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Conservation properties of the bridging domain method for coupled molecular/continuum dynamics

*** Mei Xu[1], Ted Belytschko[2]**

[1] Theoretical and Applied Mechanics
2145 Sheridan Rd., Northwestern University,
Evanston, IL 60208-3111, USA
m-xu@northwestern.edu

[2] Department of Mechanical Engineering
2145 Sheridan Rd., Northwestern University,
Evanston, IL 60208-3111, USA
tedbelytschko@northwestern.edu

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ABSTRACT

To reduce the computational cost of simulations requiring nanoscale resolution, it is often highly effective to identify regions where molecular dynamics is necessary to handle bond breaking or resolve nanostructural features and decompose the domain into a continuum and atomistic subdomains. This domain decomposition requires a coupling method to enforce compatibility between these domains. In this presentation, the conservation properties of the bridging domain method are analyzed. In the bridging domain method[1,2], Hamiltonian of the total system is defined as a linear combination of the energy of the subdomains plus a constraint term. The constraint term is implemented by Lagrange multipliers that enforce compatibility between the continuum and atomistic displacements in the overlapping region of each subdomain. The element size in the continuum model does not need to be comparable with the lattice spacing of the atomistic model, which makes it more efficient than earlier handshaking methods[3].

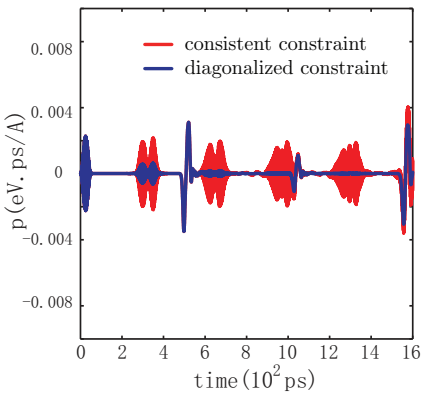

Figure 1: History of linear momentum of one dimensional coupled model with consistent and diagonalized constraints for three overlaid elements with three atoms per element.

The bridging domain method is proven to conserve momentum and energy. If the constraint equations are diagonalized, compatibility between the continuum and atomistic subdomains is not satisfied exactly, which results in energy dissipation. This approximation has useful properties of reducing spurious reflections at the interface of different resolution and reduces the computational cost of the bridging domain method.

The properties of the bridging domain method were studied in both one- and two-dimensional wave propagation problems and comparisons were drawn between solutions with consistent and diagonalized constraint matrices. In one-dimensional problems, a moderate fluctuation in both the total momentum (see Fig. 1) and energy is observed as the wave passes through the boundary of the coupling region, but it is restored perfectly after the wave passes. Both momentum and energy are perfectly conserved in two-dimensional problems with the consistent constraint. When using consistent matrix, spurious reflections are created as the wave passes through the interface of atomistic and continuum models. This spurious reflection is greatly reduced when the constraint matrix is diagonalized. Most of the reflections between the cutoff frequency of the atomistic and continuum model are eliminated (Fig. 2), although as a result, energy is dissipated. The diagonalized constraint matrix acts as a low pass filter, effectively removing 90% of the high-frequency energy while leaving the low frequency content almost unaffected.

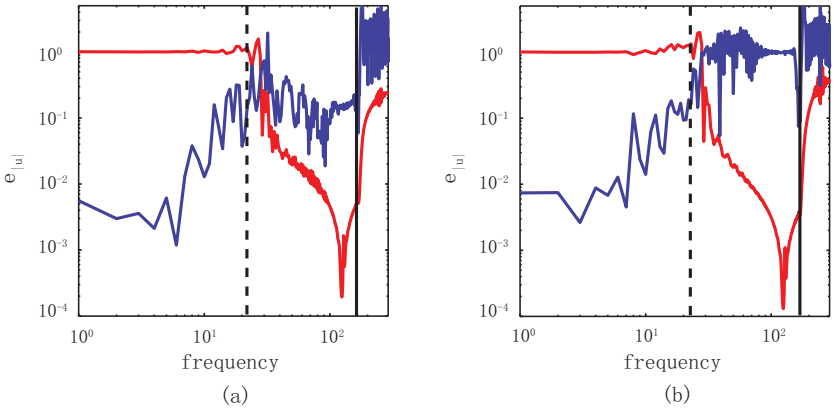

Figure 2: Reflectivity (blue) and transmission (red) for three overlaid elements with seven atoms per element. (a) diagonalized constraint; (b) consistent constraint (The dashed and solid vertical lines are the cutoff frequency of the continuum and the atomic models, respectively).

The numerical results confirm the bridging domain method retains the conservation properties when a consistent constraint matrix is used. It is also shown that the diagonalized constraint has some attractive features. It conserves system momentum, drastically suppresses spurious reflection at the interface of different resolution, and it is computationally cheaper to implement.

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