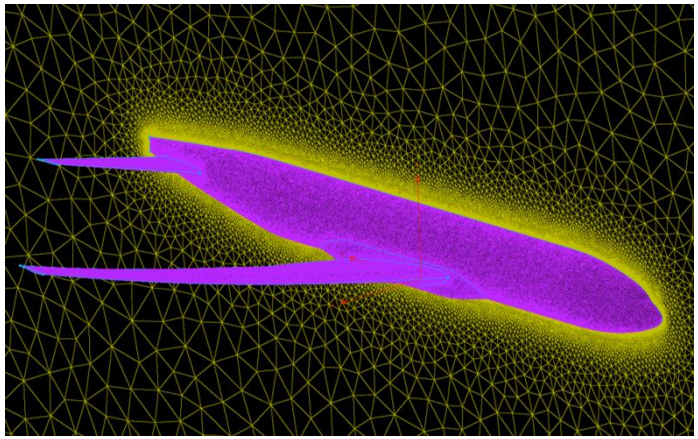
2. Can we use Molecular Dynamics to design an airplane engine ?

NO !

Why ?

Stress-strain based Design





How to link microscale MD to macroscale Thermodynamics (mechanics)?

Molecular dynamics simulations at constant pressure and/or temperature
HC Andersen - The Journal of chemical physics, 1980 - scitation.aip.org
In the molecular dynamics simulation method for fluids, the equations of motion for a collection of particles in a fixed volume are solved numerically. The energy, volume, and number of particles are constant for a particular simulation, and it is assumed that time ...
Cited by 4353 Related articles All 3 versions Cite Save

HC Andersen

Among many other things, Andersen proposed to 'scale' (multiplicative decomposition) each atom positions as

$$\mathbf{r}_I = \Omega^{1/3}(t)\mathbf{s}_I(t) \ .$$

At the initial coarse scale time,

$$\mathbf{R}_I = \Omega(0) \cdot \mathbf{s}_I(t'), \quad t' \text{the time here is fine scale time.}$$

By doing so, he was able to introduce macroscale pressure p as the work conjugate of Ω for an equilibrium MD ensemble.

The NPT ensemble MD

Parrinello-Rahman Molecular Dynamics

Polymorphic transitions in **single crystals**: A new molecular dynamics method
M Parrinello, A Rahman - Journal of Applied physics, 1981 - scitation.aip.org
A new Lagrangian formulation is introduced. It can be used to make molecular dynamics (MD) calculations on systems under the most general, externally applied, conditions of stress. In this formulation the MD cell shape and size can change according to dynamical ...
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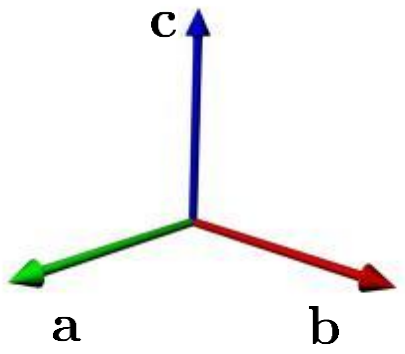


Let $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are three position vectors representing the three sides of the MD cell.

We form a second order tensor $\mathbf{h}$ by

$$\mathbf{h} = [\mathbf{a}|\mathbf{b}|\mathbf{c}] = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix} .$$

or

$$\mathbf{h} = (a_i\delta_{j1} + b_i\delta_{j2} + c_i\delta_{j3})\mathbf{e}_i \otimes \mathbf{i}_j \ .$$

We let

$$h_{i1} = a_i, \ h_{i2} = b_i, \ \text{and} \ h_{i3} = c_i, \quad \text{we have}$$

$$\mathbf{h} = h_{ij}\mathbf{e}_i \otimes \mathbf{i}_j, \quad \text{and} \ \Omega = \det\{\mathbf{h}\} \ .$$

and $\mathbf{h}_1 = \mathbf{a} = h_{i1}\mathbf{e}_i, \mathbf{h}_2 = \mathbf{b} = h_{i2}\mathbf{e}_i$, and $\mathbf{h}_3 = \mathbf{c} = h_{i3}\mathbf{e}_i$.

Parinello and Rahman proposed the following 'scaling' (multiplicative decomposition) on atomic positions:

$$\mathbf{r}_I(t) = \mathbf{h}(t) \cdot \mathbf{s}_I(t), \quad \text{or} \quad \mathbf{s}_I = \mathbf{h}^{-1} \cdot \mathbf{r}_I \; ; \quad (\text{Cf Andersen's}) \quad \mathbf{r}_I = \Omega^{1/3} \mathbf{s}_I$$

$$\mathcal{L} = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i - \frac{1}{2} \sum_i \sum_{j \neq i} \phi(r_{ij}) \quad \Rightarrow \quad m_i \ddot{\mathbf{r}}_i = - \sum_{j=1}^{N} \phi'(r_{ij}) \frac{\mathbf{r}_{ji}}{r_{ij}}$$

$$\mathcal{L}_{PR} = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{\mathbf{s}}_i \cdot \mathbf{G} \cdot \dot{\mathbf{s}}_i - \frac{1}{2} \sum_i \sum_{j \neq i} \phi(r_{ij}) + \frac{1}{2} W Tr(\dot{\mathbf{h}}^T \cdot \dot{\mathbf{h}}) - p\Omega \, ,$$

where $\mathbf{G} = \mathbf{h}^T \cdot \mathbf{h}$; $\frac{1}{2} W Tr(\dot{\mathbf{h}}^T \cdot \dot{\mathbf{h}}) = \frac{W}{2}(\dot{\mathbf{a}}^2 + \dot{\mathbf{b}}^2 + \dot{\mathbf{c}}^2)$ and $W = Tr\Big(\sum_i m_i \mathbf{s}_i \otimes \mathbf{s}_i \Big)$.

The Lagrangian equations for the Parrinello-Rahman MD:

$$\begin{aligned} \ddot{\mathbf{s}}_i &= - \sum_{j \neq i} \Big(\frac{\phi'(r_{ij})}{m_i r_{ij}} \Big) (\mathbf{s}_i - \mathbf{s}_j) - \mathbf{G}^{-1} \dot{\mathbf{G}} \dot{\mathbf{s}}_i, \\ W \ddot{\mathbf{h}} &= - (\boldsymbol{\sigma}_{virial} + p\mathbf{I}) \cdot \boldsymbol{\Pi} \end{aligned}$$

where the Virial stress,

$$\boldsymbol{\sigma}_{virial} = \frac{1}{\Omega} \sum_I \left\{ -m_I \mathbf{v}_I \otimes \mathbf{v}_I + \frac{1}{2} \sum_{I \neq J} \Big(\frac{\phi'(r_{IJ})}{r_{IJ}} \Big) \mathbf{r}_{IJ} \otimes \mathbf{r}_{IJ} \right\}$$

Parrinello-Rahman's (NσH) extended Lagrangian:

$$\mathcal{L}_{PR} = \frac{1}{2}\sum_{i=1}^{N} m_i \dot{\mathbf{s}}_i \cdot \mathbf{G} \cdot \dot{\mathbf{s}}_i - \frac{1}{2}\sum_i \sum_{j\neq i} \phi(r_{ij}) + \frac{1}{2} W \mathrm{Tr}(\dot{\mathbf{h}}^T \dot{\mathbf{h}}) - p\Omega - \frac{1}{2}\mathrm{Tr}(\boldsymbol{\Sigma} \cdot \mathbf{G})$$

where

$$\boldsymbol{\Sigma} = \mathbf{h}_0^{-1} \cdot (\mathbf{S} - p\mathbf{I}) \cdot \mathbf{h}_0^{-T} \Omega_0, \quad \mathbf{G} = \mathbf{h}^T \cdot \mathbf{h} \ .$$

Parrinello-Rahman MD:

$$\ddot{\mathbf{s}}_i = -\sum_{j\neq i} \left(\frac{\phi^{'}(r_{ij})}{m_i r_{ij}} \right) (\mathbf{s}_i - \mathbf{s}_j) - \mathbf{G}^{-1}\dot{\mathbf{G}}\dot{\mathbf{s}}_i,$$

$$W\ddot{\mathbf{h}} = (\boldsymbol{\tau} + p\mathbf{I})\boldsymbol{\Pi} - \Omega_0 \mathbf{h} \cdot \boldsymbol{\Sigma} \ , \quad \text{with} \quad \boldsymbol{\Pi} = \Omega^{-1}\mathbf{h}^{-T} \ .$$

By the way, this is NOT 100/% correct !

$$\boldsymbol{\tau} = J\boldsymbol{\sigma}$$

and

$$\boldsymbol{\tau} = \frac{1}{\Omega}\sum_{i=1}^{N} \left\{ m_i \mathbf{v}_i \otimes \mathbf{v}_i - \sum_{j\neq i} \phi^{'}(r_{ij}) \frac{\mathbf{r}_{ij} \otimes \mathbf{r}_{ij}}{r_{ij}} \right\} \ .$$

Remark: First principle Lagrangian

$$\mathcal{L} = K - V + V^{ext}$$

$$\begin{aligned} K &= \frac{1}{2}\sum_i m_i \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i = \frac{1}{2}\sum_i m_i (\dot{\mathbf{h}}\cdot\mathbf{s}_i + \mathbf{h}\cdot\dot{\mathbf{s}}_i)\cdot(\dot{\mathbf{h}}\cdot\mathbf{s}_i + \mathbf{h}\cdot\dot{\mathbf{s}}_i) \\ &= \underbrace{\frac{1}{2}\dot{\mathbf{h}}^T\dot{\mathbf{h}} : \sum_i m_i \mathbf{s}_i \otimes \mathbf{s}_i}_{K_1} + \underbrace{\frac{1}{2}\sum_i m_i \dot{\mathbf{s}}_i \cdot \mathbf{G}\cdot\dot{\mathbf{s}}}_{K_2} \\ &\quad + \underbrace{\frac{1}{2}\dot{\mathbf{h}}^T\mathbf{h} : \sum_i m_i \mathbf{s}_i \otimes \dot{\mathbf{s}}_i}_{K_3} + \underbrace{\frac{1}{2}\mathbf{h}^T\dot{\mathbf{h}} : \sum_i m_i \dot{\mathbf{s}}_i \otimes \mathbf{s}_i}_{K_4} \end{aligned}$$

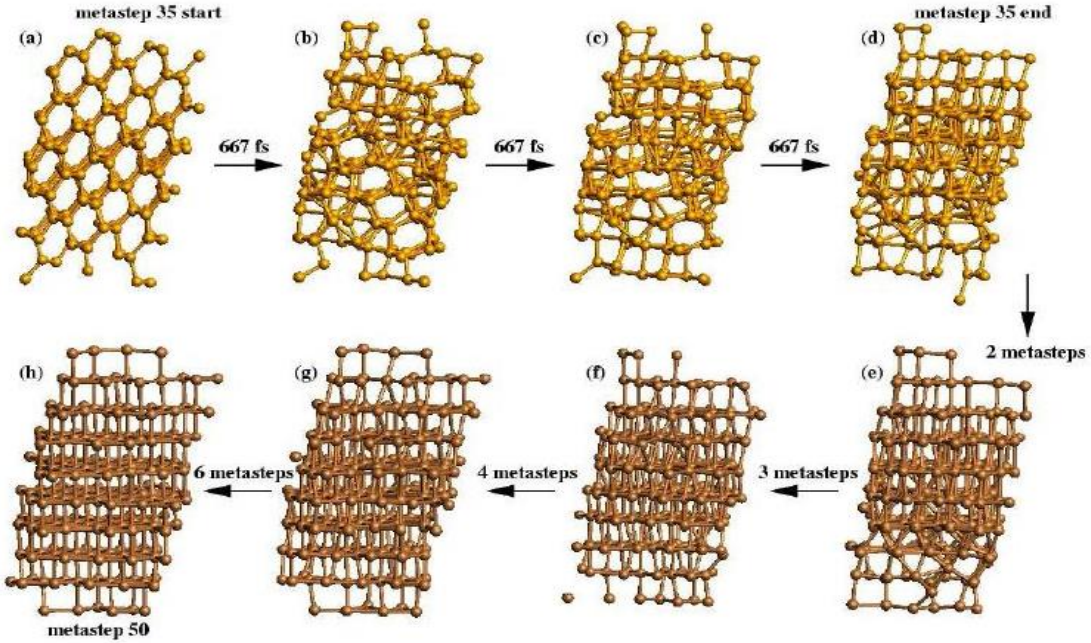
where $\mathbf{G} = \mathbf{h}^T \cdot \mathbf{h}$.

Parrinello and Rahman made the following approximation

$$K_3 \approx 0, \quad \text{and} \quad K_4 \approx 0 \ .$$

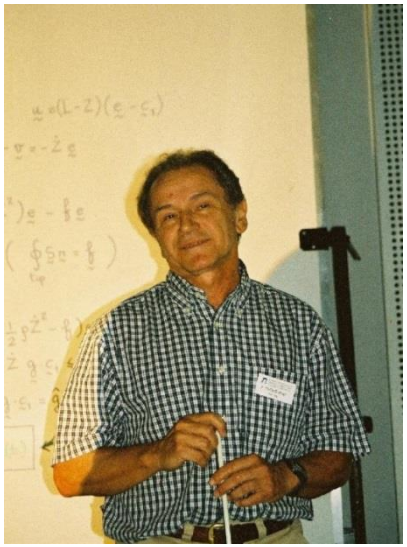
The APR-MD lagrangian has been viewed as an ad hoc choice,
as Parrinello and Rahman commented,

"..... *Whether such a Lagrangian is derivable from first principles is a question for further study; its validity can be judged, as of now, by the equations of motion and the statistical ensembles that it generates.* ....."



PR-MD can simulate the Cubic-to-Tetragonal Structure Phase Transition

Recent Developments



The (Andersen-) Parrinello-Rahman (NσH) ensemble MD was modified by Paolo Podio-Guidugli (Journal of Elasticity [2010], 145-153.)

Podio-Guidugli made the following changes:
$\mathbf{h} \to \mathbf{F}$, and $\mathbf{s}_I \to \mathbf{R}_I$ (although he still called it $\mathbf{s}_I$).

Let,

$$\mathcal{L}_{PG-PR} = \frac{1}{2}\sum_I m_I(\mathbf{F}^T \cdot \mathbf{F}) : (\dot{\mathbf{s}}_I \otimes \dot{\mathbf{s}}_I) + \frac{1}{2}W\|\dot{\mathbf{F}}\|^2 - U(\mathbf{F}\cdot\mathbf{s}_I) + \mathbf{S} : \mathbf{C}\Omega_0 \ ,$$

where $\mathbf{C} = \mathbf{F}^T \cdot \mathbf{F}$ is the right Cauchy-Green tensor.
Note that in the original paper, the last term is $\Omega_0\mathbf{S}\cdot\mathbf{F}$ may be a typo.

Consider,

$$\begin{cases} \dfrac{d}{dt}\left(\dfrac{\partial \mathcal{L}_{PG-PR}}{\partial \dot{\mathbf{s}}_I}\right) - \dfrac{\partial L_{PG-PR}}{\partial \mathbf{s}_I} = 0 \ , \\ \dfrac{d}{dt}\left(\dfrac{\partial \mathcal{L}_{PG-PR}}{\partial \dot{\mathbf{F}}}\right) - \dfrac{\partial L_{PG-PR}}{\partial \mathbf{F}} = 0 \ . \end{cases}$$

Consider,

$$\begin{cases} \dfrac{d}{dt}\left(\dfrac{\partial \mathcal{L}_{PG-PR}}{\partial \dot{\mathbf{s}}_I}\right) - \dfrac{\partial L_{PG-PR}}{\partial \mathbf{s}_I} = 0 \ , \\ \dfrac{d}{dt}\left(\dfrac{\partial \mathcal{L}_{PG-PR}}{\partial \dot{\mathbf{F}}}\right) - \dfrac{\partial L_{PG-PR}}{\partial \mathbf{F}} = 0 \ . \end{cases}$$

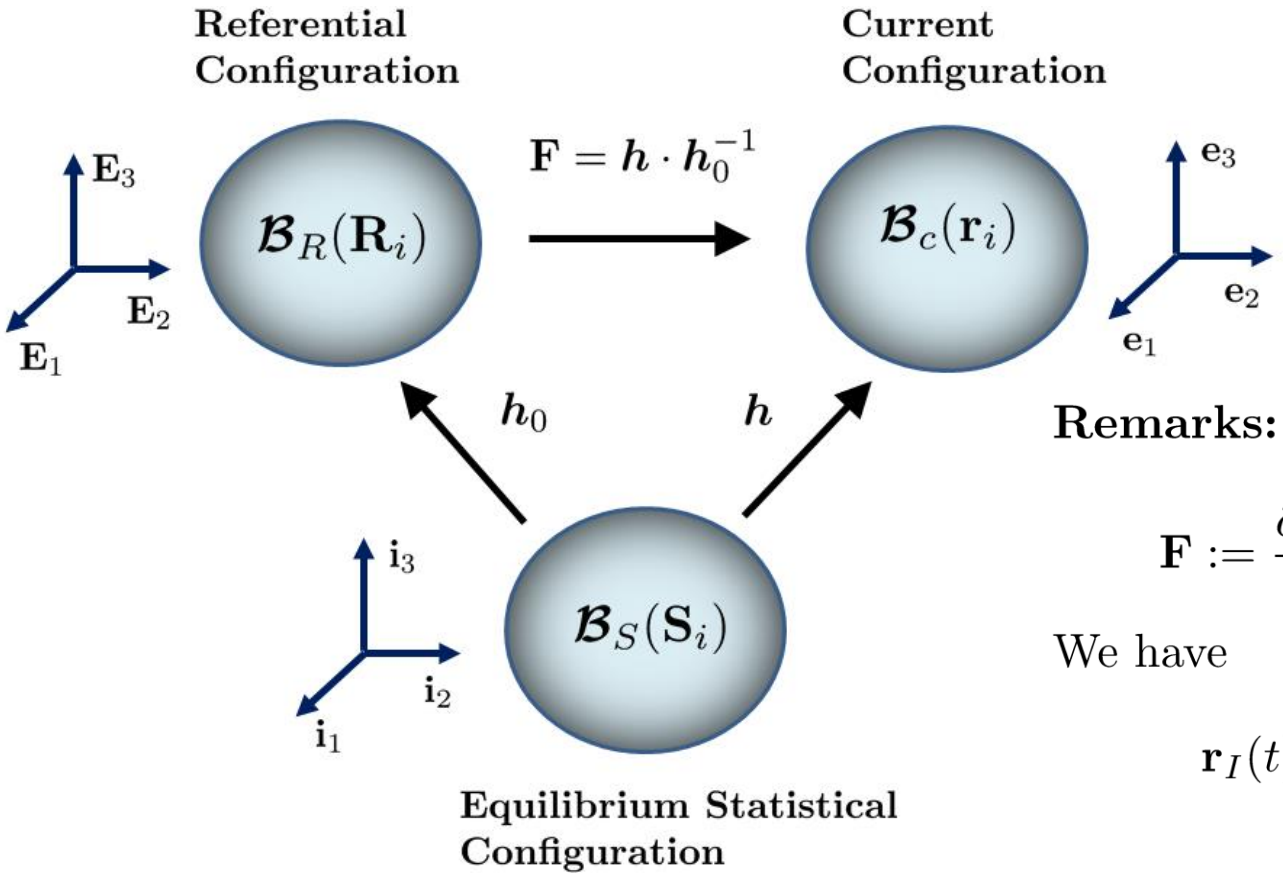
We obtain,

$$\ddot{\mathbf{s}}_I + \mathbf{C}^{-1} \cdot \dot{\mathbf{C}} \cdot \dot{\mathbf{s}}_I + \frac{1}{m_I} \sum_{J \neq I} \frac{1}{r_{IJ}} \phi^{'}(r_{IJ})(\mathbf{s}_I - \mathbf{s}_J) = 0$$

$$W\ddot{\mathbf{F}} = -\Omega_0 \mathbf{F} \cdot (\mathbf{S}_{virial} - \mathbf{S}_{ext})$$

where

$$\mathbf{S}_{virial} = \frac{1}{\Omega_0} \sum_{I=1}^{N} \left\{ -m_I \dot{\mathbf{s}}_I \otimes \dot{\mathbf{s}}_I + \sum_{J \neq I} \phi^{'}(r_{IJ})(\mathbf{s}_I - \mathbf{s}_J) \otimes (\mathbf{s}_I - \mathbf{s}_J) \right\}$$



Remarks: Define

$$\mathbf{F} := \frac{\partial \mathbf{x}(\bar{t})}{\partial \mathbf{X}},$$

We have

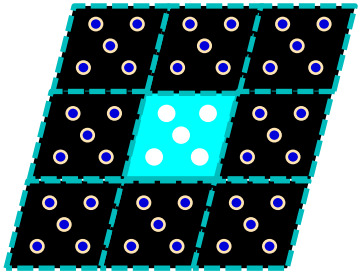
$$\begin{aligned} \mathbf{r}_I(t) &= \mathbf{F}(\bar{t}) \cdot \mathbf{R}_I(t') \\ &= \mathbf{F} \cdot \mathbf{h}_0 \cdot \mathbf{s}_I(t') \\ \rightarrow \quad & \mathbf{r}_I(t) = \mathbf{h}(\bar{t}) \cdot \mathbf{s}_I(t') \ . \end{aligned}$$

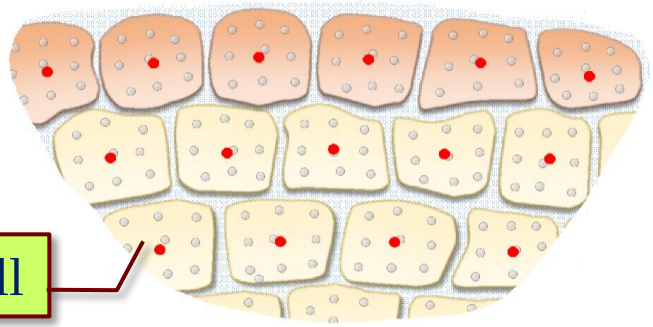
The Differential Manifold Interpretation of From Atomistic-to-Continuum MD

Multiscale Micromorphic Molecular Dynamics (MMMD)

P-R MD

MMMD





Multiscale Decomposition

$$\mathbf{r}_i = \boldsymbol{\Phi}\mathbf{S}_i$$

$$\mathbf{r}_i = \boldsymbol{\Phi}_\alpha \mathbf{S}_i + \mathbf{r}_\alpha$$

Representative unit cell
Periodic boundary condition

Individual cell has different deformation
Non-periodic, Nonequilibrium

$$\mathbf{r}_{\alpha i} = \boldsymbol{\phi}_\alpha \cdot \mathbf{S}_i \quad \text{and} \quad \boldsymbol{\phi}_\alpha := \mathbf{F}_\alpha \cdot \boldsymbol{\chi}_\alpha,$$

Multiplicative Decomposition

where $\boldsymbol{\phi}_\alpha$ is the total deformation tensor of the α-th cell, and and $\boldsymbol{\chi}_\alpha = \mathbf{h}_\alpha$.

MMMD couples three scales

1. Fine scale atomistic dynamics
2. Mesoscale micromorphic dynamics
3. Macroscale particle dynamics

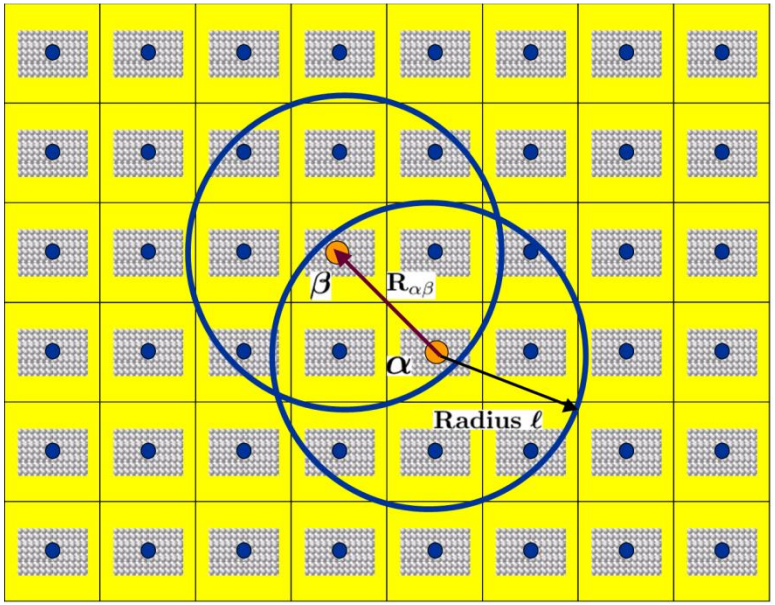
Scaled atomic coordinate $\boldsymbol{S}_i$

Cell shape $\boldsymbol{\Phi}_\alpha$

Cell center $\boldsymbol{r}_\alpha$

Multiscale Decomposition

$$\mathbf{r}_i = \mathbf{r}_\alpha + \mathbf{r}_{\alpha i}, \quad \alpha = 1, 2, \cdots M; \quad i = 1, 2, \cdots N_\alpha$$



$$\mathbf{r}_\alpha = \frac{\sum_i m_i \mathbf{r}_i}{\sum_i m_i}$$

$$\sum_i m_i \mathbf{r}_{\alpha i} = 0 \ .$$

Multiplicative Decomposition

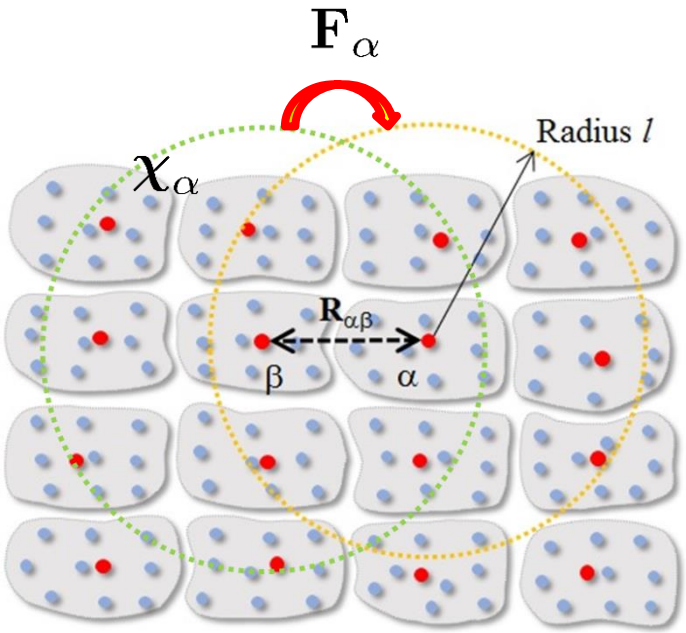
$$\mathbf{r}_{\alpha i} = \boldsymbol{\phi}_\alpha \cdot \mathbf{S}_i \quad \text{and} \quad \boldsymbol{\phi}_\alpha := \mathbf{F}_\alpha \cdot \boldsymbol{\chi}_\alpha,$$

where $\boldsymbol{\phi}_\alpha$ is the total deformation tensor of the α-th cell, and and $\boldsymbol{\chi}_\alpha = \mathbf{h}_\alpha$.

$$\mathbf{r}_{\alpha\beta} = \mathbf{r}_\beta - \mathbf{r}_\alpha, \quad \mathbf{R}_\alpha := \mathbf{r}_\alpha(0), \quad \text{and} \quad \mathbf{R}_{\alpha\beta} := \mathbf{R}_\beta - \mathbf{R}_\alpha \ .$$

$\mathbf{F}$ is determined by the positions of center of mass of MD cells.

We first define : $\mathbf{K}_\alpha = \sum_{\beta=1}^{N_h} \omega(|\mathbf{R}_{\alpha\beta}|)\mathbf{R}_{\alpha\beta} \otimes \mathbf{R}_{\alpha\beta}\Omega_{\beta 0}$



The define a two-point tensor

$$\mathbf{N} = \sum_{\beta=1}^{N_h} \omega(|\mathbf{R}_{\alpha\beta}|)\mathbf{r}_{\alpha\beta} \otimes \mathbf{R}_{\alpha\beta}\Omega_{\beta 0}$$

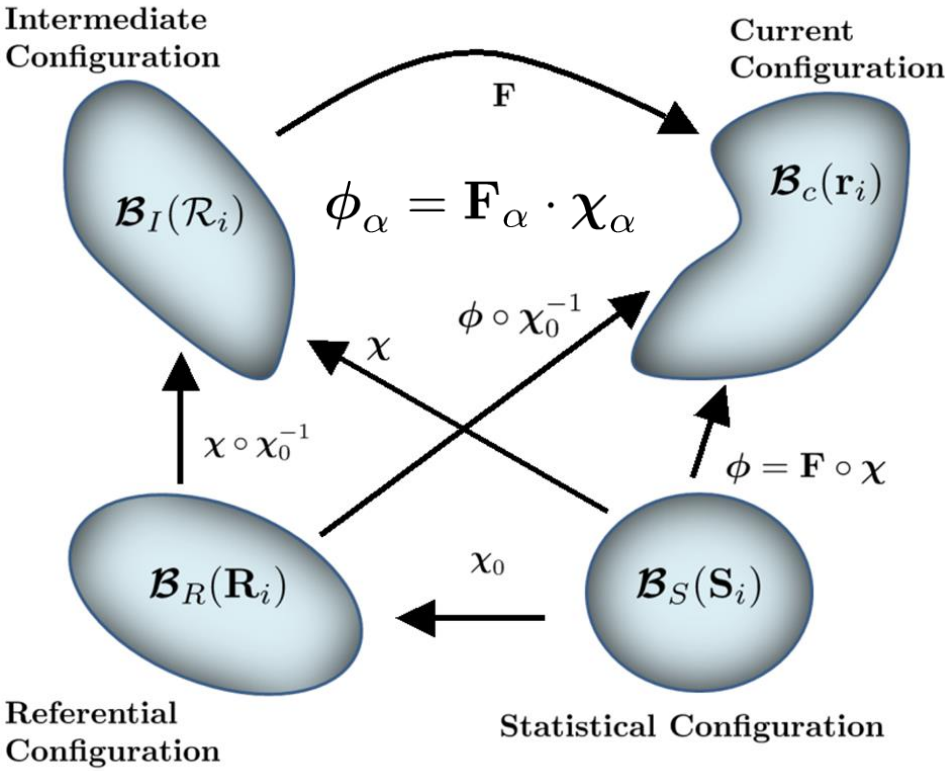
$$= \sum_{\beta=1}^{N_h} \omega(|\mathbf{R}_{\alpha\beta}|)\mathbf{F}_\alpha\mathbf{R}_{\alpha\beta} \otimes \mathbf{R}_{\alpha\beta}\Omega_{\beta 0} \ .$$

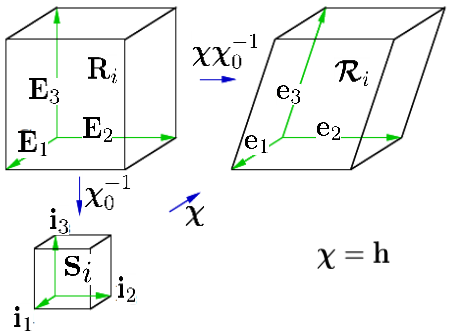
The Cauchy-Born Rule
$\mathbf{r}_{\alpha\beta} = \mathbf{F}_\alpha\mathbf{R}_{\alpha\beta};$

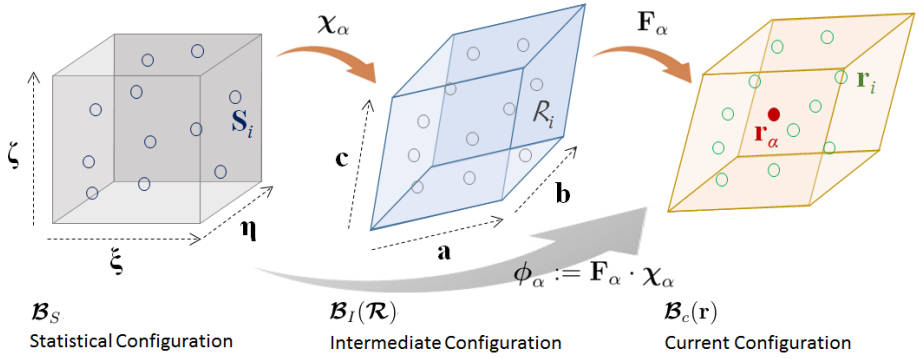
$$\mathbf{K}_\alpha = \sum_{\beta=1}^{N_h} \omega(|\mathbf{R}_{\alpha\beta}|)\mathbf{R}_{\alpha\beta} \otimes \mathbf{R}_{\alpha\beta}\Omega_{\beta 0} \quad \rightarrow \quad \mathbf{F}_\alpha = \sum_{\beta=1}^{N_h} \omega(|\mathbf{R}_{\alpha\beta}|)\mathbf{r}_{\alpha\beta} \otimes \mathbf{R}_{\alpha\beta}\Omega_{\beta 0}\Big)\mathbf{K}_\alpha^{-1}$$

$$\mathbf{r}_i = \mathbf{r}_\alpha + \mathbf{r}_{\alpha i}$$
$$= \mathbf{r}_\alpha + \mathbf{F}_\alpha \cdot \boldsymbol{\mathcal{R}}_{\alpha i}$$
$$= \mathbf{r}_\alpha + \mathbf{F}_\alpha \cdot \boldsymbol{\chi}_\alpha \mathbf{S}_i$$

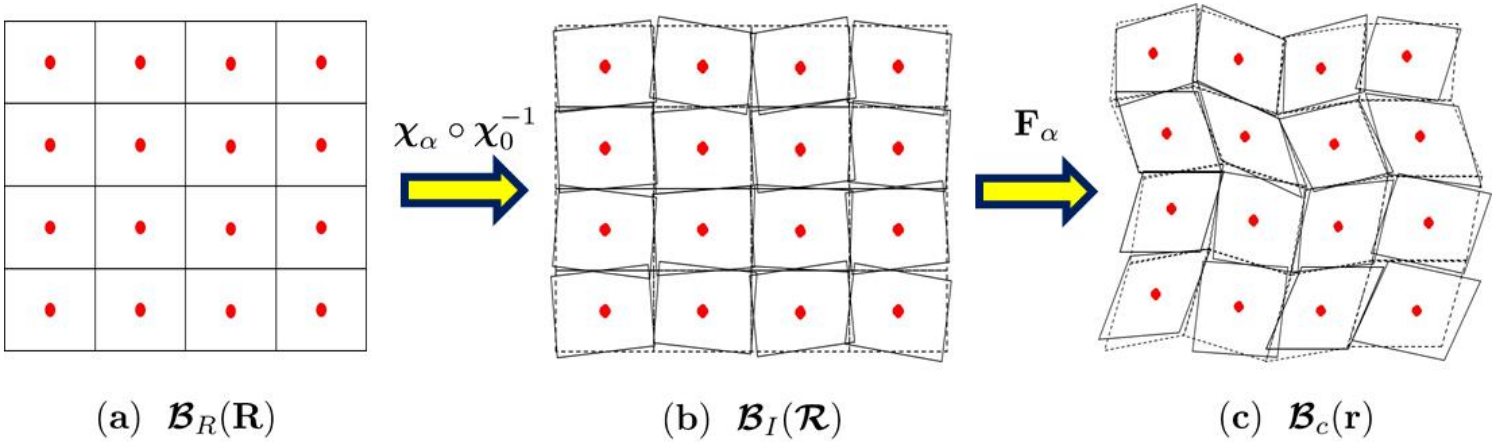
$$\boldsymbol{\mathcal{R}}_i = \mathbf{R}_\alpha + \boldsymbol{\mathcal{R}}_{\alpha i}$$
$$= \mathbf{R}_\alpha + \boldsymbol{\chi}_\alpha \cdot \mathbf{S}_i$$

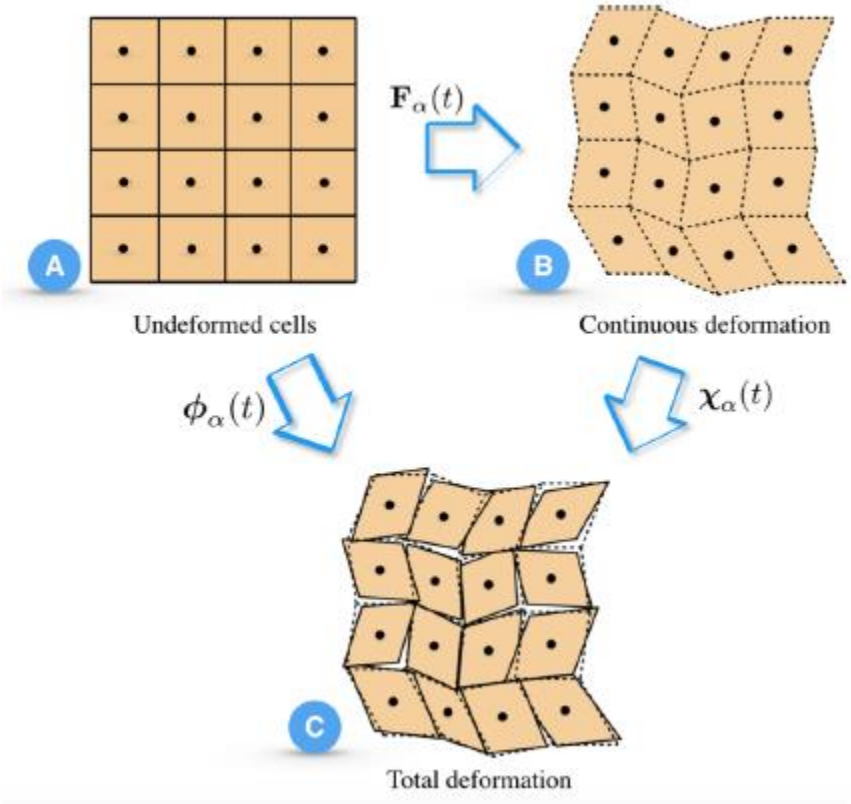


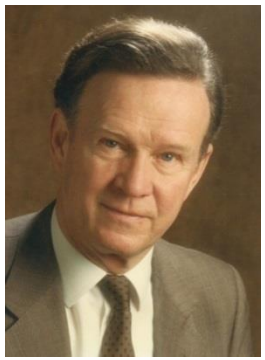




Micromorphic Multiplicative Decomposition







Recall E. Kroner's incompatible strain

Recall E. H. Lee's Decomposition

First principle Lagrangian

$$\mathcal{L}_m = \sum_\alpha K_\alpha - \sum_\alpha V_\alpha + \sum_\alpha V_\alpha^{ext}$$

Before constructing the governing equations of MMMD, we would like to revisit the statistic conditions in APR-MD and provide some explanations or interpretations. Consider the kinetic energy of the α-th cell:

$$\begin{aligned} K_\alpha &= \frac{1}{2}\sum_i m_i \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i = \frac{1}{2}\sum_i m_i (\dot{\mathbf{r}}_\alpha + \dot{\boldsymbol{\phi}}_\alpha \cdot \mathbf{S}_i + \boldsymbol{\phi}_\alpha \cdot \dot{\mathbf{S}}_i) \cdot (\dot{\mathbf{r}}_\alpha + \dot{\boldsymbol{\phi}}_\alpha \cdot \mathbf{S}_i + \boldsymbol{\phi}_\alpha \cdot \dot{\mathbf{S}}_i) \\ &= \underbrace{\frac{M_\alpha}{2}\dot{\mathbf{r}}_\alpha \cdot \dot{\mathbf{r}}_\alpha}_{K_1} + \underbrace{\frac{1}{2}\dot{\boldsymbol{\phi}}_\alpha^T \dot{\boldsymbol{\phi}}_\alpha \sum_i m_i \mathbf{S}_i \otimes \mathbf{S}_i}_{K_2} + \underbrace{\frac{1}{2}\sum_i m_i \dot{\mathbf{S}}_i \cdot \mathbf{C} \cdot \dot{\mathbf{S}}_i}_{K_3} \\ &+ \underbrace{\frac{1}{2}\dot{\boldsymbol{\phi}}_\alpha^T \boldsymbol{\phi}_\alpha \sum_i m_i \mathbf{S}_i \otimes \dot{\mathbf{S}}_i + \frac{1}{2}\boldsymbol{\phi}_\alpha^T \dot{\boldsymbol{\phi}}_\alpha \sum_i m_i \dot{\mathbf{S}}_i \otimes \mathbf{S}_i}_{K_4} \end{aligned}$$

where $M_\alpha = \sum_i m_i$ is the mass of the cell, and $\mathbf{C} = \boldsymbol{\phi}_\alpha^T \boldsymbol{\phi}_\alpha$. Introduce the following statistical assumption:

$$\begin{aligned} \mathbf{J}_\alpha^S &= \sum_i m_i \mathbf{S}_i \otimes \mathbf{S}_i = \sum_i m_i \boldsymbol{\chi}_{\alpha 0}^{-1} \cdot \mathbf{R}_{\alpha i} \otimes \mathbf{R}_{\alpha i} \cdot \boldsymbol{\chi}_{\alpha 0}^T \\ &= \boldsymbol{\chi}_{\alpha 0}^{-1} \cdot \mathbf{J}_\alpha \cdot \boldsymbol{\chi}_{\alpha 0}^{-T} = \textit{constant tensor.} \end{aligned}$$

Statistical Assumption: $\mathbf{J}^S_\alpha$ is a constant Spherical Tensor

If we choose $\mathbf{E}_I$ as principal axes, we can have a simple expression of $\mathbf{J}^S_\alpha$,

$$\mathbf{J}^S_\alpha = J^S_{11}\mathbf{E}_1 \otimes \mathbf{E}_1 + J^S_{22}\mathbf{E}_2 \otimes \mathbf{E}_2 + J^S_{33}\mathbf{E}_3 \otimes \mathbf{E}_3 \ . \tag{37}$$

Since $\mathbf{J}^S_\alpha$ is spherical, we may write $J^S_{11} = J^S_{22} = J^S_{33} = W_\alpha$. Now it becomes clear that the quantity W used in the original PR-MD is related to the component of Euler's inertia tensor. Therefore, naturally, the second term of kinetic energy becomes:

$$K_2 = \frac{1}{2} W_\alpha Tr(\dot{\phi}^T_\alpha \dot{\phi}_\alpha) \tag{38}$$

We call the expression (35) as the **First statistical condition** of APR-MD.

$$\mathbf{AC}(\tau) = < \mathbf{S}_i(t) \otimes \mathbf{S}_i(t+\tau) > := \sum_i m_i \mathbf{S}_i(t) \otimes \mathbf{S}_i(t+\tau)$$

$$\frac{d}{d\tau}\mathbf{AC}(\tau)\Big|_{\tau=0} = \sum_i m_i \mathbf{S}_i(t) \otimes \dot{\mathbf{S}}_i(t+\tau) = 0$$

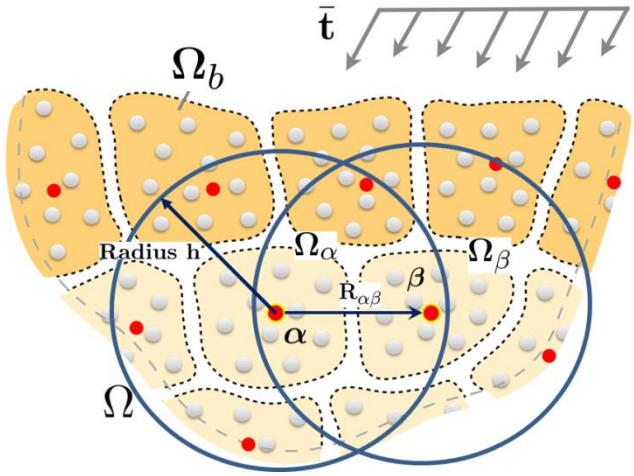
$$\text{Similarly,} \qquad \sum_i m_i \dot{\mathbf{S}}_i(t) \otimes \mathbf{S}_i = 0 \ .$$

Take into account macroscale B.C.

$$\mathcal{L}_m = \frac{1}{2}\sum_\beta M_\beta \dot{\mathbf{r}}_\beta \cdot \dot{\mathbf{r}}_\beta + \frac{1}{2}\sum_\beta \mathbf{J}^S_\beta : \left(\dot{\boldsymbol{\phi}}^T_\beta \dot{\boldsymbol{\phi}}_\beta\right)$$

$$+\frac{1}{2}\sum_\beta\sum_i m_i \dot{\mathbf{S}}_i \cdot \mathbf{C}_\beta \cdot \dot{\mathbf{S}}_i - \frac{1}{2}\sum_\beta\sum_\gamma\sum_{i\in\beta, j\in\gamma} V(r_{ij})$$

$$+\sum_\beta\sum_{i\in\beta} \mathbf{b}_i \cdot \mathbf{r}_{\beta i} + \sum_\beta S_{\beta 0}\bar{\mathbf{t}}_{\beta 0}\cdot \mathbf{r}_\beta + \sum_\beta \Omega_{\beta 0}\bar{\mathbf{b}}_{\beta 0}\cdot \mathbf{r}_\beta$$



$\mathbf{C} = \boldsymbol{\phi}^T_\alpha \boldsymbol{\phi}_\alpha$. Introduce the following statistical assumption:

$$\mathbf{J}^S_\alpha = \sum_i m_i \mathbf{S}_i \otimes \mathbf{S}_i = \sum_i m_i \boldsymbol{\chi}^{-1}_{\alpha 0}\cdot \mathbf{R}_{\alpha i} \otimes \mathbf{R}_{\alpha i}\cdot \boldsymbol{\chi}^{-T}_{\alpha 0}$$

$$= \boldsymbol{\chi}^{-1}_{\alpha 0}\cdot \mathbf{J}_\alpha \cdot \boldsymbol{\chi}^{-T}_{\alpha 0} = \textit{constant tensor}.$$

$$\boldsymbol{\phi}_\alpha = \mathbf{F}_\alpha \cdot \boldsymbol{\chi}_\alpha,$$

$$\mathbf{J}^S_\alpha = J^S_{11}\mathbf{E}_1 \otimes \mathbf{E}_1 + J^S_{22}\mathbf{E}_2 \otimes \mathbf{E}_2 + J^S_{33}\mathbf{E}_3 \otimes \mathbf{E}_3$$

Thus $\mathcal{L}_m = \mathcal{L}_m\ (\mathbf{r}_\alpha, \boldsymbol{\phi}_\alpha, \mathbf{S}_i).$

This derivation is both brilliant and splendid !

$$\frac{d}{dt}\frac{\partial \mathcal{L}_m}{\partial \dot{\mathbf{r}}_\alpha} - \frac{\partial \mathcal{L}_m}{\partial \mathbf{r}_\alpha} = 0, \quad \Rightarrow \quad M_\alpha \ddot{\mathbf{r}}_\alpha = \sum_{\beta\neq\alpha}\sum_{i\in\alpha, j\in\beta} \mathbf{f}_{ij} + S_{\alpha 0}\bar{\mathbf{t}}_{\alpha 0} + \Omega_{\alpha 0}\bar{\mathbf{b}}_{\alpha 0}.$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}_m}{\partial \dot{\boldsymbol{\phi}}_\alpha} - \frac{\partial \mathcal{L}_\alpha}{\partial \boldsymbol{\phi}_\alpha} = 0, \quad \Rightarrow \quad \ddot{\boldsymbol{\phi}}_\alpha \cdot \mathbf{J}_\alpha^S = -(\mathcal{P}_\alpha^{int} - \mathcal{P}_\alpha^{ext})\Omega_{\alpha 0} + \mathcal{M}_\alpha,$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}_m}{\partial \dot{\mathbf{S}}_i} - \frac{\partial \mathcal{L}_\alpha}{\partial \mathbf{S}_i} = 0\,. \quad \Rightarrow \quad m_i\ddot{\mathbf{S}}_i = -m_i\mathbf{C}_\alpha^{-1}\cdot\dot{\mathbf{C}}_\alpha\cdot\dot{\mathbf{S}}_i + \boldsymbol{\phi}_\alpha^{-1}\left(\sum_\beta \sum_{j\in\beta\neq i\in\alpha} \mathbf{f}_{ji} + \mathbf{b}_i\right)$$

$$\mathcal{P}_\alpha^{int} := \frac{1}{\Omega_{\alpha 0}}\sum_{i\in\alpha}\left(-\boldsymbol{\phi}_\alpha m_i \dot{\mathbf{S}}_i \otimes \dot{\mathbf{S}}_i + \frac{1}{2}\sum_{j\in\alpha, j\neq i}\mathbf{f}_{ij}\otimes\mathbf{S}_{ij}\right),$$

$$\mathcal{P}_\alpha^{ext} = \frac{1}{\Omega_{\alpha 0}}\sum_{\beta\neq\alpha}\sum_{i\in\alpha, j\in\beta}\mathbf{f}_{ij}\otimes\mathbf{S}_i$$

Virial Stress

$$\sigma_\alpha^{ext} = \frac{1}{\Omega_\alpha}\sum_{\beta\neq\alpha}\sum_{i\in\alpha, j\in\beta}\mathbf{f}_{ij}\otimes\mathbf{r}_{\alpha i}$$

$$= \frac{1}{det(\boldsymbol{\phi}_\alpha)\Omega_{\alpha 0}}\sum_{\beta\neq\alpha}\sum_{i\in\alpha, j\in\beta}\mathbf{f}_{ij}\otimes\mathbf{S}_i\cdot\boldsymbol{\phi}_\alpha^T,$$

$$\mathcal{P}_\alpha^{int} = det(\boldsymbol{\phi}_\alpha)\boldsymbol{\sigma}_\alpha^{int}\boldsymbol{\phi}_\alpha^{-T} \qquad \mathcal{P}_\alpha^{ext} = det(\boldsymbol{\phi}_\alpha)\boldsymbol{\sigma}_\alpha^{ext}\cdot\boldsymbol{\phi}_\alpha^{-T}\,.$$

The derivation is non-trivial: (Li and Tong [2015] **JAP**)

It is the journey not the destination that matters.

$$\mathcal{R}_{\alpha i} = \boldsymbol{\chi}_\alpha \cdot \mathbf{S}_i,$$

that if the length of $\mathbf{S}_i$ *is not fixed,* $\boldsymbol{\chi}_\alpha$ *may not represent the shape tensor of the* α*th cell. Therefore, we must have the constraint condition,*

$$\sum_i \mathbf{S}_i \cdot \mathbf{S}_i = const, \tag{42}$$

which is a weaker condition than conditions (40) and (41).

By utilizing above statistical conditions, we can conveniently write down the Lagrangian of the atomic system as,

$$\begin{aligned}\mathcal{L}_m = &\frac{1}{2}\sum_\beta M_\beta \dot{\mathbf{r}}_\beta \cdot \dot{\mathbf{r}}_\beta + \frac{1}{2}\sum_\beta \mathbf{J}^S_\beta : \left(\dot{\boldsymbol{\phi}}^T_\beta \dot{\boldsymbol{\phi}}_\beta\right) \\ &+ \frac{1}{2}\sum_\beta \sum_i m_i \dot{\mathbf{S}}_i \cdot \mathbf{C}_\beta \cdot \dot{\mathbf{S}}_i \\ &- \frac{1}{2}\sum_\beta \sum_\gamma \sum_{i\in\beta, j\in\gamma} V(r_{ij}) + \sum_\beta \sum_{i\in\beta} \mathbf{b}_i \cdot \mathbf{r}_i,\end{aligned} \tag{43}$$

where β, γ are cell indices, and the abbreviation $i \in \beta$ means

$$\frac{d}{dt}\left(= M_\alpha \ddot{\mathbf{r}}_\alpha + \sum_\beta \frac{\partial \mathcal{L}_m}{\partial \boldsymbol{\phi}_\beta} \cdot \frac{\partial \boldsymbol{\phi}_\beta}{\partial \mathbf{r}_\alpha} + \sum_\beta \frac{\partial \mathcal{L}_m}{\partial \dot{\boldsymbol{\phi}}_\beta} \cdot \frac{\partial \dot{\boldsymbol{\phi}}_\beta}{\partial \mathbf{r}_\alpha}.\right.$$

and

$$\ddot{\mathbf{F}}_\beta = \sum_\alpha \left(\frac{d}{dt}\left(\frac{\partial \mathbf{F}_\beta}{\partial \mathbf{r}_\alpha}\right)\dot{\mathbf{r}}_\alpha + \frac{\partial \mathbf{F}_\beta}{\partial \mathbf{r}_\alpha}\ddot{\mathbf{r}}_\alpha\right).$$

On the other hand, we may derive,

$$\ddot{\mathbf{F}}_\beta = \sum_\alpha \left(\frac{\partial \dot{\mathbf{F}}_\beta}{\partial \mathbf{r}_\alpha}\dot{\mathbf{r}}_\alpha + \frac{\partial \dot{\mathbf{F}}_\beta}{\partial \dot{\mathbf{r}}_\alpha}\ddot{\mathbf{r}}_\alpha\right).$$

Comparing Eqs. (51) and (52) and utilizing Eq. (50) obtain

$$\frac{d}{dt}\left(\frac{\partial \mathbf{F}_\beta}{\partial \mathbf{r}_\alpha}\right) = \frac{\partial \dot{\mathbf{F}}_\beta}{\partial \mathbf{r}_\alpha}.$$

Furthermore, since

$$\dot{\boldsymbol{\phi}}_\beta = \dot{\mathbf{F}}_\beta \boldsymbol{\chi}_\beta + \mathbf{F}_\beta \cdot \dot{\boldsymbol{\chi}}_\beta,$$

we can find that

$$\frac{\partial \dot{\boldsymbol{\phi}}_\beta}{\partial \dot{\mathbf{r}}_\alpha} = \frac{\partial \dot{\mathbf{F}}_\beta}{\partial \dot{\mathbf{r}}_\alpha}\boldsymbol{\chi}_\beta = \frac{\partial \mathbf{F}_\beta}{\partial \mathbf{r}_\alpha}\boldsymbol{\chi}_\beta = \frac{\partial \boldsymbol{\phi}_\beta}{\partial \mathbf{r}_\alpha}.$$

$$\beta \quad \partial \boldsymbol{\phi}_\beta \quad \partial \mathbf{r}_\alpha$$

$$= \sum_{\beta\neq\alpha}\sum_{i\in\alpha, j\in\beta} V'(r_{ij})\frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} + \sum_{i\in\alpha}\mathbf{b}_i$$

$$+ \sum_\beta \frac{\partial \mathcal{L}_m}{\partial \boldsymbol{\phi}_\beta} \cdot \frac{\partial \boldsymbol{\phi}_\beta}{\partial \mathbf{r}_\alpha} + \sum_\beta \frac{\partial \mathcal{L}_m}{\partial \dot{\boldsymbol{\phi}}_\beta} \cdot \frac{\partial \dot{\boldsymbol{\phi}}_\beta}{\partial \mathbf{r}_\alpha}.$$

MMMD Computational Algorithm (Li and Urata [2016] **CMAME**)

$$\mathbf{G_1} := \sum_i m_i \mathbf{S}_i; \quad \mathbf{G_2} := \mathbf{J}^S_\alpha(t) - \mathbf{J}^S_\alpha(0), \text{ and } \mathbf{G_3} := \mathrm{diag}(\mathbf{J}^S_\alpha(t)) - \mathrm{Tr}(\mathbf{J}^S_\alpha(0))\mathrm{diag}(\mathbf{I}^{(2)})$$

These constraints can be enforced by the Lagrangian multiplier method,

$$\mathcal{L}^*_\alpha = \mathcal{L}_\alpha - \boldsymbol{\lambda}_{\alpha 1} \cdot \mathbf{G}_{\alpha 1} - \boldsymbol{\lambda}_{\alpha 2} : \mathbf{G}_{\alpha 2} - \boldsymbol{\lambda}_{\alpha 3} \cdot \mathbf{G}_{\alpha 3} \quad \text{and} \quad \mathcal{L}^*_m = \sum_\alpha \mathcal{L}^*_\alpha \ ,$$

where $\boldsymbol{\lambda}_{\alpha 1}$ and $\boldsymbol{\lambda}_{\alpha 3}$ are vector multipliers, and $\boldsymbol{\lambda}_{\alpha 2}$ is a tensorial multiplier.

$$\mathbf{S}^{(c1)}_i(t+\Delta t) = 2\mathbf{S}_i(t) - \mathbf{S}_i(t-\Delta t) + \frac{\Delta t^2}{2m_i}\left(\mathbf{F}^{(c)}_i + \mathbf{F}^{(p)}_i\right) \tag{81}$$

$$\mathbf{S}^{(c2)}_i(t+\Delta t) = \mathbf{S}^{(c1)}_i(t+\Delta t) - \Delta t^2 \mathbf{C}^{-1}_\alpha(t) \cdot \boldsymbol{\lambda}^{(c)}_{\alpha 1}(\Delta t) \tag{82}$$

$$\mathbf{S}^{(c3)}_i(t+\Delta t) = \mathbf{S}^{(c2)}_i(t+\Delta t) - \Delta t^2 \mathbf{C}^{-1}_\alpha(t) \cdot \boldsymbol{\lambda}^{(c)}_{\alpha 2}(\Delta t) \cdot \mathbf{S}^{(c2)}_i(t+\Delta t) \ , \tag{83}$$

where the superscript "c" means the corrector phase, and the predicted velocity value is

$$\dot{\mathbf{S}}^{(c)}_i = \frac{\mathbf{S}^{(p3)}_i(t+\Delta t) - \mathbf{S}_i(t)}{\Delta t} \ \rightarrow \ \mathbf{F}^{(c)}_i := -m_i \mathbf{C}^{-1}_\alpha \cdot \dot{\mathbf{C}}_\alpha \cdot \dot{\mathbf{S}}^{(c)}_i + \phi^{-1}_\alpha \sum_\beta \sum_{\alpha_i \neq \beta_j} \mathbf{f}_{ji}(\mathbf{S}^{(p3)}_i),$$

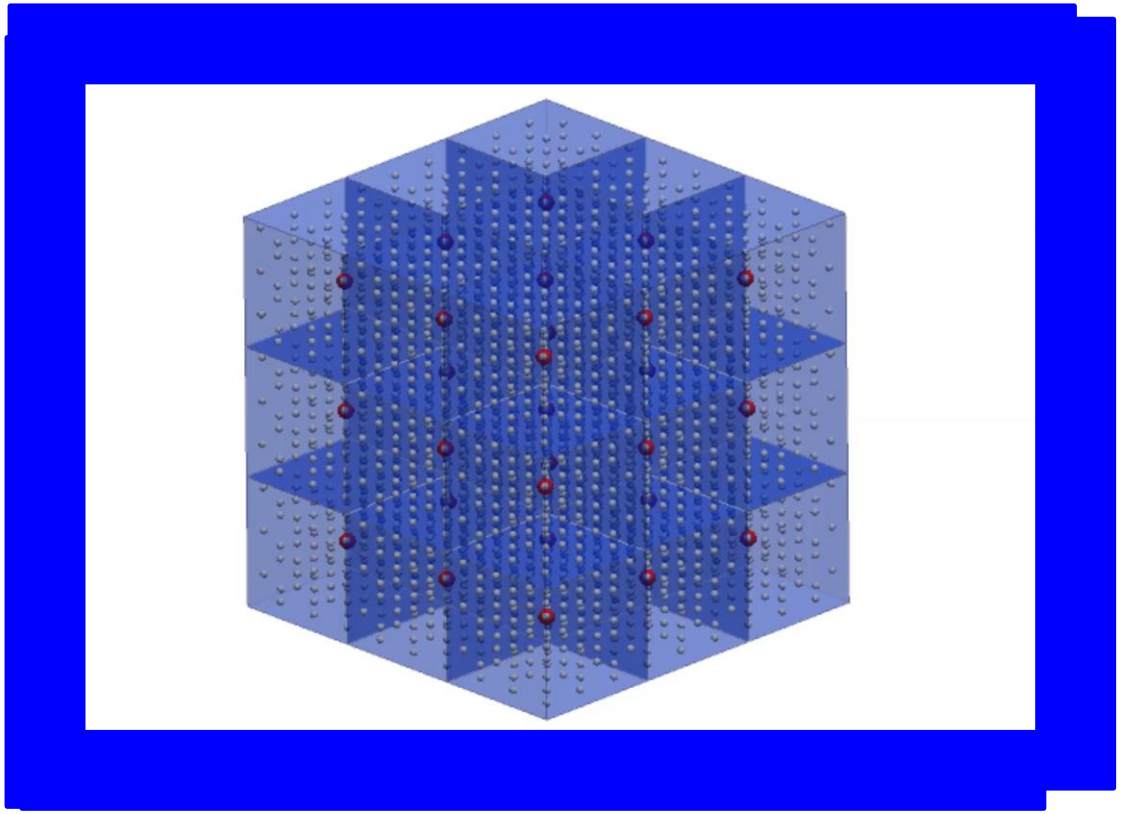
with the correction Lagrangian multipliers expressed as

$$\boldsymbol{\lambda}^{(c)}_{\alpha 1} = \mathbf{C}_\alpha(t) \cdot \left(\frac{\sum_i m_i \mathbf{S}^{(c1)}_i}{(\Delta t)^2 \left(\sum_i m_i \right)} \right), \quad \text{and} \tag{84}$$

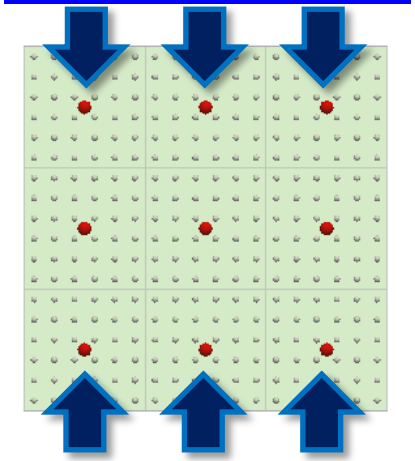
$$\boldsymbol{\lambda}^{(c)}_{\alpha 2} = \frac{1}{2(\Delta t)^2} \mathbf{C}_\alpha(t) \left\{ \sum_i m_i \mathbf{S}^{(c2)}_i \otimes \mathbf{S}^{(c2)}_i - \mathbf{J}^S_\alpha(0) \right\} \left(\sum_i m_i \mathbf{S}^{(c2)}_i \otimes \mathbf{S}^{(c2)}_i \right)^{-1} . \tag{85}$$

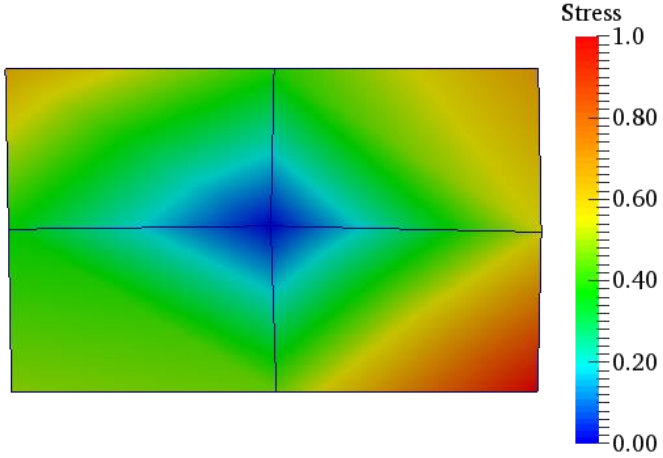
III. Validation and Numerical Examples

Ni FCC to HCP transition by compression



Displacement B.C. to cell center



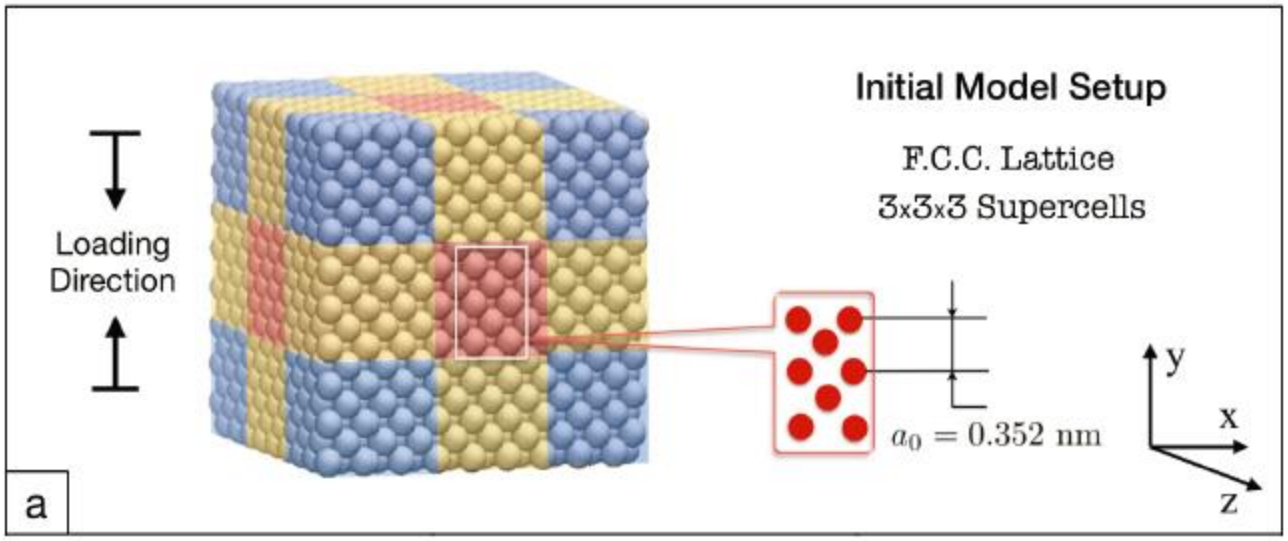


3 x 3 x 3 = 27 cells
108 atoms in each cell
2916 atoms in total.

Morse potential
350 K constant
Nose-Hoover thermostat

- Test of displacement boundary

(Tong and Li [2015] **JCP**)



Under uniaxial compression, the original FCC lattice of single crystal Nickel will go through structure change.[22,23] The interaction between atoms is modeled by Morse potential, which is plotted in Fig. 5. It has the form of

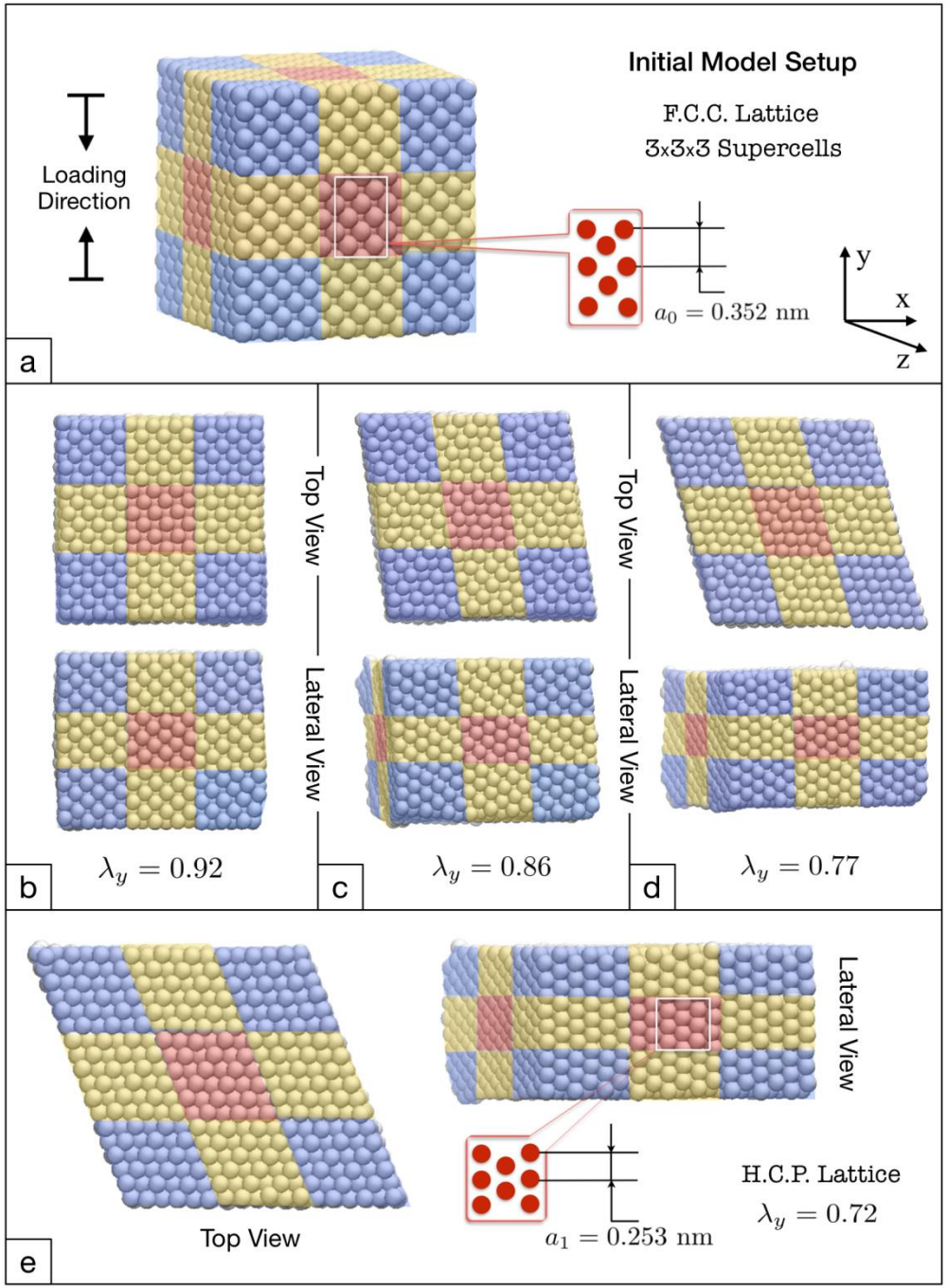
$$\phi(r) = D(e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}). \tag{85}$$

The interaction force is given by

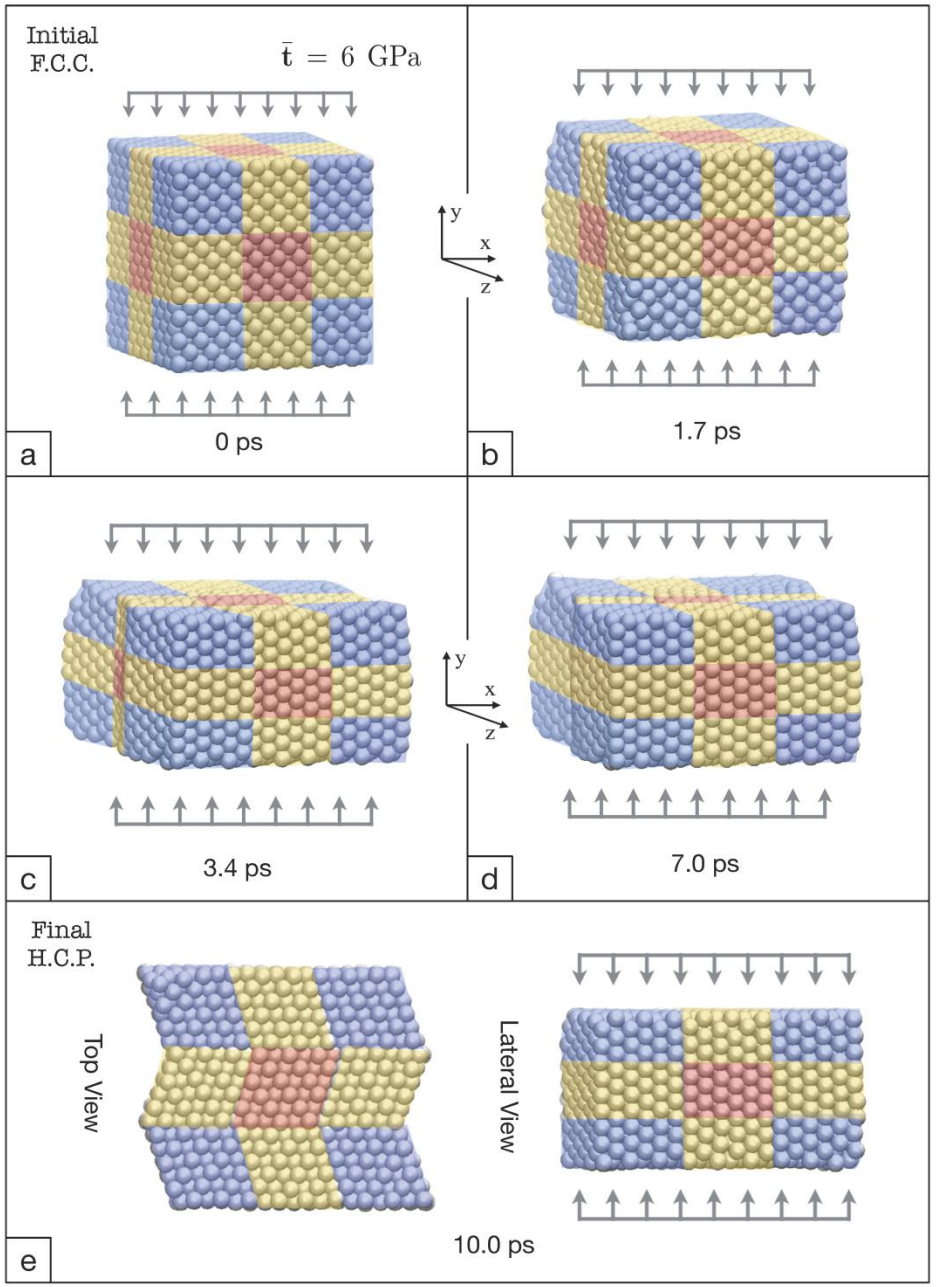
$$F(r) = -\frac{\partial\phi(r)}{\partial r} = 2D\alpha(-e^{-2\alpha(r-r_0)} + e^{-\alpha(r-r_0)}). \tag{86}$$

With the constants $D = 3.5059 \times 10^{-20}$ J, $\alpha = 8.766/a_0$, and $r_0 = 0.71727$ Å. a_0 denotes the constants of the FCC lattice of nickel, i.e., $a_0 = 3.52$ Å,[26]

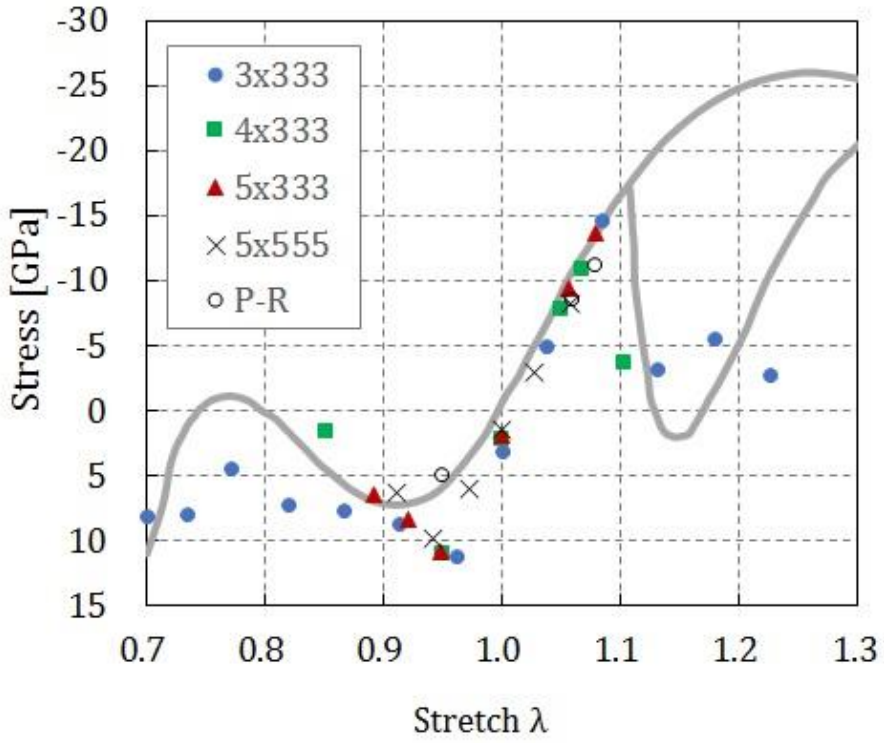
Displacement B.C.



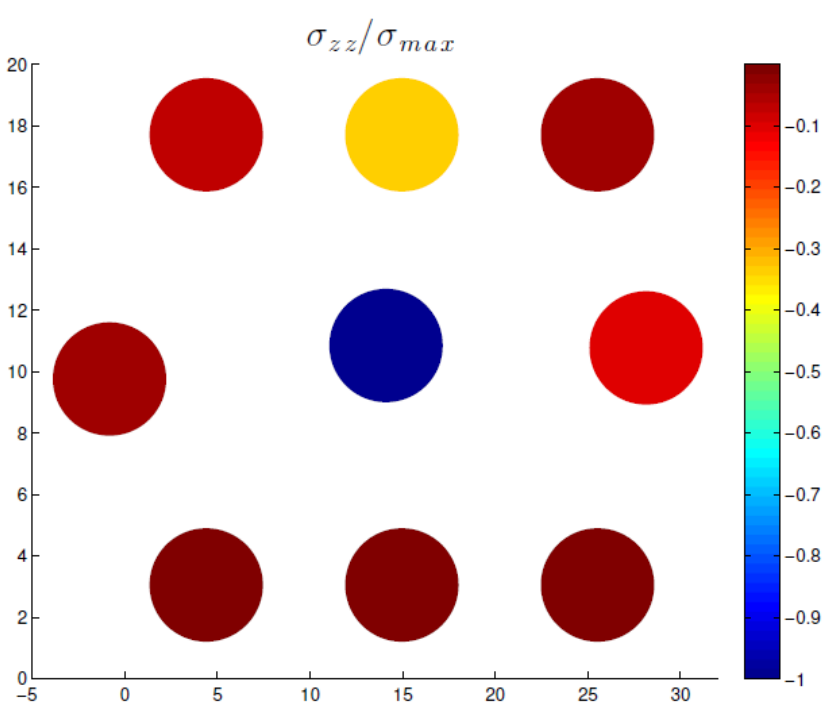
Traction B.C.

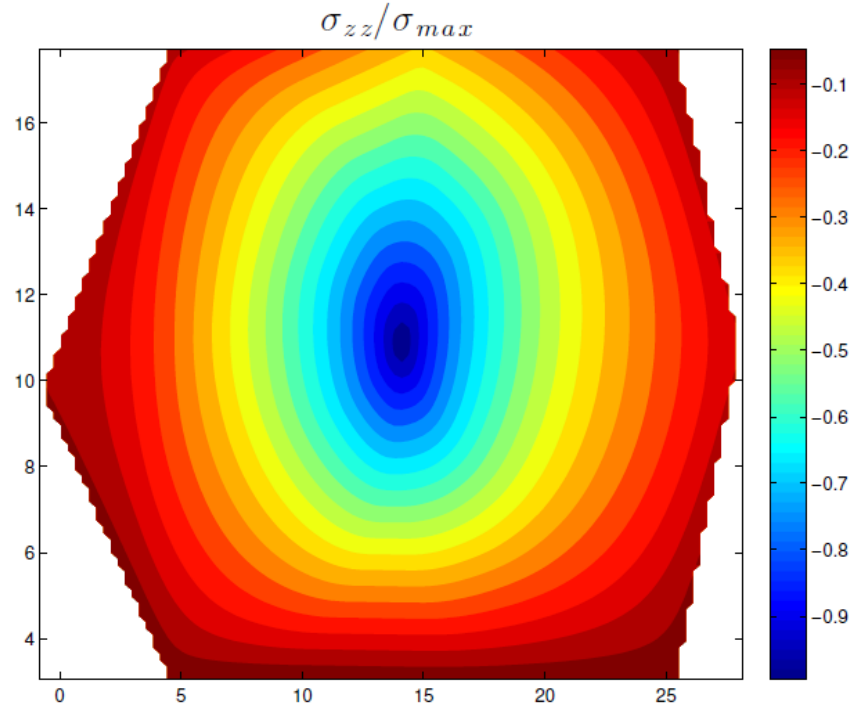

Initial
F.C.C.
$\bar{t} = 6$ GPa
y
x
z
0 ps
a
1.7 ps
b
y
x
z
3.4 ps
c
7.0 ps
d
Final
H.C.P.
Top View
Lateral View
10.0 ps
e

Supercell $3 \times 3 \times 3 = 27$ $\rightarrow$ $3 \times 3 \times 3 = 27$ unit cells
$\rightarrow$ 2916 atoms
$4 \times 4 \times 4 = 64$ $\rightarrow$ $4 \times 4 \times 4 = 64$ unit cells
$\rightarrow$ 16384 atoms
$5 \times 5 \times 5 = 125$ $\rightarrow$ $5 \times 5 \times 5 = 125$ unit cells
$\rightarrow$ 62500 atoms

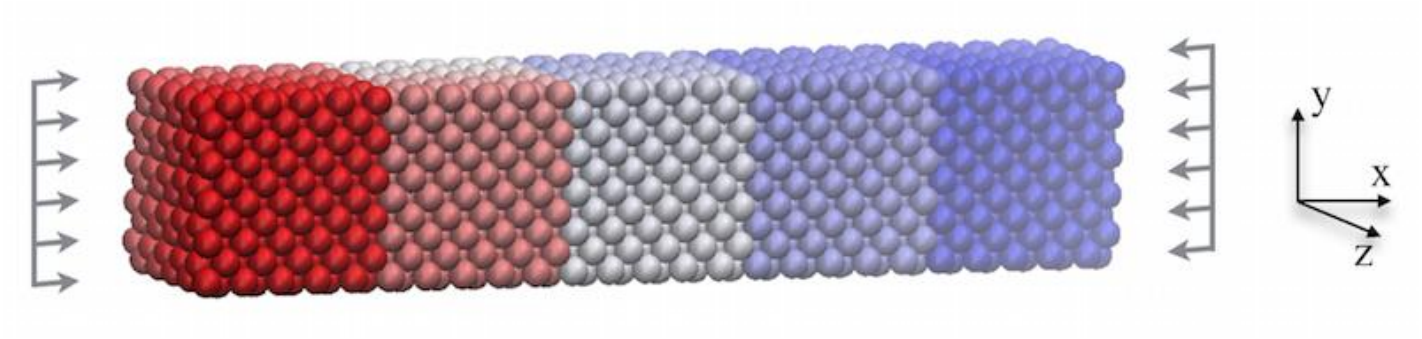


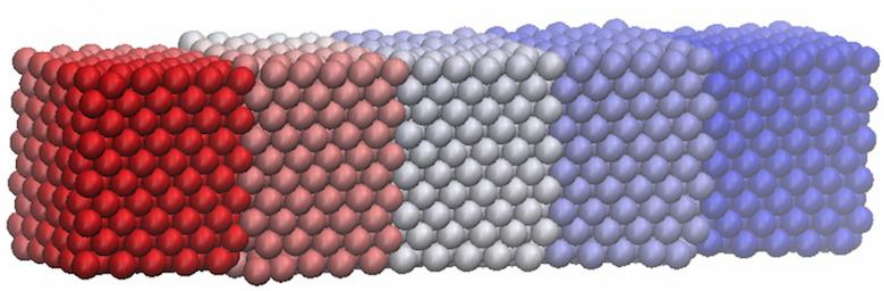
Stress Distribution

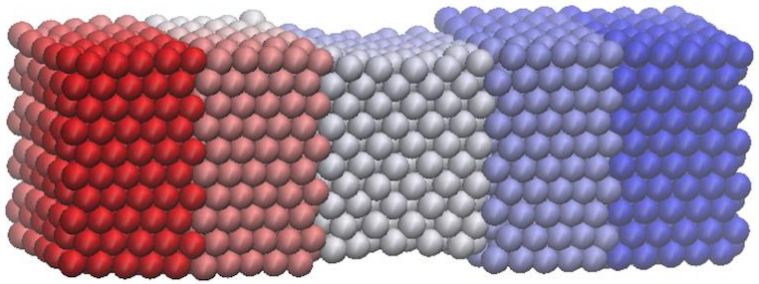


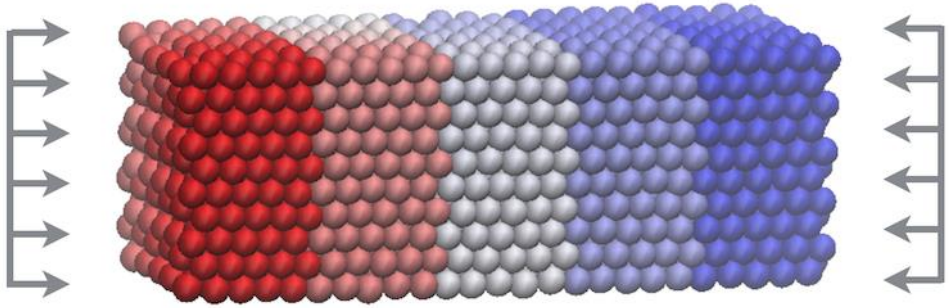


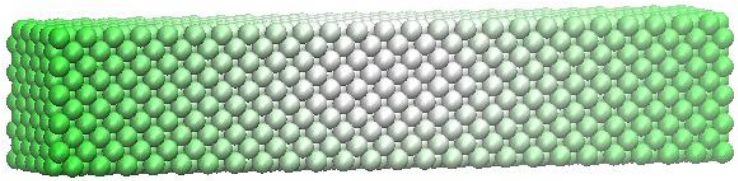
Example 2. Phase Transformation of Nano-rod

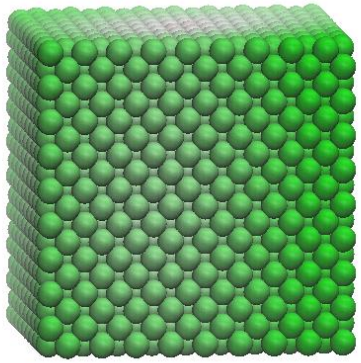




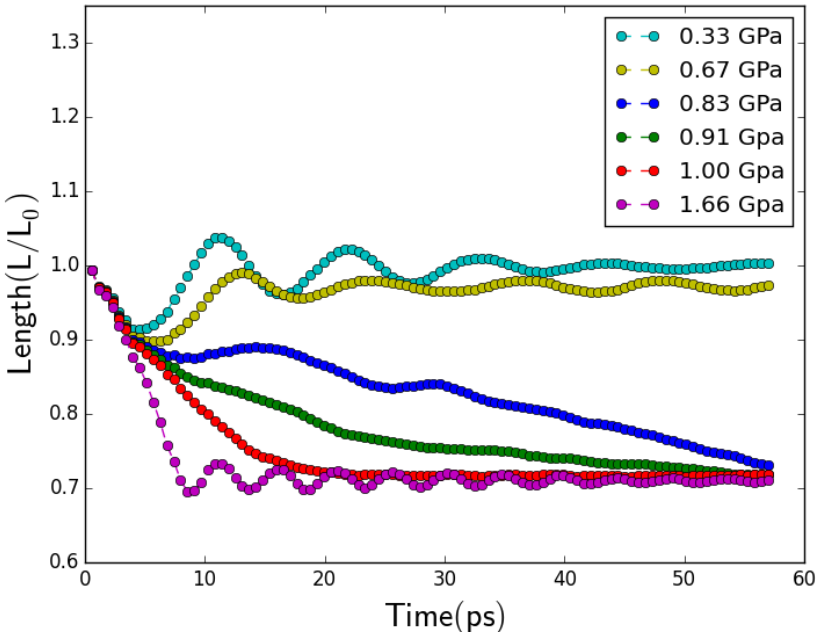


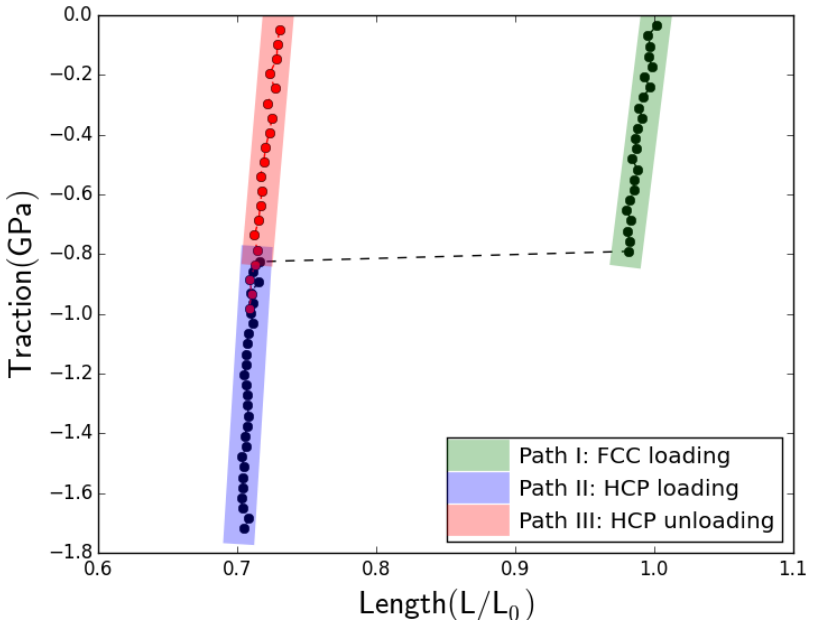






(Tong and Li [2015] **EPL**)





Example 3. Phase Transformation of Iron

In this simulation, we adopt the Finnis-Sinclair Model [52] for material BCC iron. The potential energy of the Finnis-Sinclair Model (FSM) and the Embedded Atom Model (EAM) has the following general form:

$$U = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1} V(r_{ij} + \sum_{i=1}^{N} F(\rho_i) \tag{5.3}$$

where $F(\rho_i)$ is a functional describing the energy of embedding an atom in background electron cloud, and it is defined as

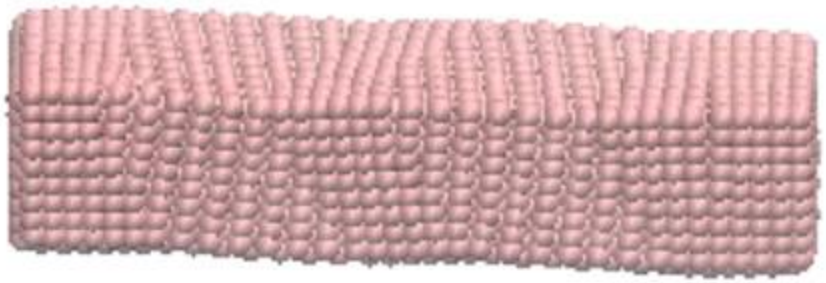
$$\rho_i = \sum_{j\neq i}^{N} \rho(r_{ij}),\ \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j,\ r_{ij} = |\mathbf{r}_{ij}| \tag{5.4}$$

The Finnis-Sinclair potential is defined as

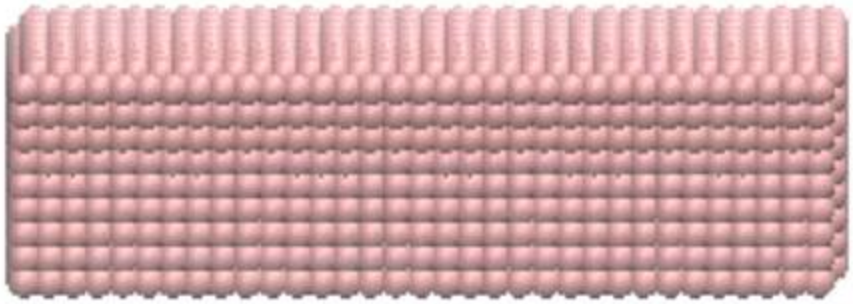
$$V(r_{ij}) = (r_{ij} - c)^2(c_0 + c_1 r_{ij} + c_2 r_{ij}^2),\ \rho(r_{ij}) = (r_{ij} - d)^2 + \beta\frac{(r_{ij} - d)^3}{d},\ F(\rho_i) = -A\sqrt{\rho_i}\,, \tag{5.5}$$

with parameters $c_0, c_1, c_2, c, A, d,$ andβ taken from [53]. Note that both c and d are cutoff distances.

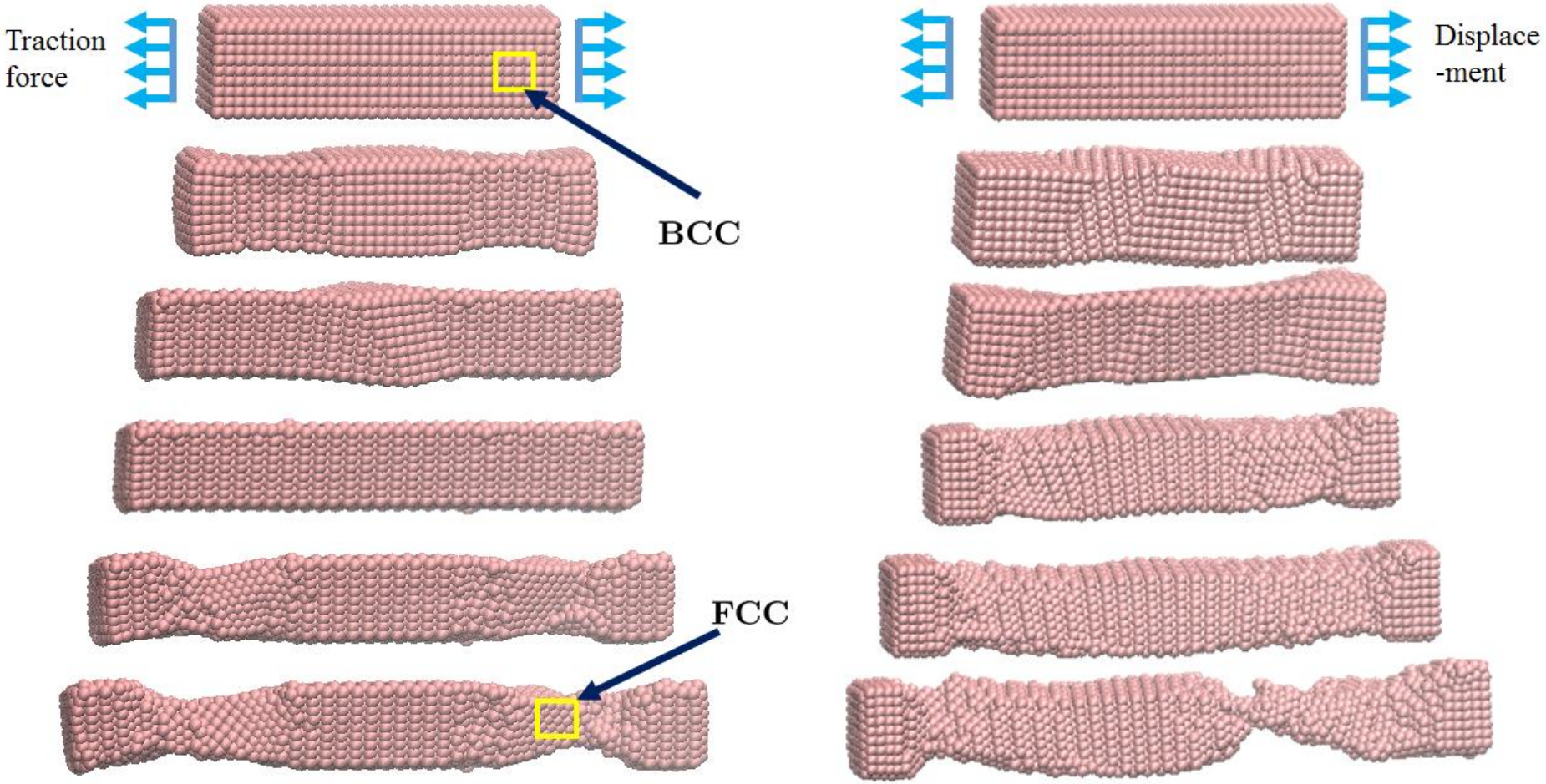
(Li and Urata [2016] **CMAME**)



Prescribed displacement boundary condition

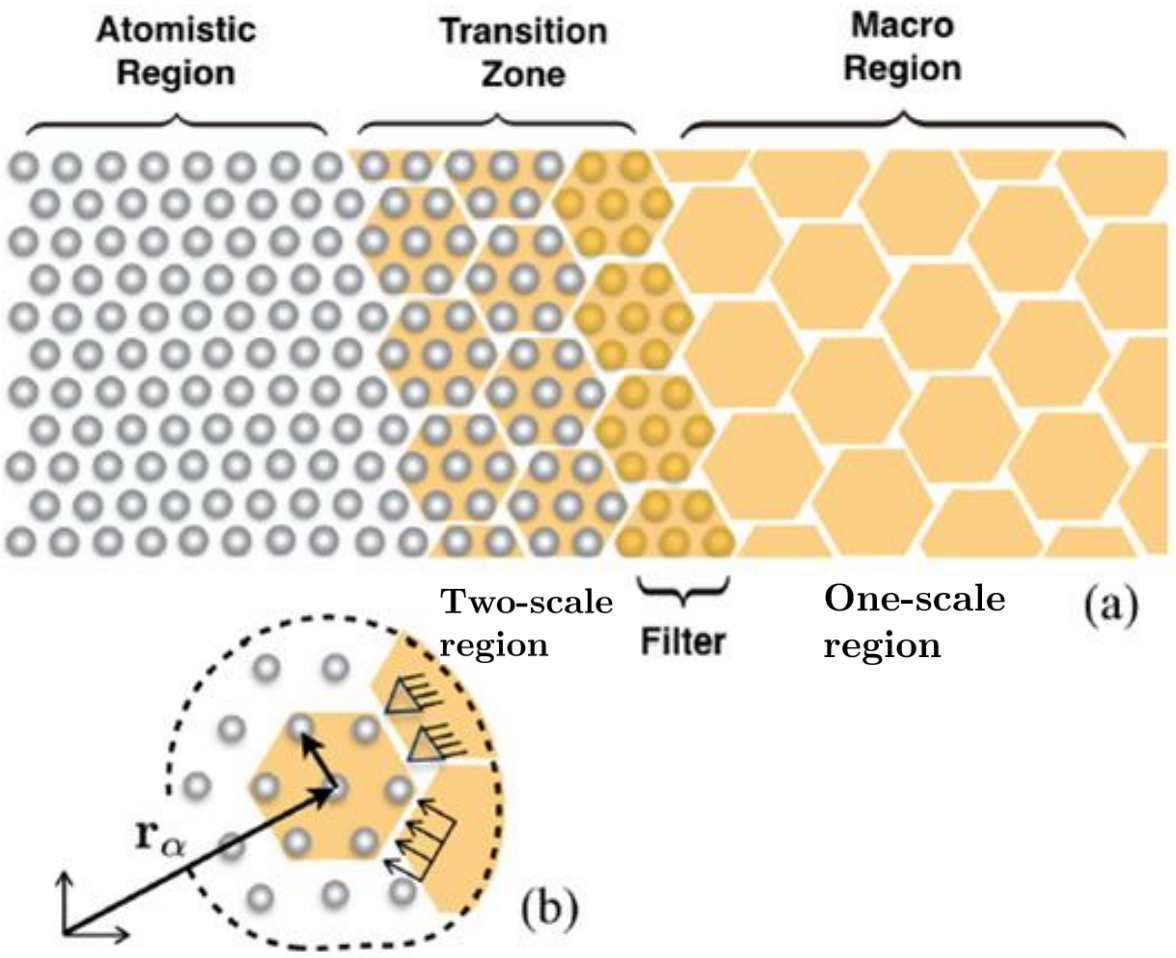


Prescribed displacement boundary condition

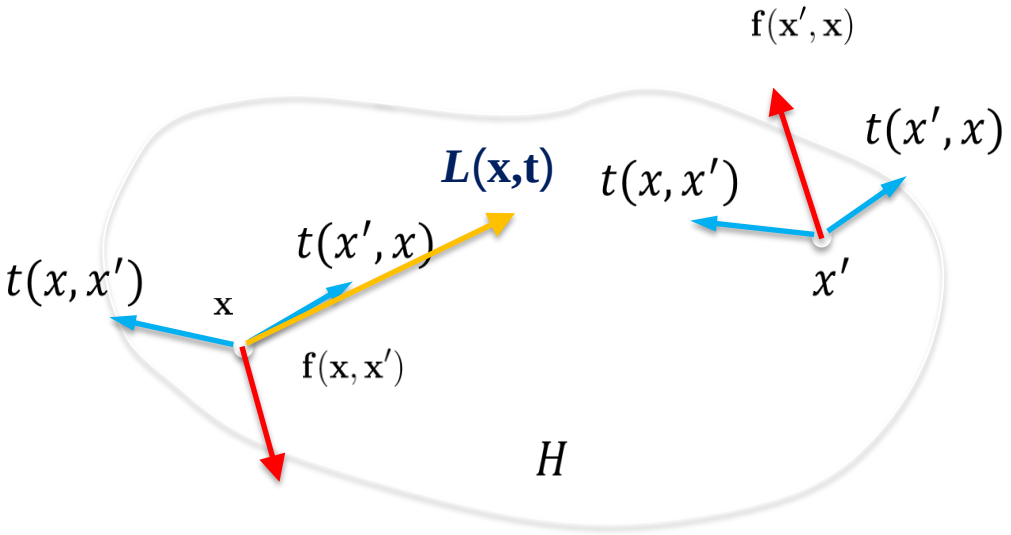

Traction
force
BCC
FCC
Displace
-ment

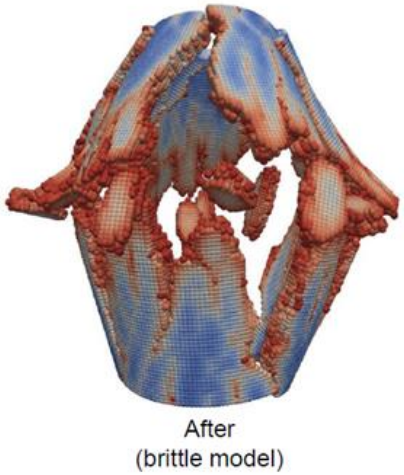
IV. Application: Coupling MD with Peridynamics

Three-scale region



State-based Peridynamics





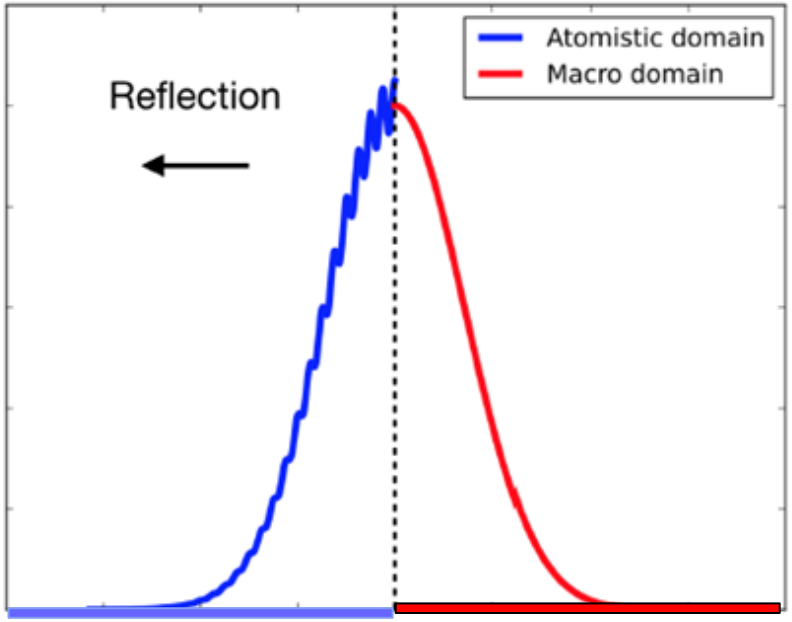
Let t(·, ·) denote a vector-valued function such that

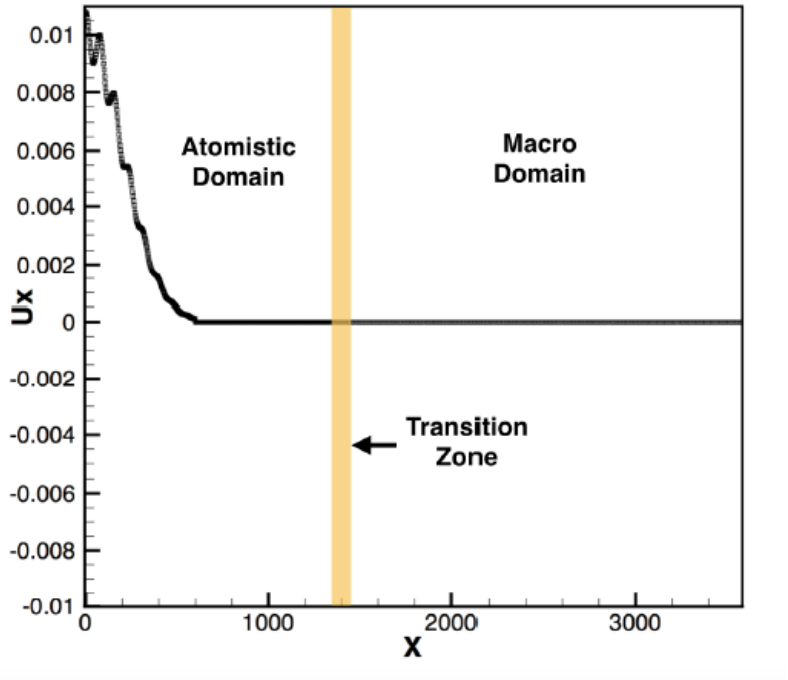
$$\mathbf{f}(\mathbf{x},\mathbf{x}') = \mathbf{t}(\mathbf{x},\mathbf{x}') - \mathbf{t}(\mathbf{x}',\mathbf{x}) \qquad \mathbf{f}(\mathbf{x}',\mathbf{x}) = -\mathbf{f}(\mathbf{x},\mathbf{x}')$$

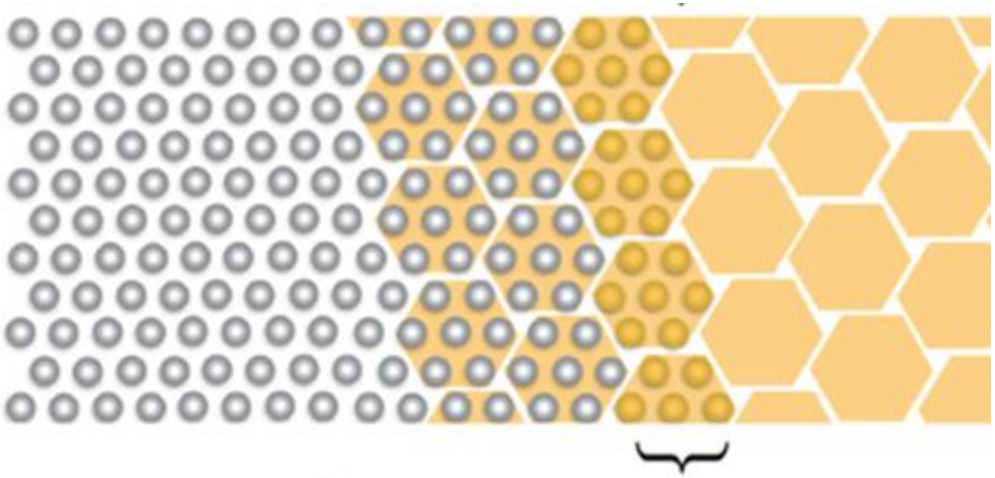
$$\rho\ddot{\mathbf{u}}(\mathbf{x}_\alpha, t) = \int_H \left\{ \mathbf{t}[\mathbf{x}_\alpha, t] < \mathbf{X}_\beta - \mathbf{X}_\alpha > - \mathbf{t}[\mathbf{x}_\beta, t] < \mathbf{X}_\alpha - \mathbf{X}_\beta > \right\} dV_{x_\beta} + \mathbf{b}[\mathbf{x}_\alpha, t]$$

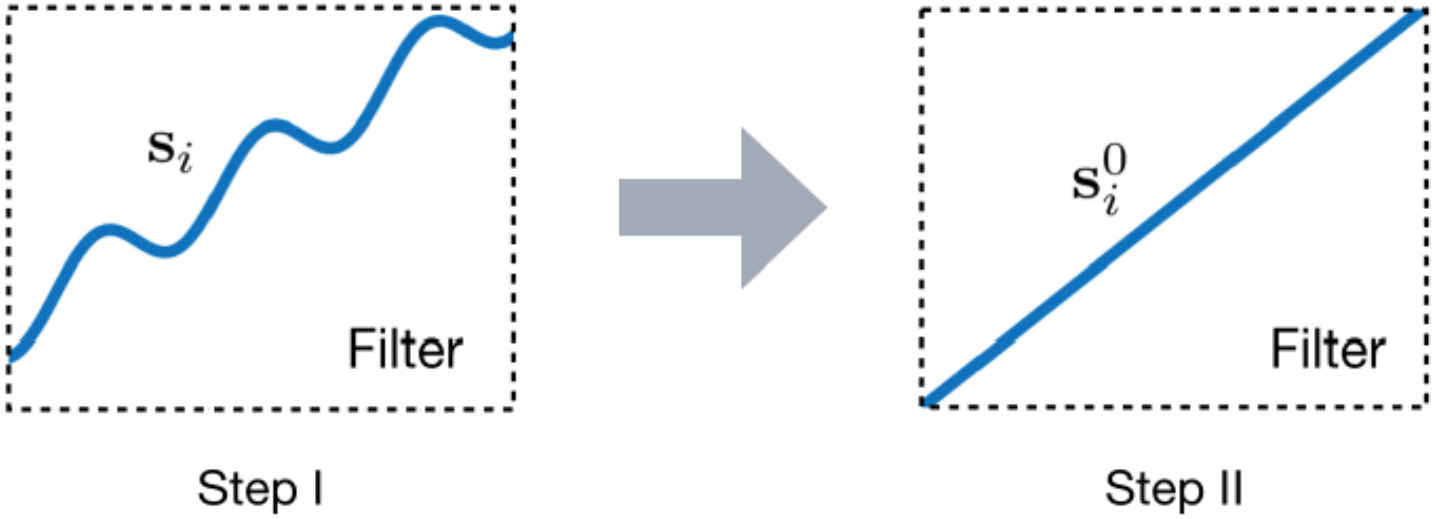
$$\rho\ddot{\mathbf{u}}_\alpha = \mathbf{L}_\alpha + \mathbf{b}_\alpha$$

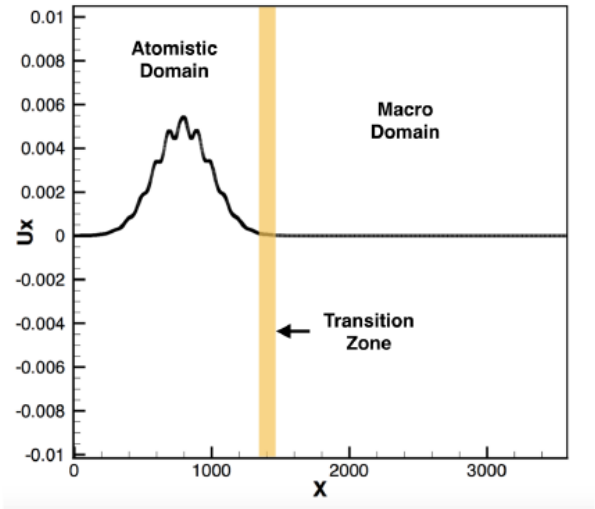
Example: An one-dimensional wave propagation



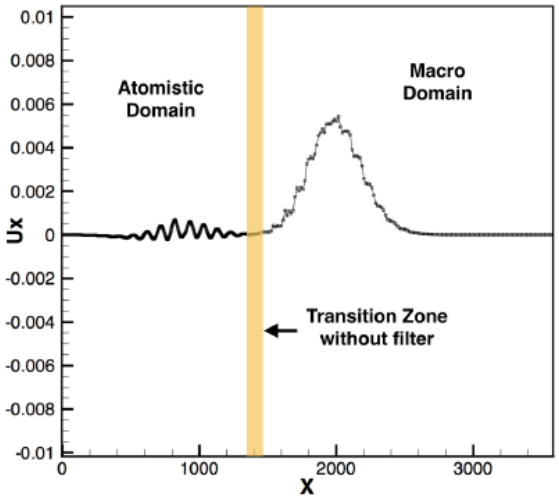





$\mathbf{s}_i$
Filter
$\mathbf{s}_i^0$
Filter
Step I
Step II



(a) t=2250



(b) t=5000

Figure 5: Displacement at (a)t=2250 and (b)t=5000 with units of macroscale step size. No filter is placed in the transition zone.

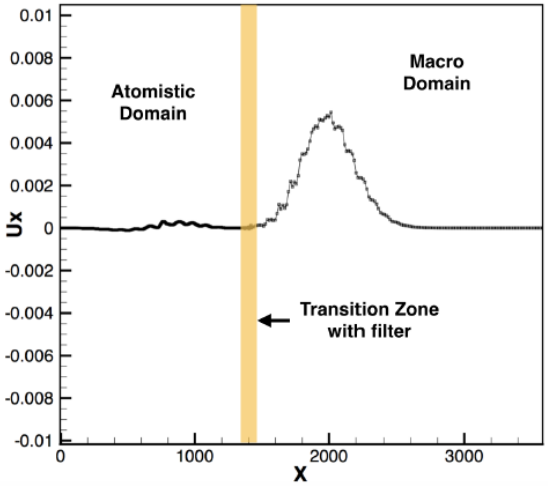
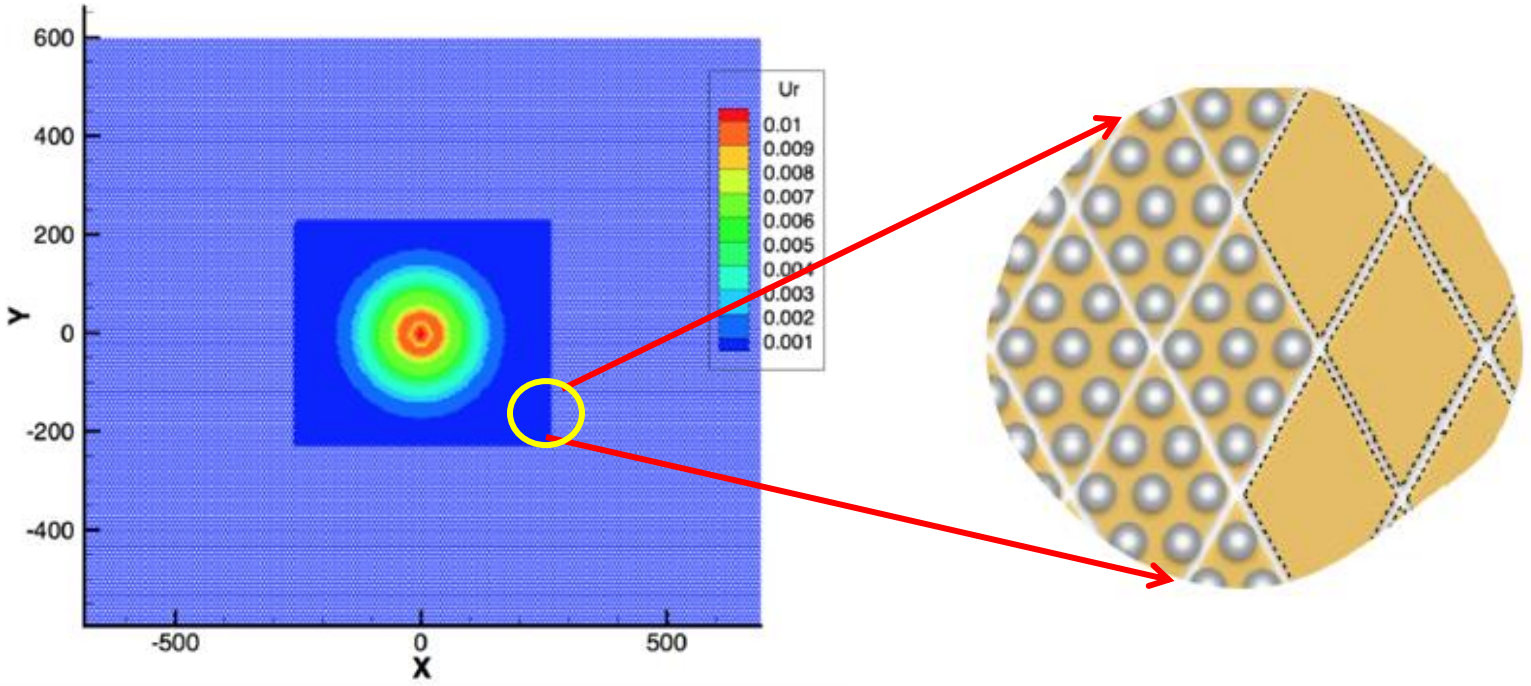


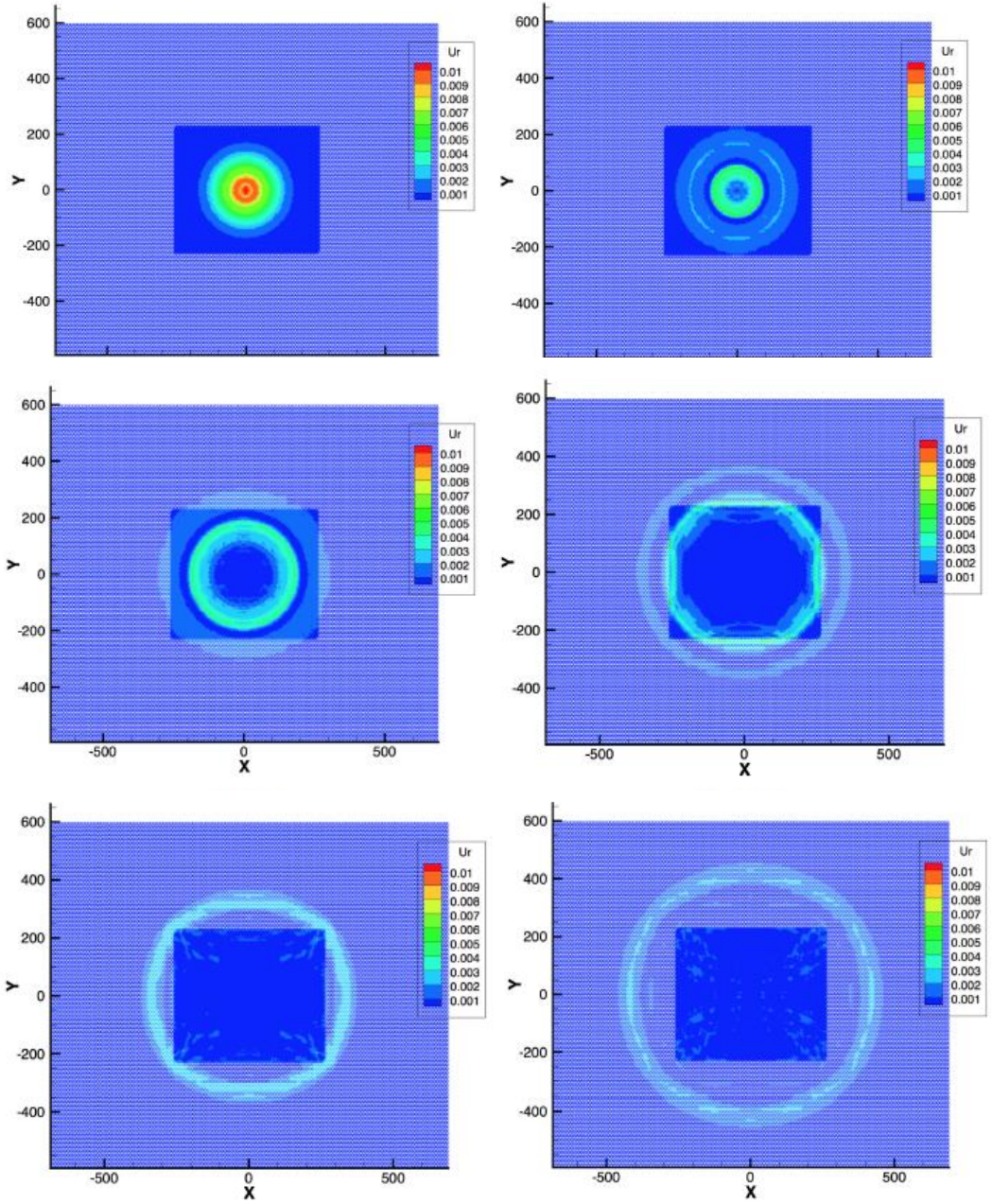
Figure 6: Displacement at t=5000 with filter in the transition zone.

(Tong and Li [2016] **JMPS**)

Example 4: A two-dimensional wave propagation

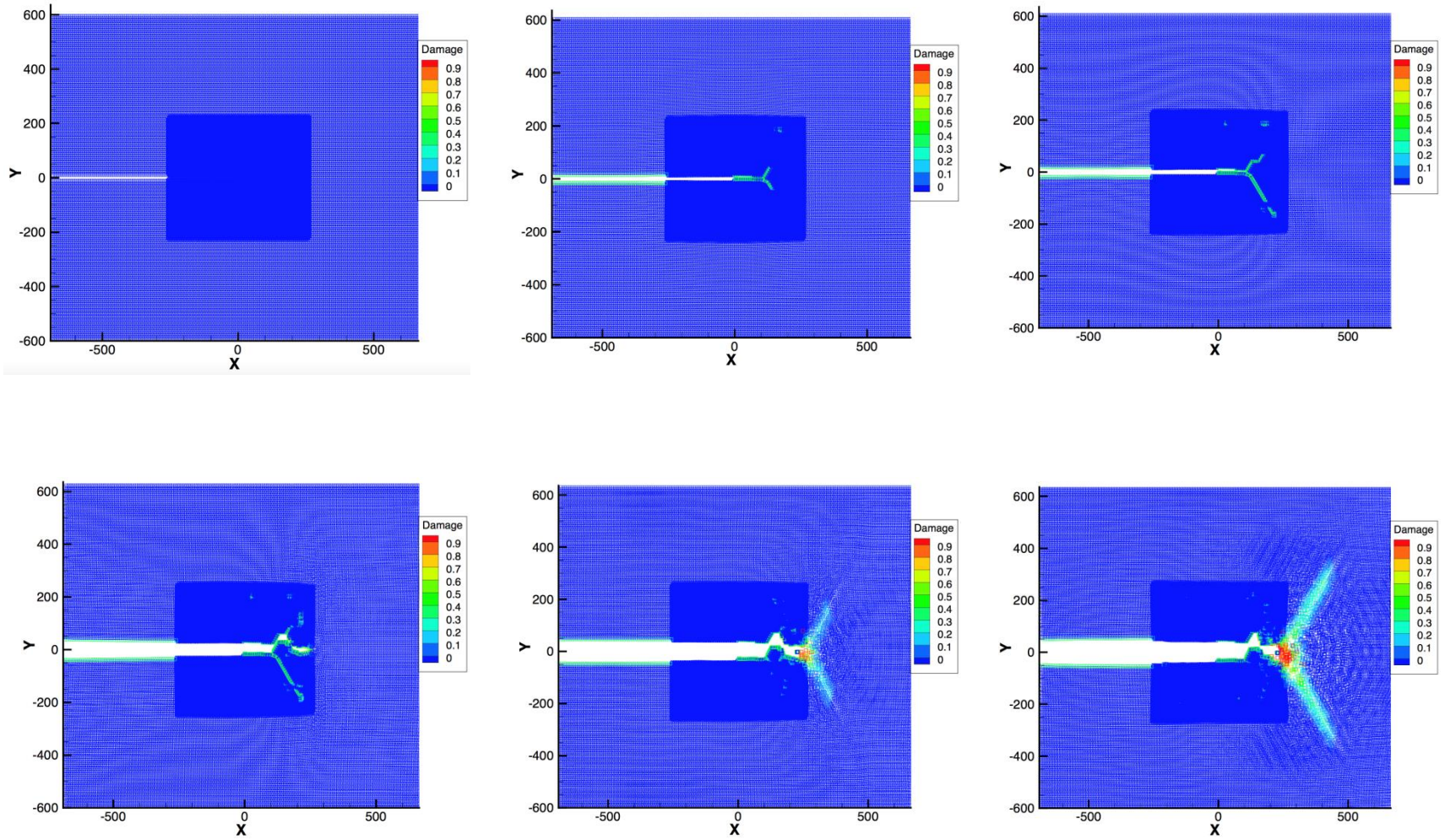
$$u(r,t=0) = \begin{cases} Ae^{-\frac{r^2}{2\sigma^2}}(1+bcos(\frac{2\pi r}{H})) & r \le L_c \\ 0 & r > L_c \end{cases}$$





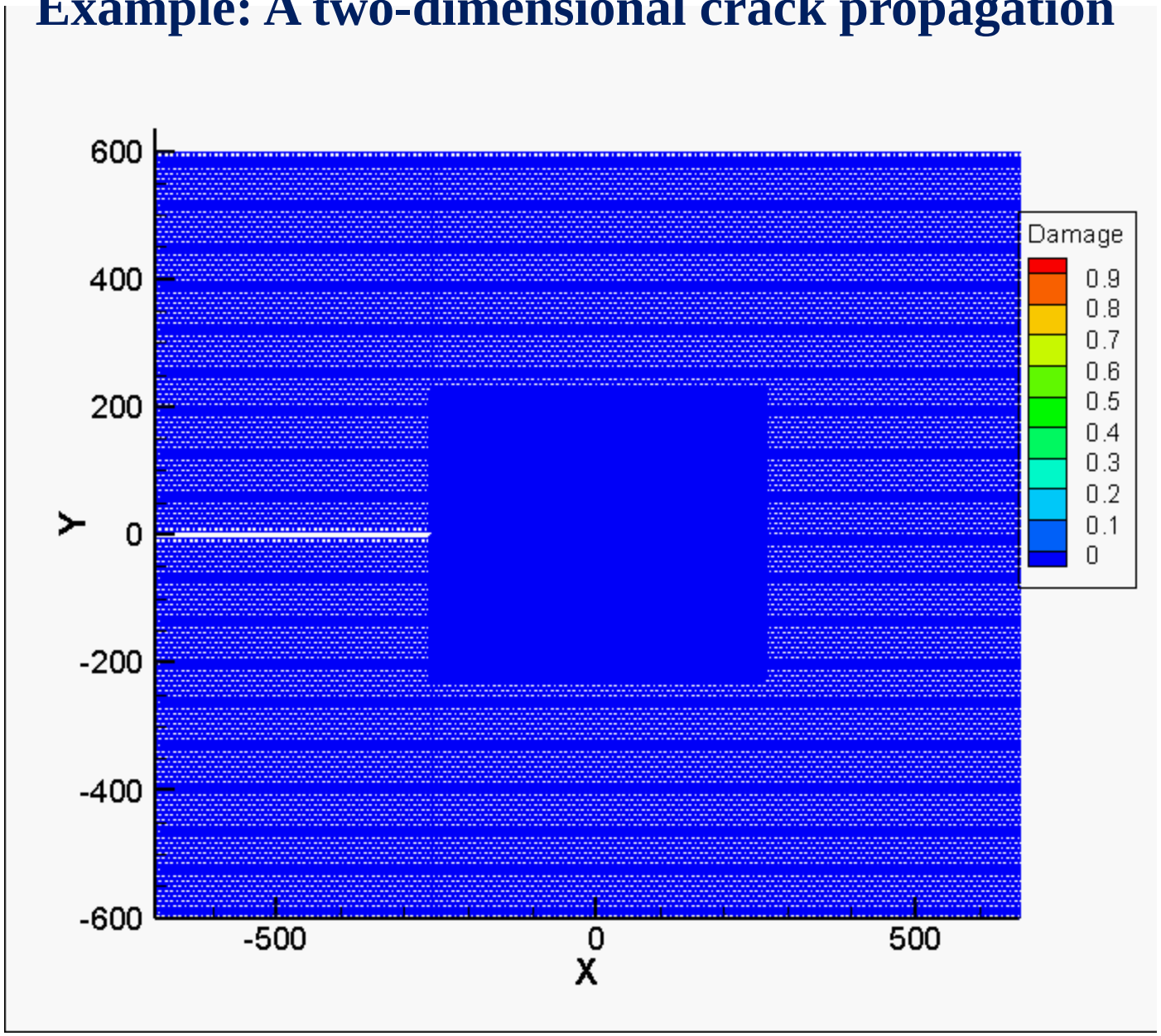
(e) t=1400

(f) t=1720



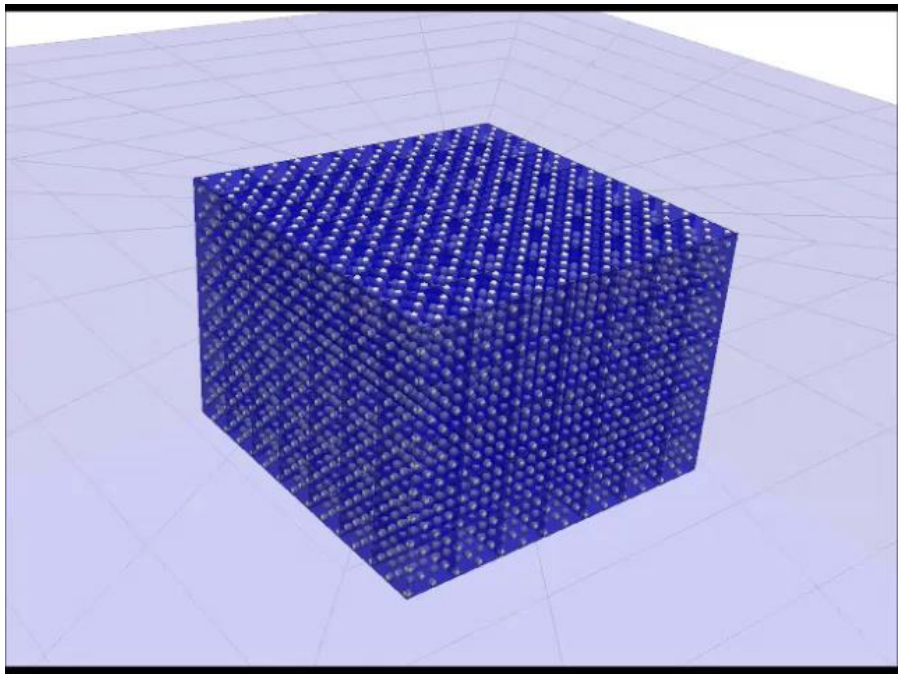
Example: A two-dimensional crack propagation

Example: A two-dimensional crack propagation

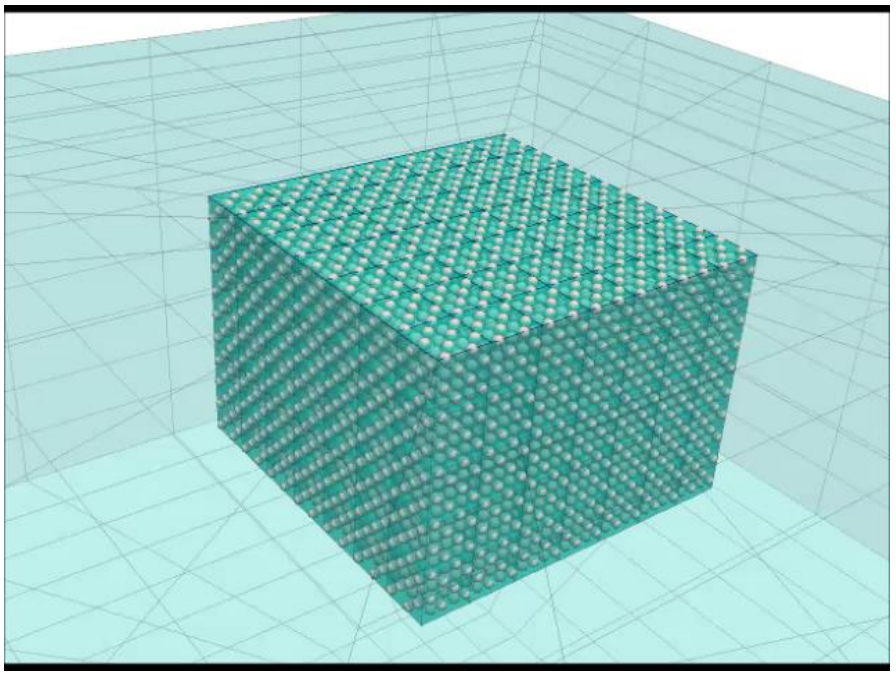


Coupling MD with FEM: Nanoindentation

Spherical Indenter



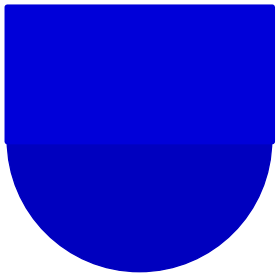
Vicker's Indenter

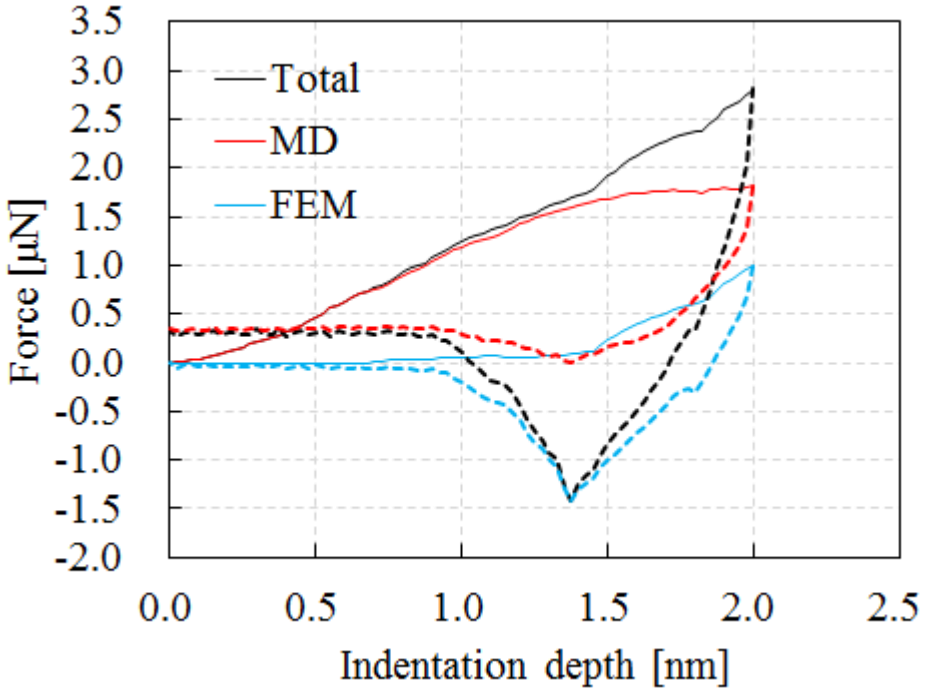


- B.C. of indenter can be applied to cell centers.
- Local pressure in each cell can be analyzed.

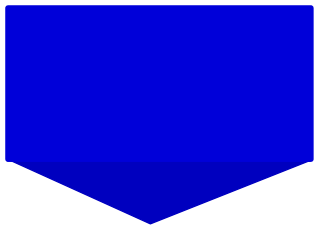
Depth vs. Force

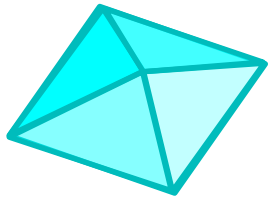
Spherical Indenter

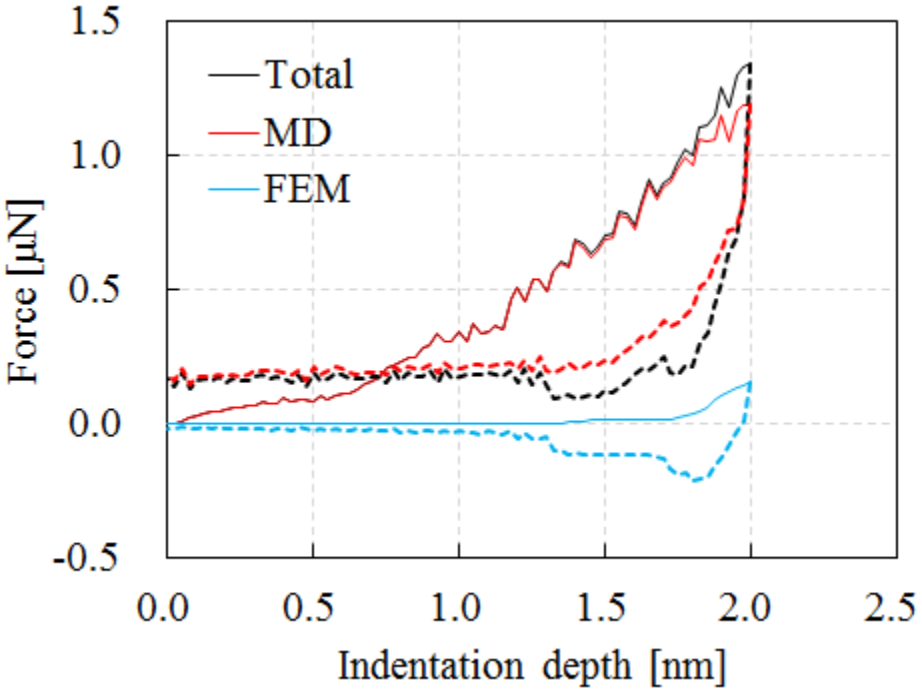




Vicker's Indenter







Conclusions

1. **We have extended the equilibrium ensemble PR-MD to a non-equilibrium atomistic-to-continuum dynamics;**

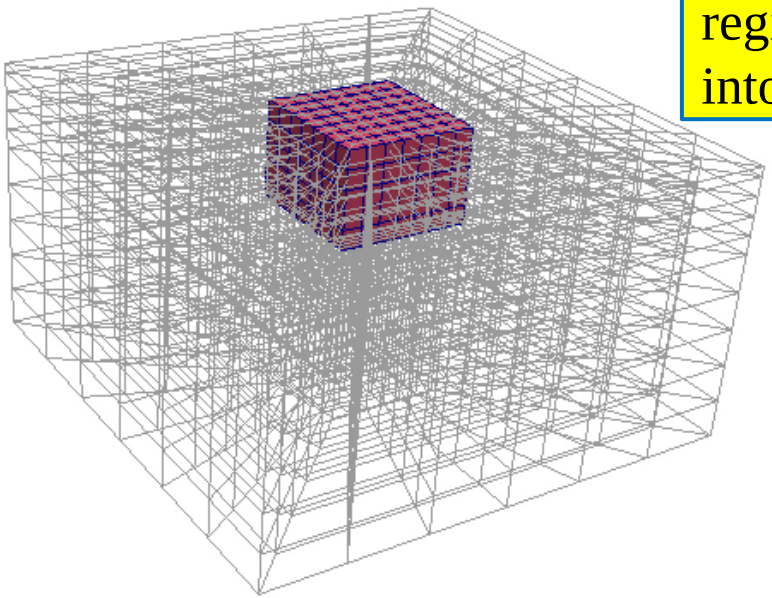
2. **We have successfully embedded macroscale boundary conditions into a finite-size microscale molecular dynamics system instead of using periodic boundary condition;**

3. **Based MMMD, we have developed the multiscale interface element to couple Molecular Dynamics with Peridynamics;**

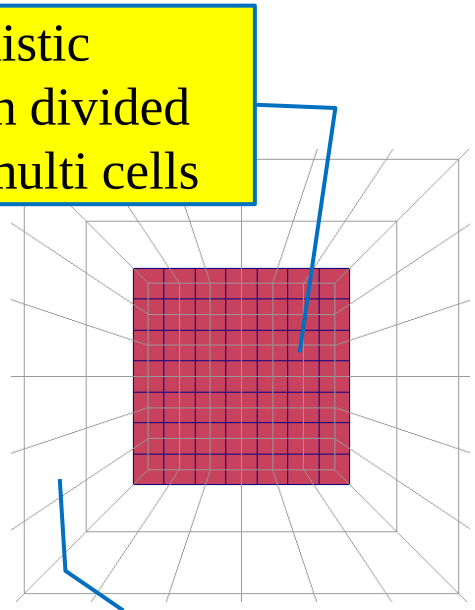
4. **MMMD touches some basic fundamental concepts of continuum mechanics and multiscale simulations.**

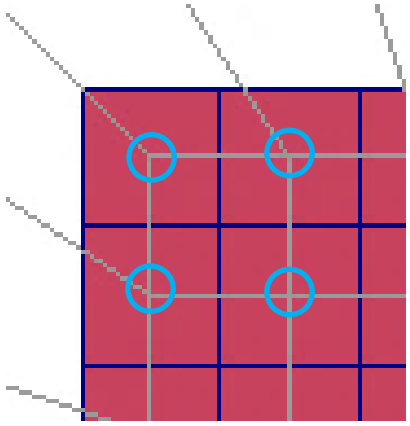
Coupling of MMMD-FEM

- To combine MMMD and FEM, position of cell centers r_α are connected to FEM nodes.
- It avoids "*Fully Refined Mesh* ", at the boundary, because nodes are connected to coarse scale positions but not atoms



MMMD + FEM system





MD cells

FEM elements

MD cell centers & FEM nodes

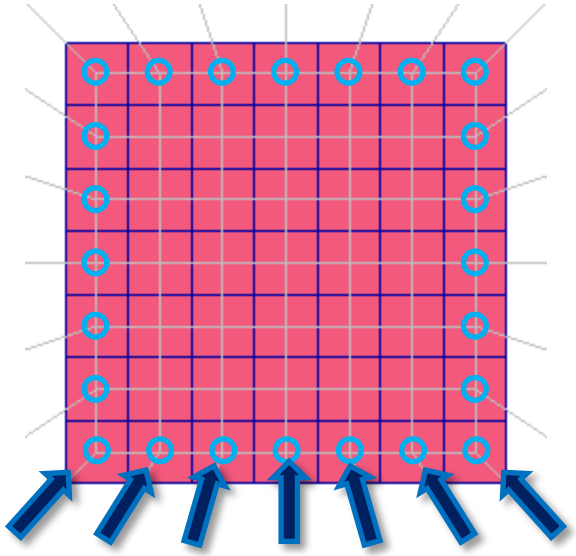
Algorithm

i. Define intermediate nodes (○) to connect FEM & MD regions.

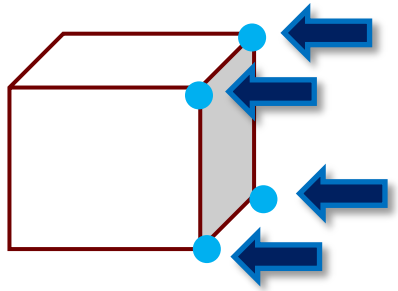
ii. Force from FEM elements are considered as traction force $\mathbf{T}_k$ for boundary condition of MD cell centers.

$$\mathbf{M}_\alpha \ddot{\mathbf{r}}_\alpha = -\sum_{\beta \neq \alpha} \mathbf{f}_{\alpha\beta} + \mathbf{T}_k$$

iii. Displacement of MD cell center $\Delta \boldsymbol{r}_\alpha$ is utilized to estimate deformation gradient $\boldsymbol{F}$ of the boundary elements.

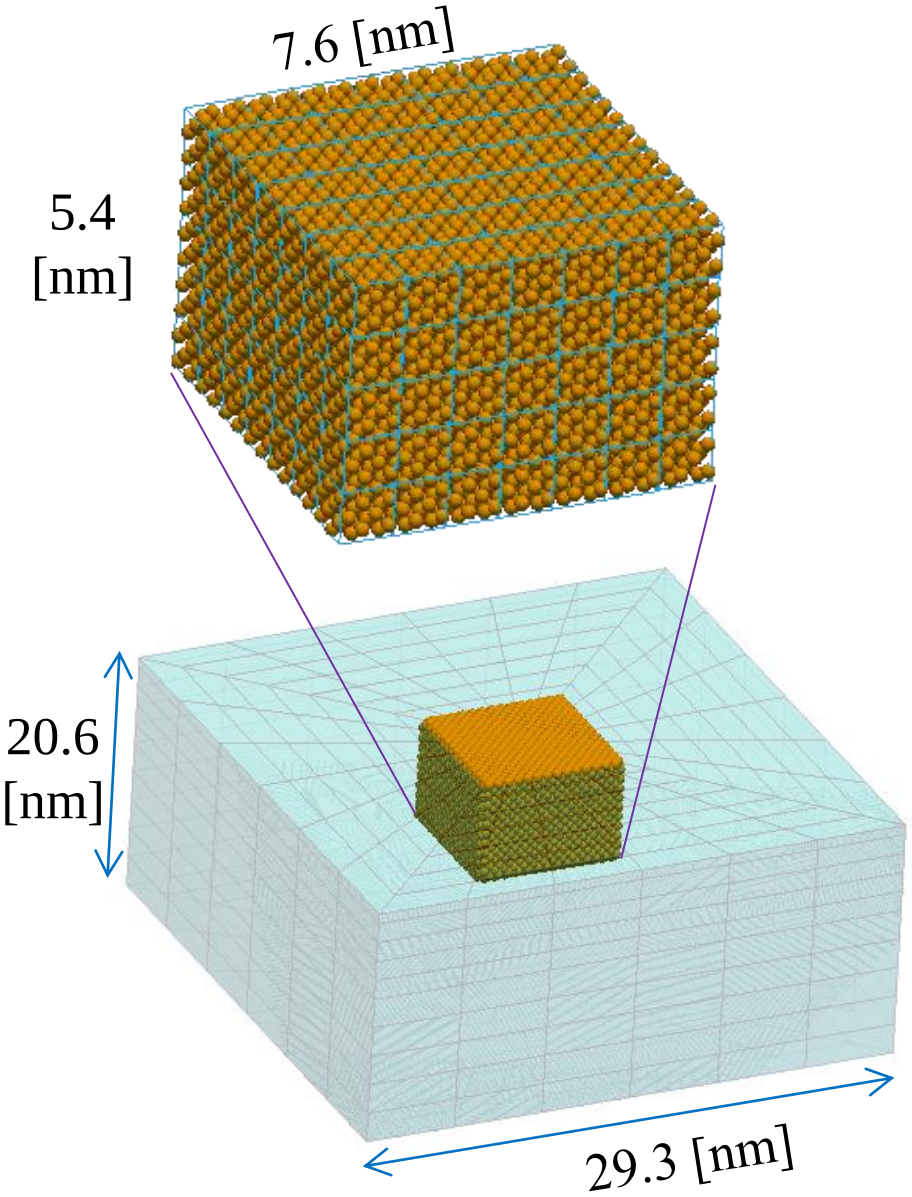


Traction force B.C.
from FEM to celll center



Displacement B.C. from
celll center to FEM node

Multiscale system



MD region

7 x 7 x 5 = 245 cells

64 ***Silicon*** atoms in each cell

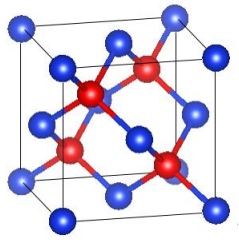
15680 atoms in total

Tersoff Potential for silicon

FEM region

14-14-5 extra elements around MD cells 1860 elements in FEM

method with cubic crystal unit cel



Indenter

Spherical (20nmϕ)

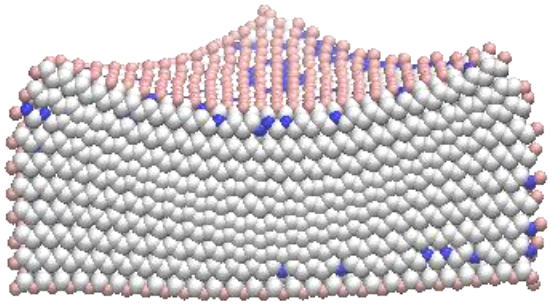
& Vicker's indenters.

applied as displacement B.C. analytically

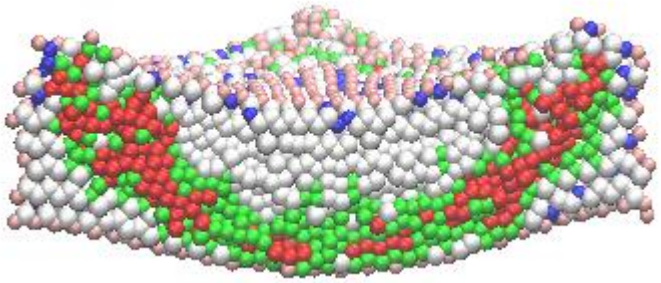
Crystal phase under indenters

Spherical Indenter

2nm



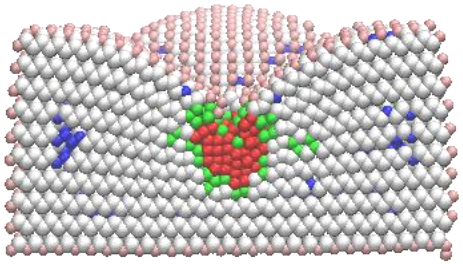
4nm



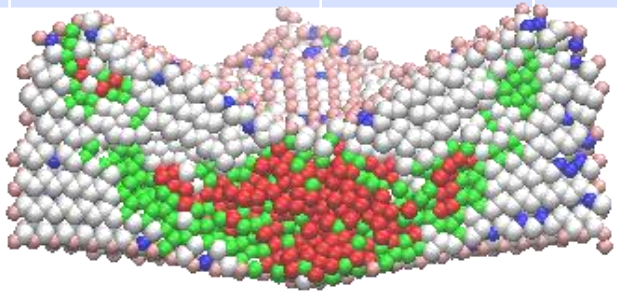
	Crystal	Bond [A]	Coord. No
●	Surface/ Amorphous	2.35	<4
●	Si-I	2.35	4
●	bct-5	2.31	4
		2.44	1
●	Si-III, XII	2.39	4
		3.2-3.4	1
●	Si-II	2.42	4
		2.57	2

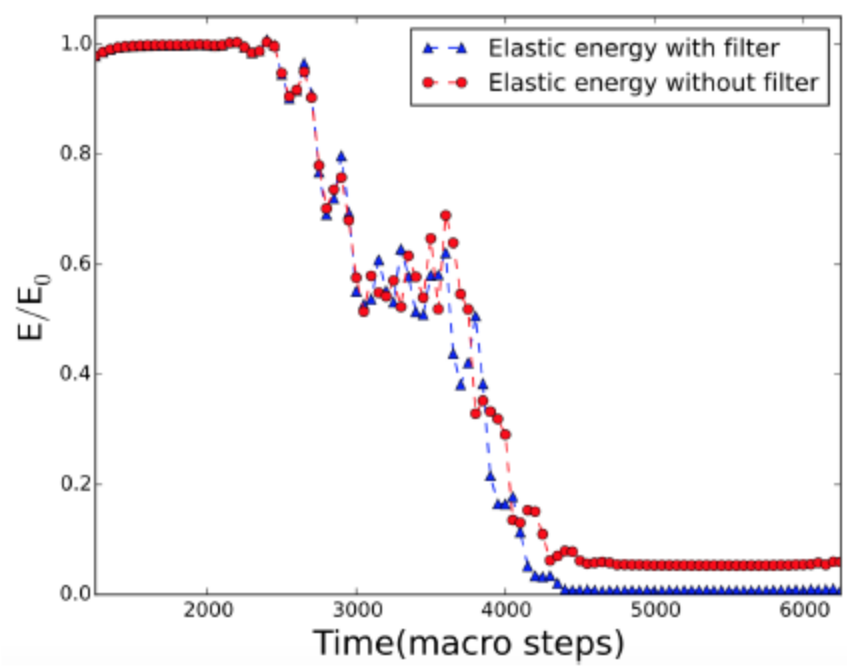
Vicker's Indenter

2nm

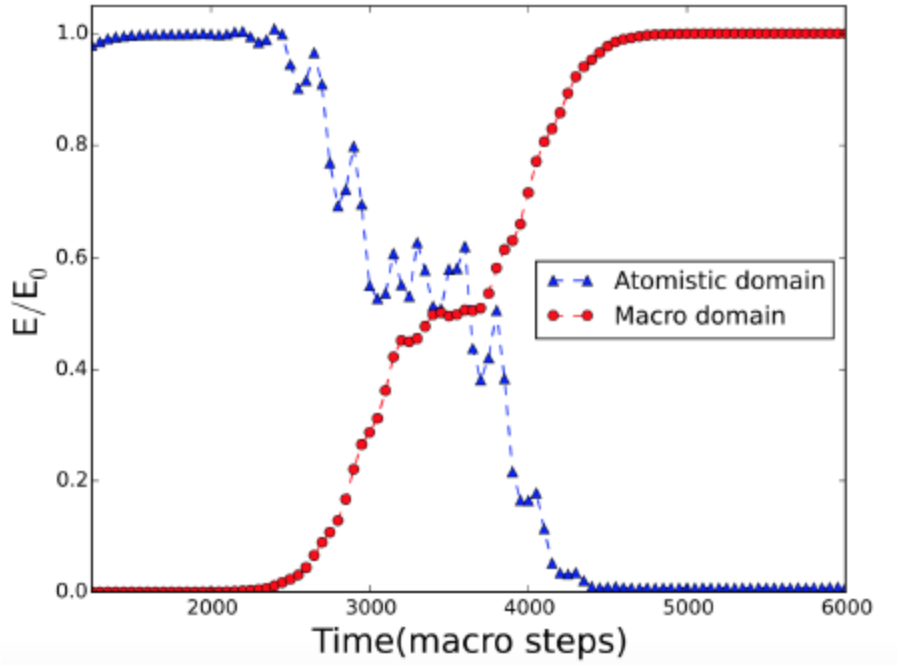


4nm



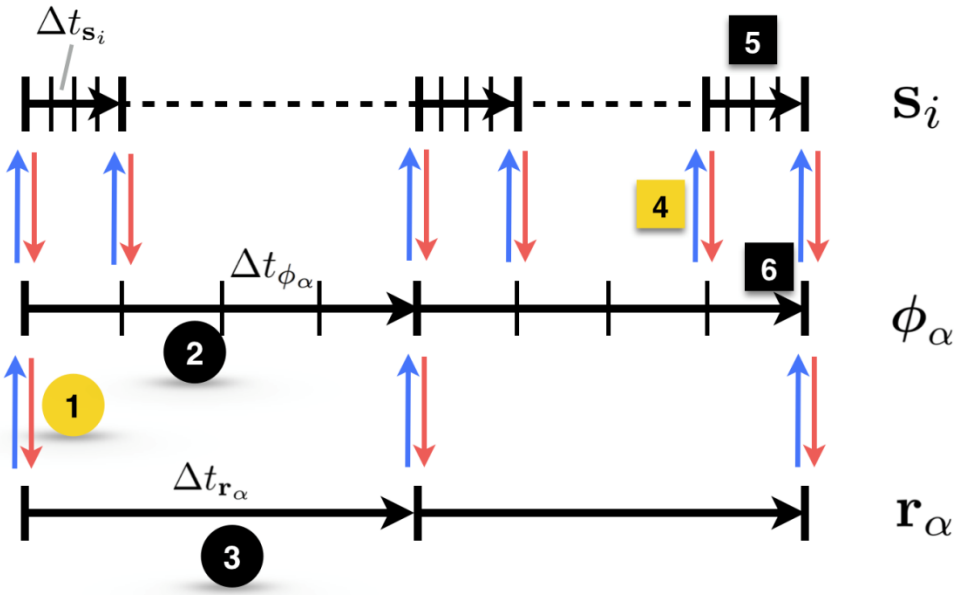


(a) Energies of atomistic domain with and without filter



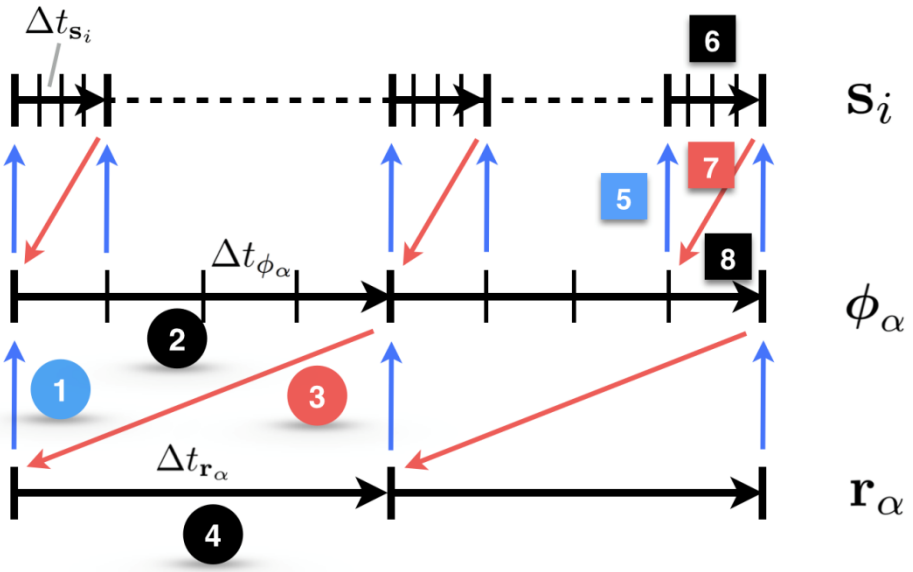
(b) Comparison of energies of atomistic and macro domain

Figure 7: Evolution of energy in each domain.



Computer Implementation

Parallel Computation



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2. Tong, Q. and Li, S., 2015. From molecular systems to continuum solids: A multiscale structure and dynamics, *The Journal of Chemical physics*, ***143***(6), p.064101.

3. Tong, Q. and Li, S., 2015. A multiscale molecular dynamics allowing macroscale Mechanical loads. *EPL (Europhysics Letters)*, ***110***(6), p.60005.

4. Li, S. and Urata, S., 2016. An atomistic-to-continuum molecular dynamics: Theory, algorithm, and applications. *Computer Methods in Applied Mechanics and Engineering, **311**, 452-478.*

5. Tong, Q. and Li, S. , 2016. Multiscale coupling of molecular dynamics and peridynamics, *Journal of Mechanics and Physics of Solids*, **95**, 169-187.