Conservation Properties of the Bridging Domain Method for Coupled Molecular/Continuum Dynamics

Mei Xu

Collaborator: Ted Belytschko

Theoretical and Applied Mechanics

1851

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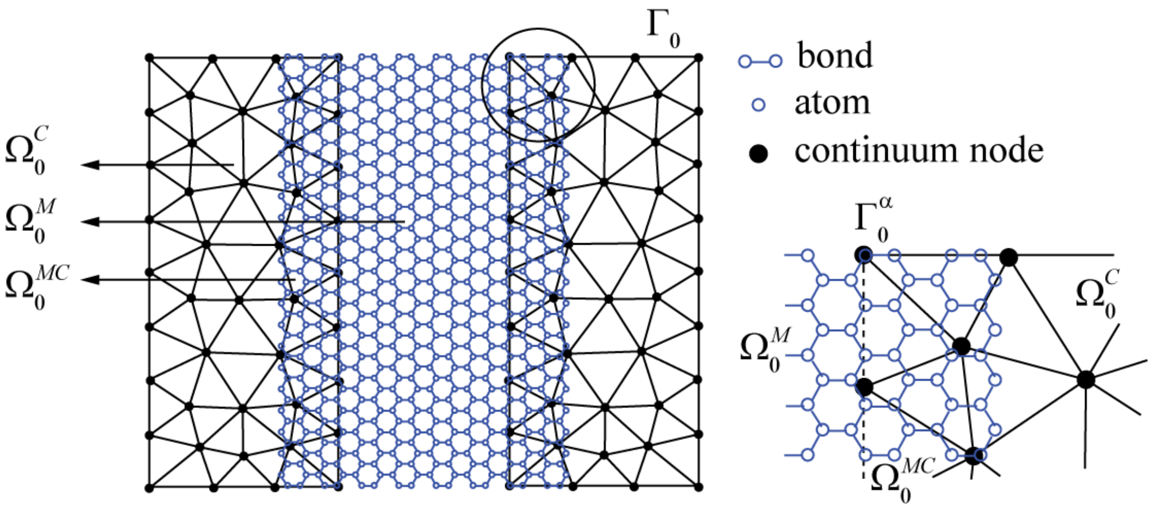
Outline

- Bridging domain method
- Conservation properties
  - Linear momentum
  - Angular momentum
  - Energy
- Numerical tests
  - One-dimensional
  - Two-dimensional
- Conclusions

Bridging Domain Method



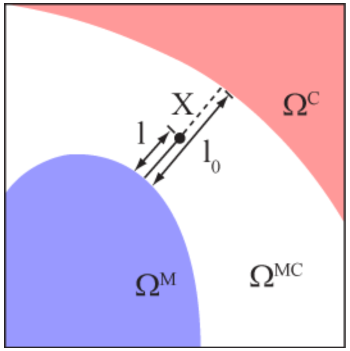
- Main features
  - Couples atomistic and continuum model
  - Scaling factor function is introduced to the coupling region
  - Total energy of the system is the combination of the energy of the atomistic and continuum model
  - Lagrange multipliers are used to enforce the compatibility between the models

Xiao, S.P. and Belytschko, T., Int. J. Numer. Meth. Engng., Vol 1 pp 115-126, 2003

Bridging Domain Method

- Scaling factor (linear)

$$\alpha(\mathbf{X}) = \begin{cases} 0 & if \quad \mathbf{X} \in \Omega_0^M / \Omega_0^{MC} \\ l(\mathbf{X}) / l_0(\mathbf{X}) & if \quad \mathbf{X} \in \Omega_0^{MC} \\ 1 & if \quad \mathbf{X} \in \Omega_0^C / \Omega_0^{MC} \end{cases}$$

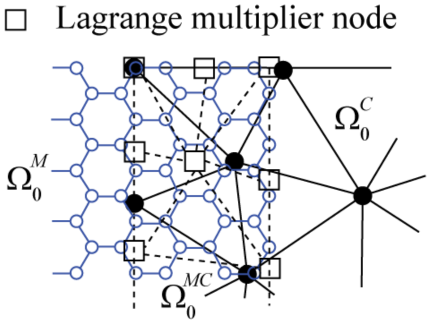


- Lagrange multiplier
  - Interpolated from a continuum field

$$W = W^{\text{int}} - W^{\text{ext}} + \boldsymbol{\lambda}^T \mathbf{g}$$

$$g_{iI} = \sum_J \underbrace{N_J(\mathbf{X}_I)}_{N_{JI}} u_{iJ} - d_{iI}$$

$$\lambda(\mathbf{X}_I) = \sum_J N_{JI}^{\lambda} \bar{\lambda}_I$$



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Conservation Properties of Dynamic Systems

- Equations of motion

$$\bar{M}_I^M \ddot{d}_{iI} + \bar{f}_{iI}^{\,\mathrm{int}\,M} + \bar{f}_{iI}^{\,GM} = 0$$

$$\bar{M}_I^M \ddot{u}_{iI} + \bar{f}_{iI}^{\,\mathrm{int}\,C} + \bar{f}_{iI}^{\,GC} = 0$$

$$\sum_{I\in S} N_{IJ} u_{iI} - d_{iJ} = 0$$

where

$$\bar{f}_{iI}^{\,\mathrm{int}\,M} = \sum_{J\in M} \left(1-\alpha_{IJ}\right)\frac{\partial w_{IJ}^M}{d_{iI}} \qquad \bar{f}_{iI}^{\,GM} = \frac{\partial G}{\partial d_{iI}} = -\lambda_{iI}$$

$$\bar{f}_{iI}^{\,\mathrm{int}\,C} = \int_{\Omega_0^C} \alpha \frac{\partial N_I}{\partial X_j} P_{ji}\, d\Omega_0^C \qquad \bar{f}_{iI}^{\,GC} = \frac{\partial G}{\partial u_{iI}} = \sum_{J\in M} \lambda_{iJ} N_{IJ}$$

- Conservation properties
  - Linear momentum

$$\boxed{\mathbf{p} = \sum_{I\in M} \bar{M}_I^M \dot{\mathbf{d}}_I + \sum_{I\in S} \bar{M}_I^C \dot{\mathbf{u}}_I}$$

  - Angular momentum

$$\boxed{\mathbf{L} = \sum_{I\in M} \bar{M}_I^M \mathbf{x}_I^M \times \dot{\mathbf{d}}_I + \sum_{I\in S} \bar{M}_I^C \mathbf{x}_I^C \times \dot{\mathbf{u}}_I}$$

  - Energy

$$\boxed{E = \frac{1}{2}\sum_{I\in M} \bar{M}_I^M \dot{d}_{iI}\dot{d}_{iI} + \frac{1}{2}\sum_{I\in S} \bar{M}_I^C \dot{u}_{iI}\dot{u}_{iI}\,] + \sum_{I<J\in M} \bar{w}_M\left(\mathbf{x}_I, \mathbf{x}_J\right) + \int_{\Omega_0^C} \bar{w}_C\left(\mathbf{F}\right) d\Omega_0^C}$$

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Conservation of Linear Momentum

$$\frac{dp_i}{dt}=\frac{d}{dt}\left(\sum_{I\in M}\bar{M}_I^M\dot{d}_{iI}+\sum_{I\in S}\bar{M}_I^C\dot{u}_{iI}\right)$$

$$=\sum_{I\in M}\lambda_{iI}-\sum_{I,J\in M}\left(1-\alpha_{IJ}\right)\frac{\partial w_{IJ}^M}{\partial d_{iI}}-\sum_{I\in M}\lambda_{iI}\sum_{J\in S}N_{JI}-\sum_{I\in S}\int_{\Omega_0^C}\alpha\frac{\partial N_I}{\partial X_i}P_{ji}\,d\Omega_0^C$$

cancel

vanish

$$\sum_{J\in M}N_J\left(\mathbf{X}\right)=1$$

partition of unity

$$\sum_{I,J\in M}\frac{\partial w_{IJ}^M}{\partial d_{iI}}=\frac{1}{2}\sum_{I,J\in M}\left(\frac{\partial w_{IJ}^M}{\partial d_{iI}}+\frac{\partial w_{IJ}^M}{\partial d_{iJ}}\right)=0$$

anti-symmetry

Conservation of Angular Momentum

$$\frac{d\mathbf{L}}{dt}=\frac{d}{dt}\left(\sum_{I\in M}\bar{M}_I^M\mathbf{x}_I^M\times\dot{\mathbf{d}}_I+\sum_{I\in S}\bar{M}_I^C\mathbf{x}_I^C\times\dot{\mathbf{u}}_I\right)\Rightarrow\frac{dL_k}{dt}=\varepsilon_{jik}\left(\sum_{I\in M}\bar{M}_I^M x_{jI}^M\ddot{d}_{iI}+\sum_{I\in S}\bar{M}_I^C x_{jI}^C\ddot{u}_{iI}\right)$$

$$\frac{dL_k}{dt}=\varepsilon_{jik}\left(\sum_{I\in M}\left[\lambda_{iI}-\sum_{J\in M}\left(1-\alpha_{IJ}\right)\frac{\partial w_{IJ}^M}{\partial d_{iI}}\right]x_{jI}^M+\sum_{I\in S}\left[\sum_{J\in M}\lambda_{iJ}N_{IJ}-\int_{\Omega_0^C}\alpha\frac{\partial N_I}{\partial X_l}P_{li}\,d\Omega_0^C\right]x_{jI}^C\right)$$

cancel

$$\boxed{F_{jl}}$$

$$\sum_{I\in S}\varepsilon_{jik}F_{jl}P_{li}=\frac{1}{2}\sum_{I\in S}\varepsilon_{jik}\left(F_{jl}P_{li}-F_{il}P_{lj}\right)=\frac{1}{2}\sum_{I\in S}\varepsilon_{jik}J\left(\sigma_{ji}-\sigma_{ij}\right)=0$$

Cauchy stress is symmetric

$$\varepsilon_{jik}\sum_{J\in M}\left(1-\alpha_{IJ}\right)\frac{\partial w_{IJ}^M}{\partial d_{iI}}x_{jI}^M=\frac{1}{2}\varepsilon_{jik}\sum_{J\in M}\left(1-\alpha_{IJ}\right)\frac{\partial w_{IJ}^M}{\partial d_{iI}}\left(x_{jI}^M-x_{jJ}^M\right)=\frac{1}{2}\sum_{J\in M}\left(1-\alpha_{IJ}\right)\mathbf{r}_{IJ}\times\frac{\partial w_{IJ}^M}{\partial\mathbf{d}_I}=0$$

Bond force is co-axial with the bond vector

Conservation of Energy

$$\frac{dE}{dt}=\sum_{I\in M}\bar{M}_I^M\ddot{d}_{iI}\dot{d}_{iI}+\sum_{I\in S}\bar{M}_I^C\ddot{u}_{iI}\dot{u}_{iI}+\frac{1}{2}\sum_{I,J\in M}(1-\alpha_{IJ})\left(\frac{\partial w_{IJ}^M}{\partial d_{iI}}\dot{d}_{iI}+\frac{\partial w_{IJ}^M}{\partial d_{iJ}}\dot{d}_{iJ}\right)+\int_{\Omega_0^C}\alpha\boxed{\frac{\partial w^C}{\partial F_{ij}}}\boxed{\dot{F}_{ij}}d\Omega_0^C$$

$$\frac{dE}{dt}=-\sum_{I\in M}\left(\bar{f}_{iI}^M+\bar{f}_{iI}^{GM}\right)\dot{d}_{iI}-\sum_{I\in S}\left(\bar{f}_{iI}^{GC}+\bar{f}_{iI}^C\right)\dot{u}_{iI}+\sum_{J\in M}(1-\alpha_{IJ})\frac{\partial w_{IJ}^M}{\partial d_{iI}}\dot{d}_{iI}+\int_{\Omega_0^C}\alpha\underline{P}_{ji}\underline{\frac{\partial N_I}{\partial X_j}}\dot{u}_{iI}d\Omega_0^C$$

cancel

cancel

$$\frac{dE}{dt}=-\sum_{I\in M}\bar{f}_{iI}^{GM}\dot{d}_{iI}-\sum_{I\in S}\bar{f}_{iI}^{GC}\dot{u}_{iI}=\dot{G}$$

⇒ always zero

Numerical Test

- Constraint Matrix

$$\sum_{J\in M} \lambda_{iJ} A_{IJ} = B_{iI}$$

$$\boxed{A_{IJ} = -\sum_{L\in S} \frac{N_{LI} N_{LJ}}{\bar{M}_L^C} - \frac{\delta_{IJ}}{\bar{M}_I^M}} \longrightarrow \boxed{A_{II} = \sum_{J\in S} A_{IJ}}$$

consistent constraint matrix

-compatibility is satisfied exactly

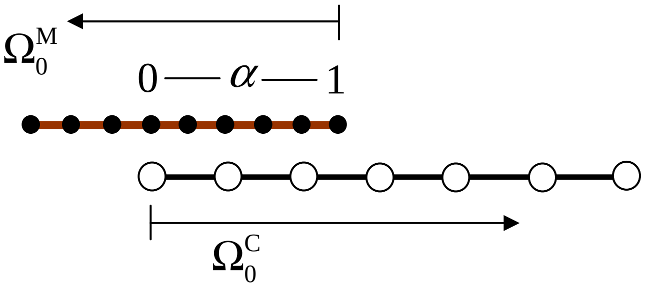
-computationally more expensive

diagonalized constraint matrix

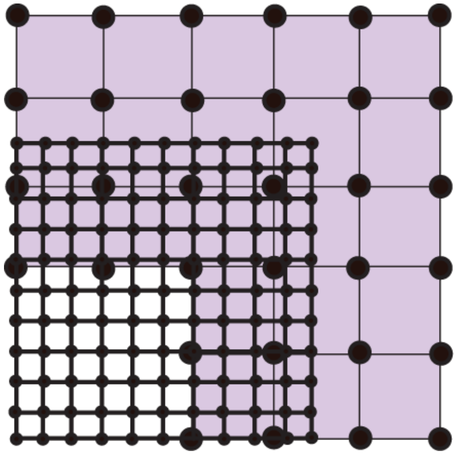
-compatibility is weakly enforced

-cheaper in computation

- Numerical Models



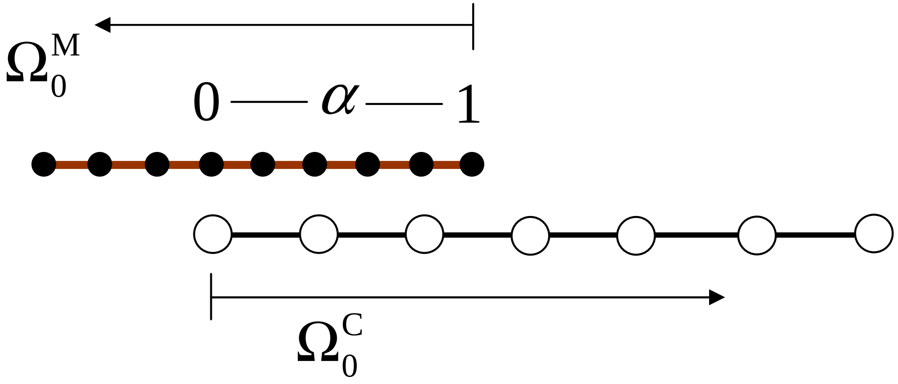
1D bridging domain model
(Lennard-Jones potential)



2D bridging domain model
(Quadratic potentials)

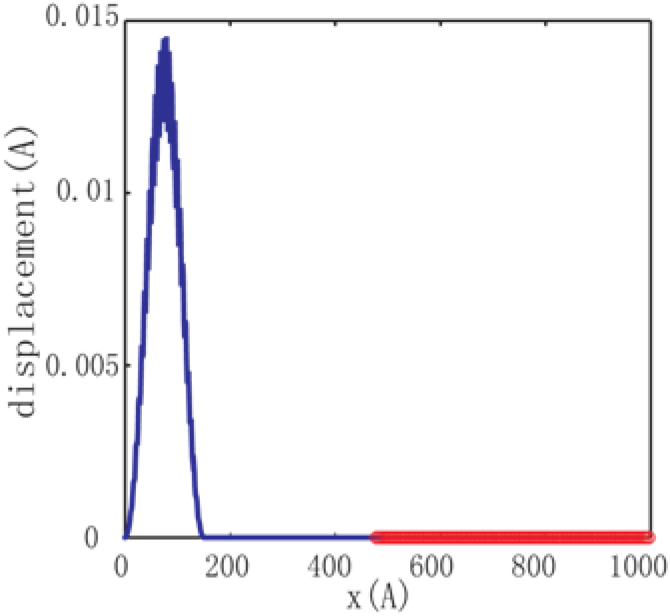
Numerical Test – 1D

- One-dimensional example
  - Lennard-Jones potential

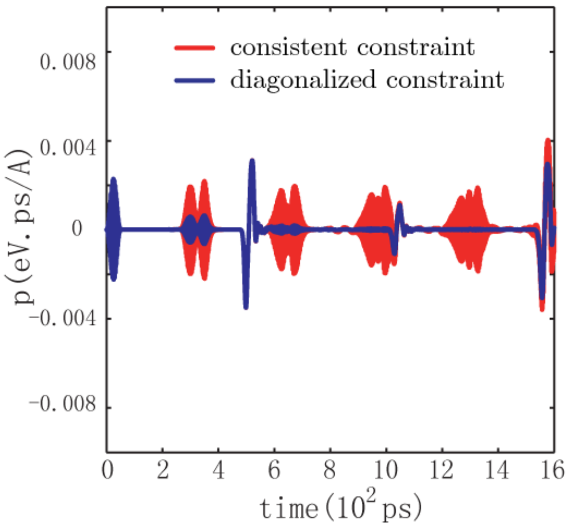


$$w(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

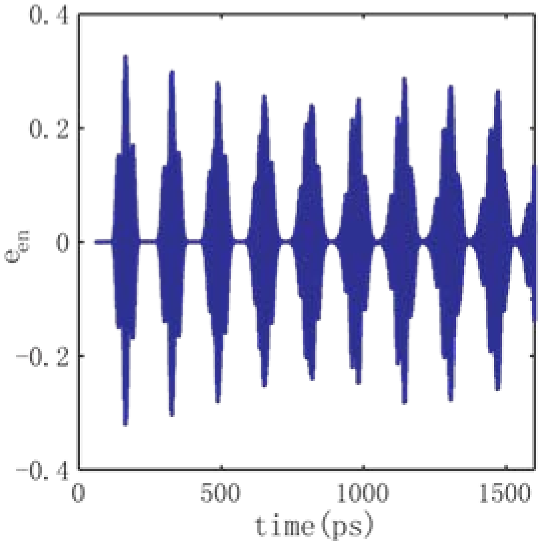
  - Initial condition



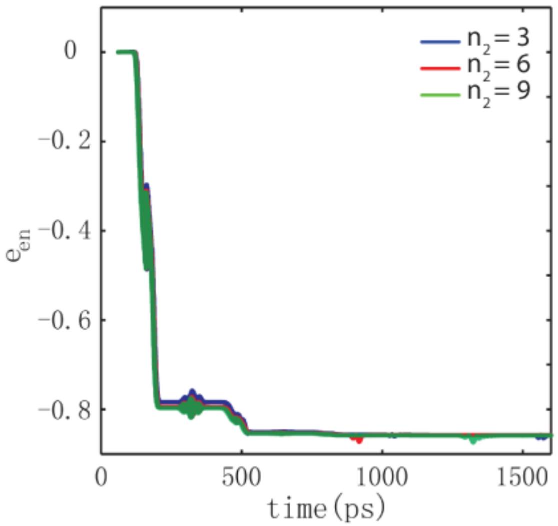
Numerical Test – 1D



linear momentum history



error in energy with consistent constraint

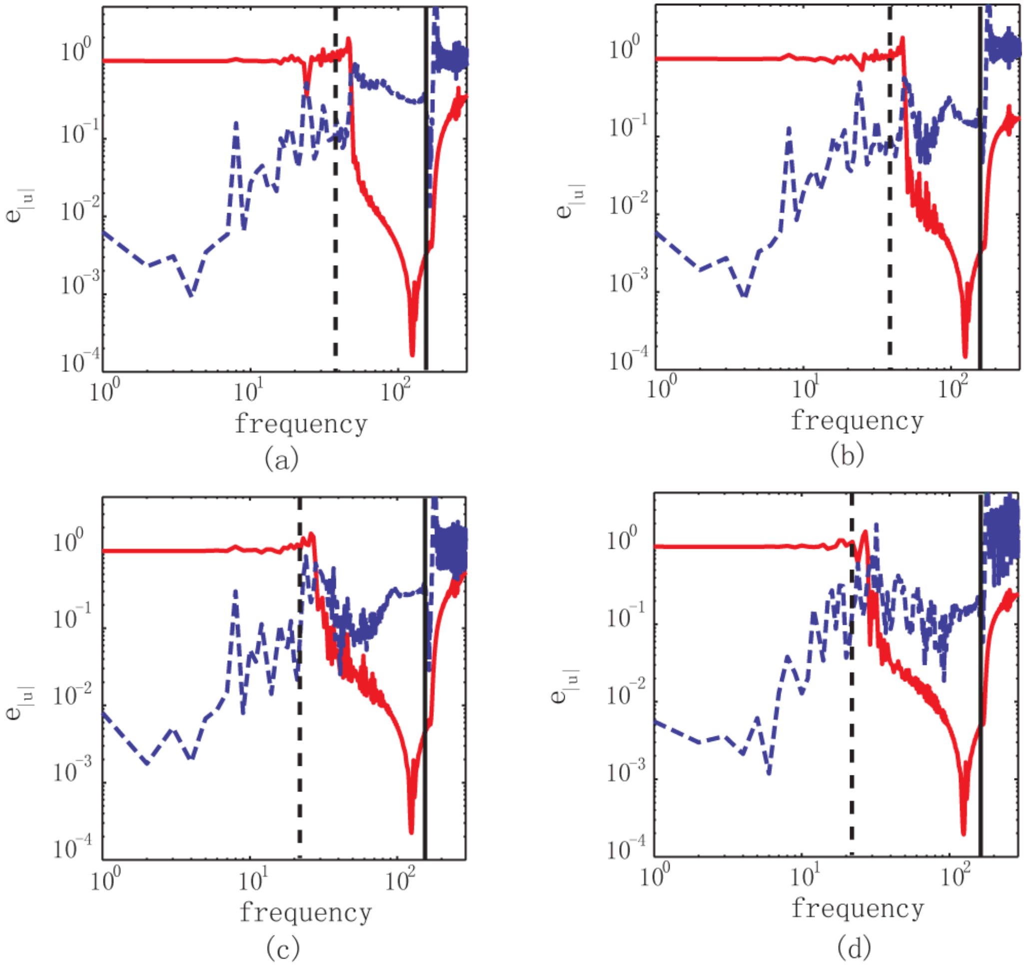


error in energy with diagonalized constraint

$$\boxed{error = \frac{A(t) - A_0}{A_0}}$$

Numerical Test – 1D

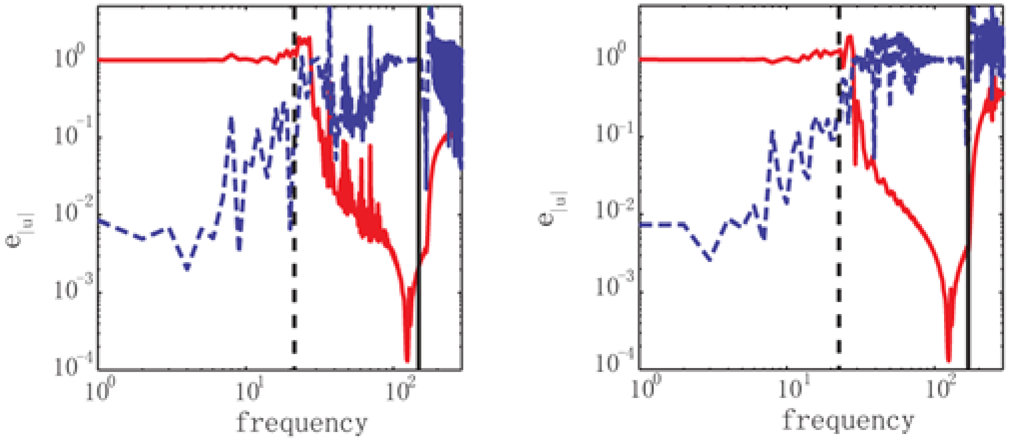
- Spurious Reflection



Reflectivity and transmission for n_2 overlaid elements with n_1 atoms per element with ***diagonalized constraint matrix***. (a) $n_1 = 4, n_2 = 3$ (b) $n_1 = 4, n_2 = 6$ (c) $n_1 = 7, n_2 = 3$ (d) $n_1 = 7, n_2 = 6$

Numerical Test – 1D

- Spurious Reflection



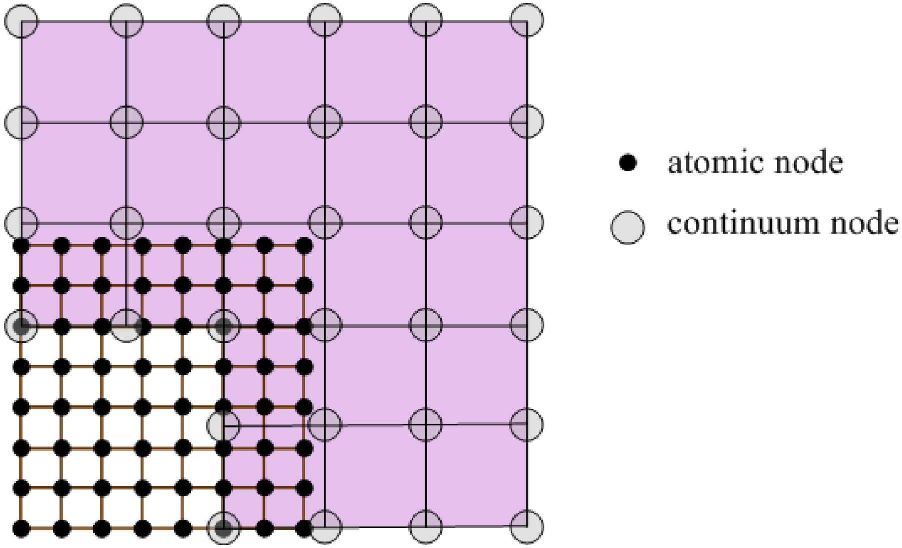
Reflectivity and transmission for the ***consistent constraint matrix***. (a) $n_1 = 7, n_2 = 3$ (b) $n_1 = 7, n_2 = 6$

  - *Low frequencies smoothly propagate into coarser scale.*
  - *The diagonalized constraint matrix can effectively eliminate the spurious reflection at the atomistic/continuum interface.*
  - *One-dimensional examples show that bigger overlapping domain gives better transmission of the low frequency wave.*

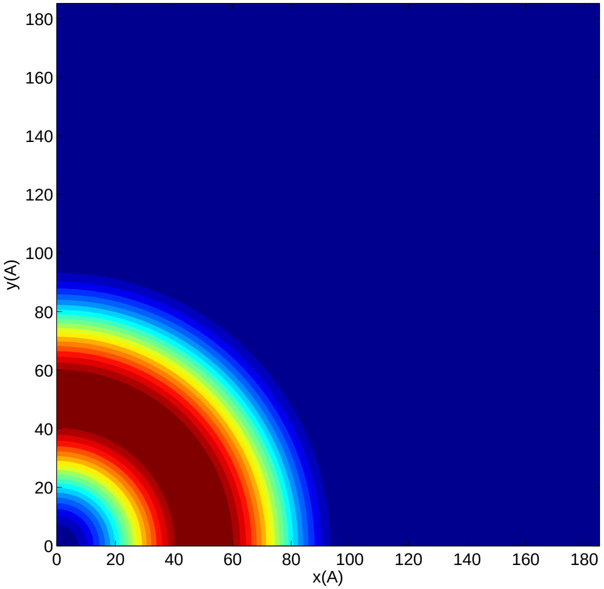
Numerical Test – 2D

- Two-dimensional example
  - Quadratic potential

$$U\left(r,\theta\right)=\frac{1}{2}k_a\left(r-r_0\right)^2+\frac{1}{2}k_\theta\left(\theta-\theta_0\right)^2$$

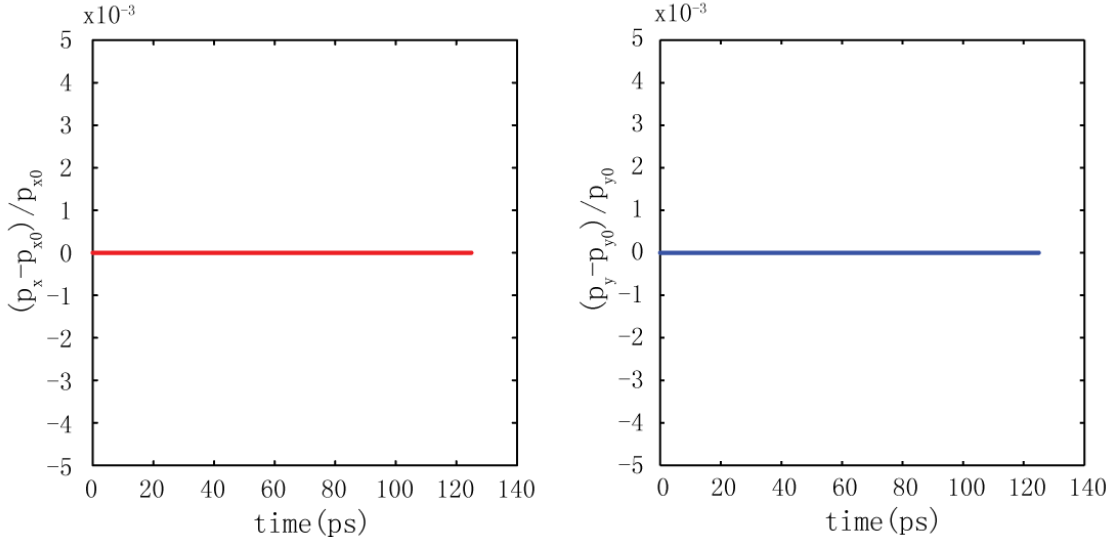


Coupling model



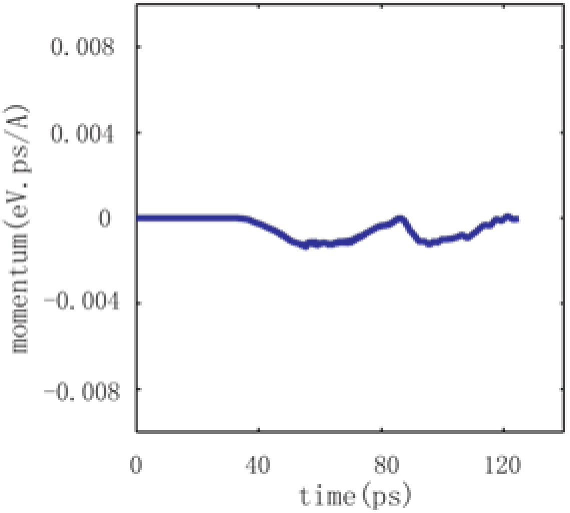
Initial displacement field

Numerical Test – 2D



error in linear momentum of 2D tests

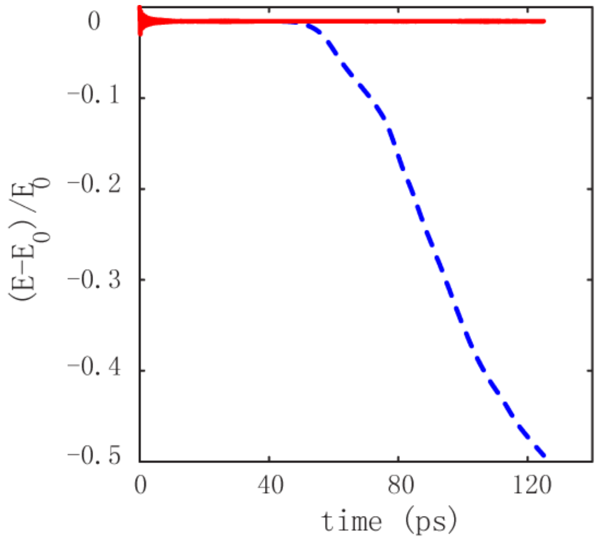
$$n_1 = 4, n_2 = 1$$



time history angular momentum of 2D tests

Numerical Test – 2D

- *Both linear momentum and angular momentum are conserved.*
- *Energy conservation depends on the compatibility condition between the atomistic and continuum models. The consistent constraint matrix conserves energy while the diagonalized constraint matrix dissipates energy.*



error in energy of

two-dimensional tests

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Conclusions

- The bridging domain method conserves energy and momentum
- Oscillation of linear momentum and energy (1D), and angular momentum (2D) is observed as waves pass through the coupling domain
  - These quantities are restored after the wave exits the coupling domain
- Energy conservation depends on the constraint implementation:
  - The consistent constraint conserves total energy
  - The diagonalized constraint dissipates high frequency energy, eliminating reflections at the interface between different scales