Bridging Domain Multiscale Method

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Summary

A bridging domain method for coupling continuum models with molecular models is described. In this method, the continuum and molecular domains are overlapped in a bridging subdomain, where the Hamiltonian is taken to be a linear combination of the continuum and molecular Hamiltonians. We enforce the compatibility in the bridging domain by Lagrange multipliers or by the augmented Lagrangian method. An explicit algorithm for dynamic solutions is developed. In this paper, the bridging domain multiscale method is employed to study nanotube-based composites.

Introduction

Concurrent methods for coupling molecular dynamics models with continuum or quasicontinuum models are useful for studying local phenomena such as fracture. They permit the use of far fewer equations than in strict molecular dynamics models, since the resolution in the subdomain modeled by continuum mechanics can be far coarser than in the molecular dynamics model. In these coupled models, the continuum subdomain serves primarily as a boundary model that provides the low frequency impedance and a sink for the energy associated with outgoing waves of the molecular dynamics model. Such models are often called multiscale because the spectra (and the resolution) of the continuum model have much smaller cutoff frequencies than the molecular dynamics model.

Abraham et al. [1], in a pioneering work, developed a methodology that couples a tight-binding quantum mechanics approximation with molecular dynamics and in turn with a finite element continuum model. The molecular dynamics model was coupled with the continuum model in a "handshake" domain in which the two Hamiltonians were averaged. To reduce spurious reflections into the molecular dynamics domain, damping was used in the handshake region, although the damping was not based on any rigorous theory. In most cases, it appears that the finite element continuum model had to be nearly of the scale of interatomic distances at the atomistic/continuum interface to perform well.

A coupling method called the bridging domain method is developed in this paper. In this method, the molecular model and continuum model overlap at their junctions in a bridging domain. This method can avoid spurious wave reflection without any additional filtering or damping. In effect, the method projects the fine scale solution onto the coarse scale solution in the bridging domain at each time

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step. Thus it filters the high frequency components at the interface. Furthermore, since the method is not based on linearization, it was surmised that it would apply to nonlinear problems. Based on the test problems we have studied so far, this appears to be the case.

Bridging Domain Multiscale Method

In an isolated system of atoms or molecules, the total energy, the sum of the kinetic and potential energies of the molecules, is constant in time and identified as the Hamiltonian H^M, which is given by

$$H^M\left(\mathbf{x}_I^{(}t), \mathbf{p}_I^M(t)\right) = \sum_I \frac{1}{2m_I}\mathbf{p}_I^M \cdot \mathbf{p}_I^M + W^M\left(\mathbf{x}_I(t)\right) = constant \qquad (1)$$

where m_I is the mass of atom I, $\mathbf{x}_I$ is the position of atom I and $\mathbf{x}_I = \mathbf{X}_I + \mathbf{d}_I$ ($\mathbf{X}_I$ is the original position of atom I and $\mathbf{d}_I$ is the displacement of atom I); $\mathbf{p}_I^M$ is the momentum and defined by $\mathbf{p}_I^M = m_I\dot{\mathbf{x}}_I = m_I\dot{\mathbf{d}}_I$. $W^M(\mathbf{x})$ is the potential function which is the sum of the energies due to any force fields, such as pair-wise interaction of the atoms, three-body potentials or others. The total potential is

$$W^M = -W_M^{ext} + W_M^{int} = -\sum_I \mathbf{f}_I^{ext}\mathbf{d}_I + \sum_{I,J>I} w_M\left(\mathbf{x}_I, \mathbf{x}_J\right) \qquad (2)$$

The well known Hamiltonian canonical equations of motion are

$$\dot{\mathbf{p}}_I^M = -\frac{\partial H}{\partial \mathbf{x}_I} = -\frac{\partial W^M}{\partial \mathbf{x}_I}, \quad \dot{\mathbf{x}}_I = \dot{\mathbf{d}}_I = \frac{\partial H}{\partial \mathbf{p}_I^M} = \frac{\mathbf{p}_I^M}{m_I} \qquad (3)$$

Eq. (3) can be combined to yield

$$m_I\ddot{\mathbf{d}}_I = -\frac{\partial W^M}{\partial \mathbf{x}_I} = \frac{\partial W_M^{ext}}{\partial \mathbf{d}_I} - \frac{\partial W_M^{int}}{\partial \mathbf{d}_I} = \mathbf{f}_I^{ext} - \mathbf{f}_I^{int} \qquad (4)$$

where $\mathbf{f}_I^{int} = \partial W_M^{int}/\partial \mathbf{d}_I$.

In the continuum domain, the Hamiltonian is given by

$$H^C = K^C + W^C = \int_{\Omega_0^C} \frac{1}{2}\rho\mathbf{v}^T\mathbf{v}d\Omega_0^C + W^C \qquad (5)$$

$$W^C = -W_C^{ext} + W_C^{int} = -\sum_I \mathbf{f}_I^{extC}\mathbf{u}_I + \int_{\Omega_0^C} \rho_0 w_C\left(\mathbf{F}\right)d\Omega_0^C \qquad (6)$$

Note that we use the same symbol for the nodal forces for the continuum model once it is discretized by a finite element method.

The model for the bridging domain coupling method is shown in Figure 1. The complete domain in the initial configuration is denoted by Ω_0. The domain is subdivided into two subdomains: the molecular subdomain denoted by Ω_0^M, and the continuum subdomain, denoted by Ω_0^C. The overlap of these two domains is denoted by Ω_0^{int} in the initial configuration; Ω_0^{int} is called the bridging domain and it corresponds to the overlap of the two subdomains; Γ_0^α denotes the edges of the continuum subdomains and Γ_1^α denotes the edges of the molecular subdomain.
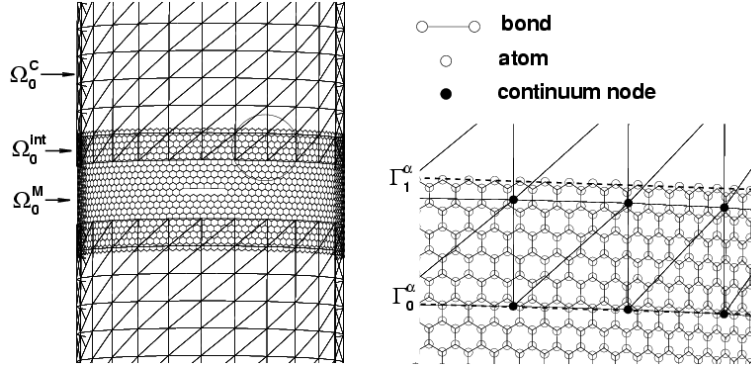

Figure 1: Bridging domain model for a nanotube; finite elements are indicated by lines that connect continuum nodes

In the bridging domain method, the total energy is taken to be a linear combination of the molecular and continuum energies. A scaling parameter α is introduced in the bridging subdomain, i.e. the overlapping subdomain. The parameter α is defined as $\alpha = l(\mathbf{X})/l_0$ where $l(\mathbf{X})$ is the orthogonal projection of $\mathbf{X}$ onto Γ_0^α and l_0 is the length of this orthogonal projection to Γ_1^α. The Hamiltonian for the complete domain is taken to be a linear combination of the molecular and continuum Hamiltonians

$$
\begin{aligned}
H &= (1 - \alpha) H^M + \alpha H^C \\
&= \sum_I (1 - \alpha(\mathbf{X}_I)) \frac{\mathbf{p}_I^M \cdot \mathbf{p}_I^M}{2m_I} + (1 - \alpha) W^M + \sum_I \alpha(\mathbf{X}_I) \frac{\mathbf{p}_I^C \cdot \mathbf{p}_I^C}{2M_I} + \alpha W^C
\end{aligned} \tag{7}
$$

The two models are constrained on the overlapping subdomain Ω_0^{int} by

$$
\mathbf{g}_I = \{g_{iI}\} = \{u_i(\mathbf{X}_I) - d_{iI}\} = \left\{ \sum_J N_J(\mathbf{X}_I) u_{iJ} - d_{iI} \right\} = 0 \tag{8}
$$

i.e. the atomic displacements are required to conform to the continuum displacements at the positions of the atoms. The constraints are applied to all components of the displacements. In the Lagrange multiplier method [2], the total Hamiltonian

is written as:

$$H_L = H + \lambda^T \mathbf{g} = H + \sum_I \lambda_I^T \mathbf{g}_I \tag{9}$$

where $\lambda_I = \{\lambda_{iI}\}$ is a vector of Lagrange multipliers whose components correspond to the components of the displacement of atom I. Note that the Lagrange multipliers are assigned to the discrete positions of atoms.

The equations of motion for the Lagrange multiplier method are

$$\alpha(\mathbf{X}_I)\dot{\mathbf{p}}_I^C = -\frac{\partial H_L}{\partial \mathbf{u}_I}, \quad \alpha(\mathbf{X}_I)\dot{\mathbf{u}}_I = \frac{\partial H_L}{\partial \mathbf{p}_I^C} \quad in \quad \Omega_0^C \tag{10}$$

$$(1 - \alpha(\mathbf{X}_I))\dot{\mathbf{p}}_I^M = -\frac{\partial H_L}{\partial \mathbf{d}_I}, \quad (1 - \alpha(\mathbf{X}_I))\dot{\mathbf{d}}_I = \frac{\partial H_L}{\partial \mathbf{p}_I^M} \quad in \quad \Omega_0^M \tag{11}$$

These can be combined to yield

$$\begin{aligned} \bar{M}_I \ddot{\mathbf{u}}_I &= \mathbf{f}_I^{extC} - \mathbf{f}_I^{intC} - \mathbf{f}_I^{LC} &&in \quad \Omega_0^C \\ \bar{m}_I \ddot{\mathbf{d}}_I &= \mathbf{f}_I^{ext} - \mathbf{f}_I^{int} - \mathbf{f}_I^{L} &&in \quad \Omega_0^M \end{aligned} \tag{12}$$

where $\bar{M}_I = \alpha(\mathbf{X}_I)M_I$, $\bar{m}_I = (1 - \alpha(\mathbf{X}_I))m_I$

The internal forces are

$$\mathbf{f}_I^{intC} = \int_{\Omega_0^C} \alpha(\mathbf{X})\rho_0 \frac{\partial w_C(\mathbf{F})}{\partial \mathbf{u}_I} d\Omega_0^C, \quad \mathbf{f}_I^{int} = (1 - \alpha(\mathbf{X}_I)) \sum_{I,J>I} \frac{\partial w_M(\mathbf{x}_I, \mathbf{x}_J)}{\partial \mathbf{d}_I} \tag{13}$$

The forces $\mathbf{f}_I^{LC}$ and $\mathbf{f}_I^{L}$ are due to the constraints enforced by the Lagrange multipliers and they are:

$$\mathbf{f}_I^{LC} = \sum_J \lambda_J^T \frac{\partial \mathbf{g}_J}{\partial \mathbf{u}_I} = \sum_J \lambda_J^T \mathbf{G}_{JI}^C \quad \mathbf{f}_I^{L} = \sum_J \lambda_J^T \frac{\partial \mathbf{g}_J}{\partial \mathbf{d}_I} = \sum_J \lambda_J^T \mathbf{G}_{JI}^M \tag{14}$$

where $N_{IJ} = N_I(\mathbf{X}_J)$ and $\mathbf{G}_{JI}^C = \left[\frac{\partial \mathbf{g}_J}{\partial \mathbf{u}_I}\right] = [N_{JI}\mathbf{I}]$, $\mathbf{G}_{JI}^M = \left[\frac{\partial \mathbf{g}_J}{\partial \mathbf{d}_I}\right] = [-\delta_{IJ}\mathbf{I}]$

Explicit Algorithm

The Verlet algorithm is used here for time-integration of above equations of motion. the accelerations are obtained from Eq. (12) without considering the forces due to the constraints, so

$$\begin{aligned} \ddot{\mathbf{u}}_{I(n+1)} &= \frac{1}{M_I}\left[\mathbf{f}_{I(n+1)}^{extC} - \mathbf{f}_{I(n+1)}^{intC}\right] &&in \quad \Omega_0^C \\ \ddot{\mathbf{d}}_{I(n+1)} &= \frac{1}{\bar{m}_I}\left[\mathbf{f}_{I(n+1)}^{ext} - \mathbf{f}_{I(n+1)}^{int}\right] &&in \quad \Omega_0^M \end{aligned} \tag{15}$$

We then obtain the trial velocities:

$$
\begin{aligned}
\dot{\mathbf{u}}^*_{I(n+1)} &= \dot{\mathbf{u}}_{I(n)} + \tfrac{1}{2}\left[\ddot{\mathbf{u}}_{I(n)} + \ddot{\mathbf{u}}_{I(n+1)}\right]\Delta t \quad in \quad \Omega^C_0 \\
\dot{\mathbf{d}}^*_{I(n+1)} &= \dot{\mathbf{d}}_{I(n)} + \tfrac{1}{2}\left[\ddot{\mathbf{d}}_{I(n)} + \ddot{\mathbf{d}}_{I(n+1)}\right]\Delta t \quad in \quad \Omega^M_0
\end{aligned}
\tag{16}
$$

The velocities at time step $n+1$ can be alternatively expressed as:

$$
\dot{\mathbf{u}}_{I(n+1)} = \dot{\mathbf{u}}^*_{I(n+1)} - \bar{M}_I^{-1}\Delta t \sum_J \mathbf{G}^C_{JI}\lambda_J
\tag{17}
$$

$$
\dot{\mathbf{d}}_{I(n+1)} = \dot{\mathbf{d}}^*_{I(n+1)} - \bar{m}_I^{-1}\Delta t \sum_J \mathbf{G}^M_{JI}\lambda_I
\tag{18}
$$

The above velocities must satisfy the constraints (their time derivatives). Therefore, the unknown Lagrange multipliers can be obtained by solving the following equations:

$$
\sum_L \mathbf{A}_{IL}\lambda_L = \mathbf{g}^*_I
\tag{19}
$$

where $\mathbf{A}_{IL} = \Delta t\bar{M}_I^{-1}\sum_J N_{JI}\mathbf{G}^C_{LJ} - \Delta t\bar{m}_I^{-1}\mathbf{G}^M_{LI}$ and $\mathbf{g}^*_I = \sum_J N_{JI}\dot{\mathbf{u}}^*_J - \dot{\mathbf{d}}^*_I$. To reduce the computational cost, the matrix $\mathbf{A}$ consisting of submatrices $\mathbf{A}_{IL}$ is diagonalized as a diagonal matrix. Once the lagrange multipliers is calculated, they are substituted into Eqs. (17) and (18) to update the velocities of nodes/atoms in the bridging domain.
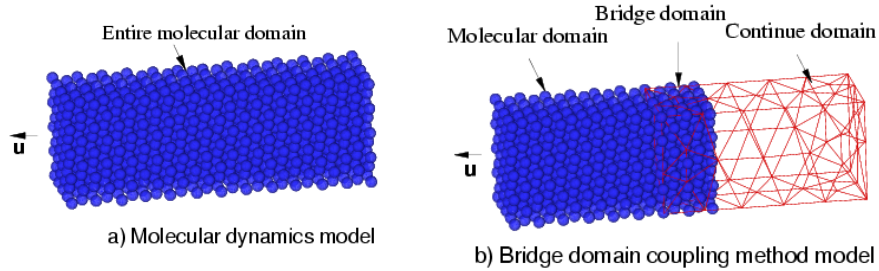
Verification of Multiscale Method

Figure 2: Numerical models of an Al crystalline bar

We consider an Aluminum (Al) crystalline bar with the following dimensions: the length of 5.6 nm, the width of 1.6 nm, and the thickness of 1.6 nm. There are 2025 atoms in this bar. Figure 2 illustrates the molecular and bridging domain multiscale models of this Al crystalline bar. In the multiscale model, there are 1377 atoms and 55 finite elements. The calculated stress-strain evolution at the room temperature is illustrated in Figure 3 when the bar is under uniaxial tension or compression. The stress-strain relation is almost linear and the calculated Young's modulus is around 74 GPa. It can be seen that the multiscale simulation gives the same results as molecular dynamics.
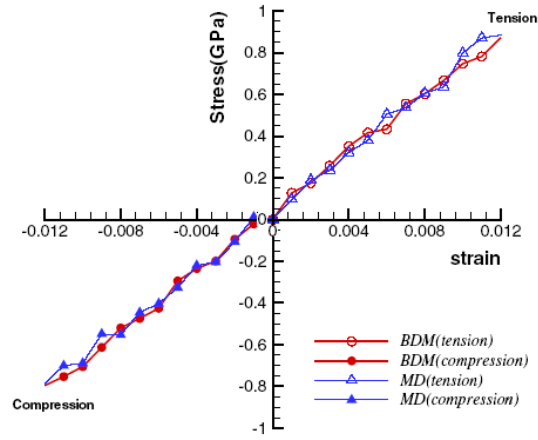
Figure 3: Comparison of stress-strain evolutions at the room temperature

Multiscale Modeling and Simulation of Nanocomposites

We employ the bridging domain coupling method to study the failure behavior of fracture mode I for nanotube-based aluminum composites, shown in Figure 4. Figure 5 illustrates that when even 2% pristine nanotubes are embedded into the aluminum matrix, the strength of nanocomposites can be improved by two times.
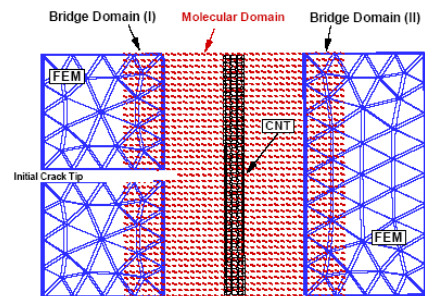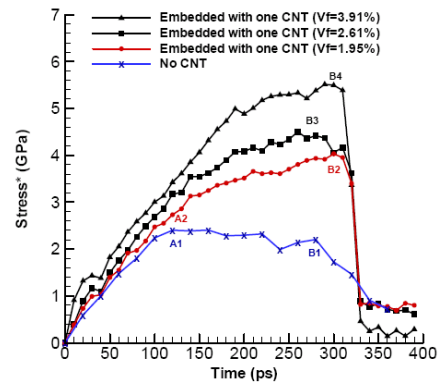

Figure 4: Coupling model of nanocomposites.

Figure 5: The effect of the volume of embedded nanotubes on strength.

References

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2. Belytschko, T., Liu, W. K. and Moran, B. (2001): *Nonlinear Finite Elements for Continua and Structures*, Wiley: New York