MULTISCALE COUPLING OF MESHLESS METHOD AND MOLECULAR DYNAMICS

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Abstract

A multiscale modeling procedure, combining meshless method with molecular dynamics is developed in this paper. An intermediate oscillator is introduced to act as a media for the energy transfer between atom and continuum domains. Very smooth energy transfer is observed in our calculations for both 1D and 2D examples.

Keywords: multiscale, meshless, atomistic, intermediate oscillator.

Introduction

Most physical phenomena in nature involve a hierarchy of both spatial and temporal scales at different levels. Typical cases include protein folding, chemical reaction, turbulence, crack propagation in solid, or shear localization. To solve such kind of problems is often beyond the capability of one theoretical frame valid within a single scale, such as molecular dynamics and continuum mechanics.

Efforts seeking for multiscale methodologies spanning from atomistic to continuum domains can be traced back to the work by Sinclair (1971). Mullins *et al.* (1982) used finite element method to model the continuum domain slight away from the region near the crack tip where atomistic calculation is performed. Tadmor *et al*. (1996) developed the quasicontinuum (QC) method with capability to remesh according to the variation of the deformation gradient. Rudd *et al*. (1998) formulated a coarse-grained molecular dynamics (CGMD) method, derived directly from finite temperature MD through a statistical coarse graining procedure. Xiao *et al*. (2004) proposed a bridging domain method with linear combination of the continuum and atomic Hamiltonians at the overlapping domain, avoiding spurious wave reflections. Till now, most of the multiscale methods belong to handshaking approach. Recently, Cai *et al*. (2000) and Park *et al*. (2004) introduced a general Langevin equation as a boundary to atom region, also to eliminate wave reflections.

In this paper, motivated by Xiao *et al.* (2004), we study wave propagation with a modified multiscale modeling method, coupling meshless method with molecular dynamics. Very smooth energy transfer between atom and continuum domains is achieved.

Coupling Model

The coupled model (Fig.1) includes atomistic and continuum domains, and an intermediate oscillator. The oscillator acts as a
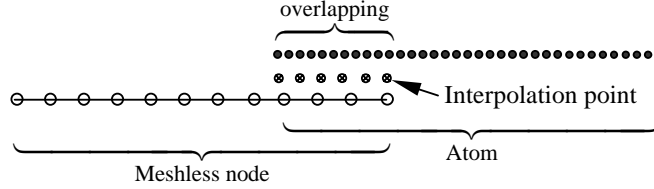

Figure 1. Coupling model

media for the energy transfer between atomistic and continuum domains. The total Hamiltonian of the extended system is a combination of the Hamiltonians of the atomistic and continuum domains, and the intermediate oscillator,

$$H = \sum_{i}^{atom} \frac{\mathbf{p}_i^{\mathrm{T}}\mathbf{p}_i}{2(1-\alpha)m_i} + (1-\alpha)V + \sum_{I}^{node} \frac{\mathbf{p}_I^{\mathrm{T}}\mathbf{p}_I}{2\alpha m_I} + \alpha W + \sum_{\Theta}^{Media}\left(\frac{\mathbf{p}_{g\Theta}^{\mathrm{T}}\mathbf{p}_{g\Theta}}{2Q} + \lambda_{\Theta}^{\mathrm{T}}\mathbf{g}_{\Theta} + \frac{K}{2}\mathbf{g}_{\Theta}^{\mathrm{T}}\mathbf{g}_{\Theta}\right) \qquad (1)$$

where i stands for the atoms, I for meshless node, and Θ for the interpolation point in the overlapping region. $\alpha\,(\in[0,1])$ is the scale parameter, allowing for a grade energy transfer between atomistic and continuum domains. In practice, α takes the form of arctangent function. Q, K, λ, $\mathbf{p}_{g\Theta}$ and $\mathbf{g}_{\Theta}$ are the generalized mass, stiffness, Lagrange force, momentum, and coordinate of the intermediate oscillator respectively. $\mathbf{p}_{g\Theta}$ and $\mathbf{g}_{\Theta}$ are obtained by the following,

$$\mathbf{g}_{\Theta} = \sum_{I} N_{\Theta I}\mathbf{u}_I - \sum_{i} N_{\Theta i}\mathbf{u}_i \qquad\qquad \mathbf{p}_{g\Theta} = Q\left(\sum_{I}\frac{N_{\Theta I}}{\alpha m_I}\mathbf{p}_I - \sum_{i}\frac{N_{\Theta i}}{(1-\alpha)m_i}\mathbf{p}_i\right) \qquad (2)$$

At each point Θ, there is a "particle" with mass Q (a small value for quick energy transfer in calculations), subjected to a constant force (penalty method) and variable Lagrange force (Lagrange multiplier method). $N_{\Theta I}$ and $N_{\Theta i}$ are shape functions of node I and atom i respectively evaluated at point Θ. The shape function is constructed via MLS approach (Belytschko *et al.*, 1994). The equations of motion, derived from Hamiltonian canonical equations, can be integrated with velocity Verlet integrator, using multiple- time step algorithm**:**

$$\mathbf{u}_{I(n+1)} = \mathbf{u}_{I(n)} + \dot{\mathbf{u}}_{I(n)}\Delta T + \frac{1}{2}\frac{\mathbf{f}_{I(n)}}{m_I}\Delta T^2 \qquad\qquad \mathbf{u}_{i\left(n+\frac{j+1}{N}\right)} = \mathbf{u}_{i\left(n+\frac{j}{N}\right)} + \dot{\mathbf{u}}_{i\left(n+\frac{j}{N}\right)}\Delta t + \frac{1}{2}\frac{\mathbf{f}_{i\left(n+\frac{j}{N}\right)}}{m_i}\Delta t^2$$

$$\mathbf{f}_{I\left(n+\frac{j+1}{N}\right)} = \mathbf{f}_{I(n+1)}^{\mathrm{int}} + \left(\mathbf{f}_{I\left(n+\frac{j+1}{N}\right)}^{\lambda} + \mathbf{f}_{I\left(n+\frac{j+1}{N}\right)}^{g}\right)/\alpha \qquad \mathbf{f}_{i\left(n+\frac{j+1}{N}\right)} = \mathbf{f}_{i\left(n+\frac{j+1}{N}\right)}^{\mathrm{int}} + \left(\mathbf{f}_{i\left(n+\frac{j+1}{N}\right)}^{\lambda} + \mathbf{f}_{i\left(n+\frac{j+1}{N}\right)}^{g}\right)/(1-\alpha) \qquad (3)$$

$$\dot{\mathbf{u}}_{I\left(n+\frac{j+1}{N}\right)} = \dot{\mathbf{u}}_{I\left(n+\frac{j}{N}\right)} + \frac{\Delta t}{2m_I}\left(\mathbf{f}_{I\left(n+\frac{j}{N}\right)} + \mathbf{f}_{I\left(n+\frac{j+1}{N}\right)}\right) \qquad \dot{\mathbf{u}}_{i\left(n+\frac{j+1}{N}\right)} = \dot{\mathbf{u}}_{i\left(n+\frac{j}{N}\right)} + \frac{\Delta t}{2m_i}\left(\mathbf{f}_{i\left(n+\frac{j}{N}\right)} + \mathbf{f}_{i\left(n+\frac{j+1}{N}\right)}\right)$$

where, $j = 0,1,2\cdots,N-1$. ΔT is the time step for continuum, Δt for atomistic region. $\mathbf{f}_I^{\mathrm{int}}$, $\mathbf{f}_i^{\mathrm{int}}$ are the interal force for continuum and atom respectively. The generalized forces are

$$\mathbf{f}_I^{\lambda} = -\sum_{\Theta}\lambda_{\Theta}N_{\Theta I} \qquad\qquad \mathbf{f}_I^{g} = -K\left(\sum_{\Theta}\sum_{J}N_{\Theta I}N_{\Theta J}\mathbf{u}_J - \sum_{\Theta}\sum_{j}N_{\Theta I}N_{\Theta j}\mathbf{u}_j\right)$$

$$\mathbf{f}_j^{\lambda} = \sum_{\Theta}\lambda_{\Theta}N_{\Theta j} \qquad\qquad \mathbf{f}_i^{g} = K\left(\sum_{\Theta}\sum_{J}N_{\Theta i}N_{\Theta J}\mathbf{u}_J - \sum_{\Theta}\sum_{j}N_{\Theta i}N_{\Theta j}\mathbf{u}_j\right) \qquad (4)$$

Results and Discussion

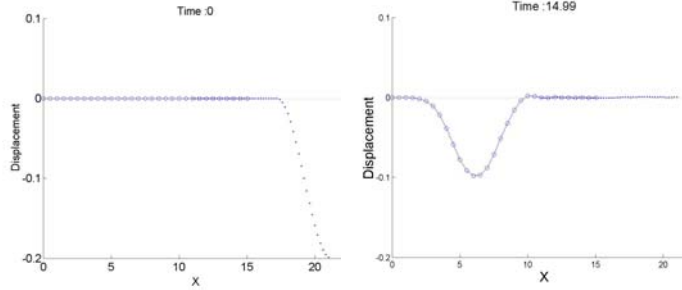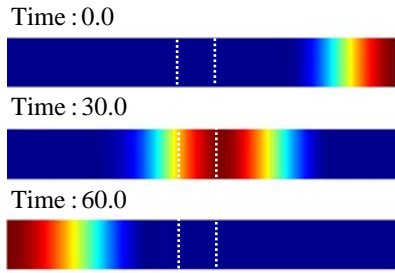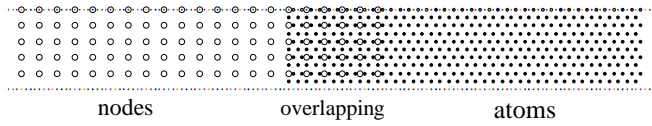**Figure 2.** A wave propagates in 1D domain with overlapping area.

Figure 3. Time history of energy transfer in 1D domain.

nodes   overlapping   atoms

Figure 4. The 2D model.

Time : 0.0

Time : 30.0

Time : 60.0

Figure 5. A plane wave propagates in a 2D domain with overlapping area.
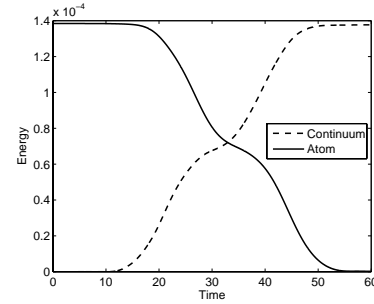

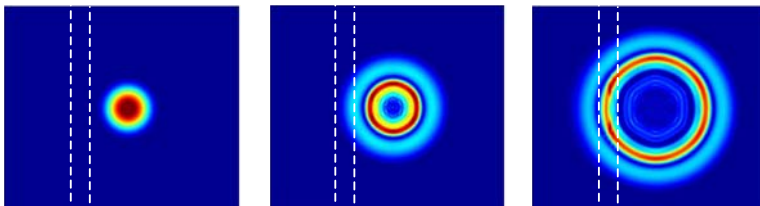**Figure 6.** Time history of energy transfer in 2D domain. (plane wave)

Figure 7. A circular wave propagates in 2D domain with overlapping area.

In the 1D and 2D models, nearest neighbor (NN) interaction in atom domain is represented with harmonic potential. The elastic properties of continuum domain are equivalent to that of atomistic domain. The units are reduced.

The lognitudinal wave propagation in 1D model is shown in Fig.2. The distances between the NN atoms and NN nodes are 0.2 and 0.5, respectively. There are 30 nodes and 75 atoms in 1D model. The two ends are traction free. An initial displacement of one-quarter of sinusoid is applied as in Fig.2 (time=0.0). The time steps for atoms and nodes are 0.01

and 0.05, respectively. Figure 3 shows a smooth energy (sum of kinetic and potential energy) transfer from atom to continuum.

Figure 4 is a 2D slab model, with 105 nodes and 400 atoms. The distances between the NN atoms and NN nodes are 0.2 and 0.4, respectively. Periodic boundary condition is applied along the vertical direction and the two horizontal ends are traction free. The initial displacement is similar to that in 1D model. Figure 5 demonstrates the plane wave propagation in the slab model. Again, energy transfers smoothly between the two domains (Fig. 6).

Figure 7 exhibits the propagation of a circle wave in a square model. The overlapping zone locates between the dashed lines, the left to which is continuum domain, and the right to which is atom domain. The wave crosses the bridging domain in a good manner, with minor wave reflection observed. For comparison, Park et al. (2004) adopted generalized Langevin equation as the boundary condition for atom domain, where the refection wave is not neglectable.

Conclusions

A multiscale modeling method, combining meshless method with molecular dynamics, is developed in this paper, in which an intermediate oscillator is introduced acts as a media for the energy transfer between atom and continuum domains. 1D and 2D models are studied with our approach. Smooth energy transfer is observed in our calculations.

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