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MULTISCALE SIMULATION BASED ON MOVING KRIGING METHOD

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ABSTRACT

A multiscale simulation is developed for coupling molecular dynamics (MD) and continuum mechanics models by incorporating Moving Kriging (MK) interpolation [1] and Lagrange multiplier technique. In this proposed method, the MK interpolation in conjunction with *layered domain of influence* concept [2] is employed over the entire domain, while the MD simulation is utilized only in the localize region. In the bridging subdomain, the Hamiltonian is postulated as the combination of the continuum and molecular Hamiltonians by using quadratic spline scaling parameter. Also, the compatibility of two simulations in the aforementioned subdomain is enforced by applying Lagrange multiplier technique.

The effectiveness of the proposed method is reported through the numerical results in one dimensional lattice with Lennard-Jones (LJ) 6-12 potential. Additionally, a multiple-time-step Verlet algorithm is used for time integration in the entire domain.

As a result, the proposed method can diminish the spurious wave reflection compare with edge-to-edge method, where the high frequency wave is reflected back into the

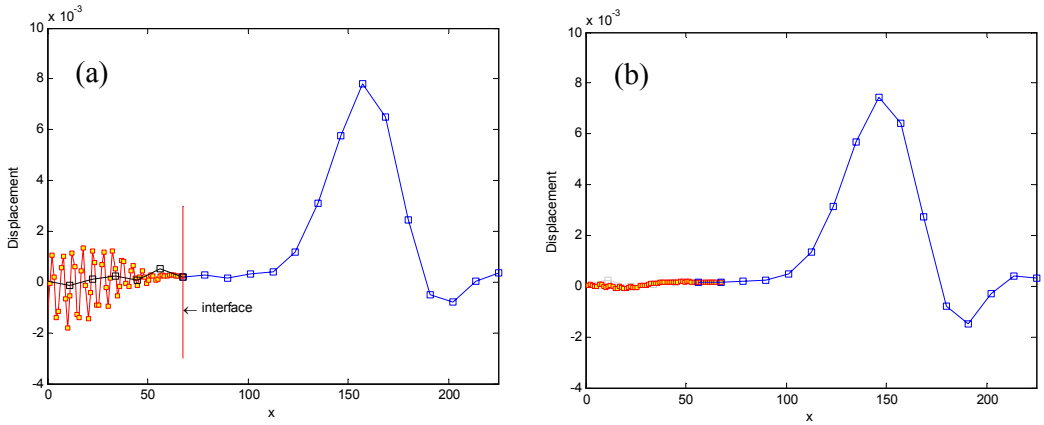

Figure1. Comparison of displacement between (a) edge-to-edge method and (b) proposed method (1-element overlapping).

molecular region at the interface as illustrated in Figure 1. Furthermore, the time history of energy remains in molecular domain is also studied as depicted in Figure 2. It was found that only 0.1% and 0.06% of normalized energy remain in molecular domain by using 1- and 2-element overlapping respectively.

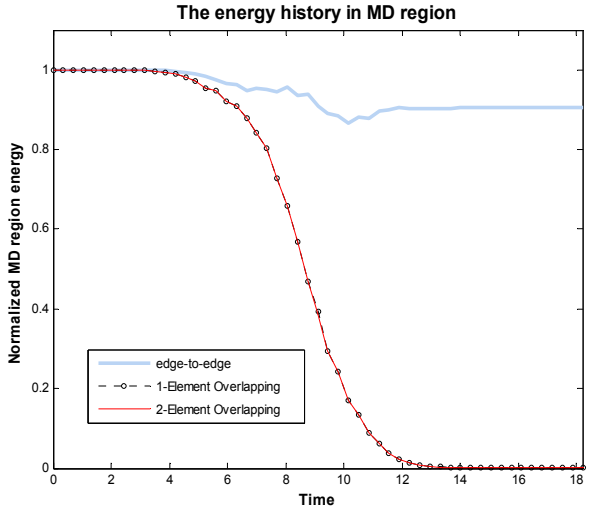

Figure2. The energy history in molecular region

A multiscale based on MK has been successfully proposed as an alternative technique to couple MD and continuum simulations. It does not require any filtering or damping function, simply to implement and can be straightforward extended to 2- and 3-dimensional analysis problems. Using this method, it can be eliminated spurious wave reflection in molecular domain. Consequently, the information at atomistic level can be transferred to continuum level without losing any significant phenomenon which is very crucial in multiscale or nanomechanics problems.

REFERENCES

[1] L. Gu, "Moving Kriging interpolation and element-free Galerkin method", *Int. J. Numer. Meth. Eng.*, Vol. **56**, pp. 1-11, (2003).

[2] K. Plengkhom and W. Kanok-Nukulchai, "An enhancement of finite element method with moving Kriging shape functions", *Int. J. Comp. Meth.*, Vol. **2**, pp. 451-475, (2005).

[3] G.J. Wagner and W.K. Liu, "Coupling of atomistic and continuum simulations using a bridging scale decomposition", *J. Comp. Phys.*, Vol. **190**, pp. 249-274, (2003).

[4] S.P. Xiao and T. Belytschko, "A bridging domain method for coupling continua with molecular dynamics", *Comput. Methods Appl. Mech. Eng.*, Vol. **193**, pp. 1645-1669, (2004).

[5] D. Qian, G.J. Wagner and W.K. Liu, "A multiscale projection method for the analysis of carbon nanotubes", *Comput. Methods Appl. Mech. Eng.*, Vol. **193**, pp. 1603-1632, (2004).

[6] H.S. Park and W.K. Liu, "An introduction and tutorial on multiple-scale analysis in solids", *Comput. Methods Appl. Mech. Eng.*, Vol. **193**, pp. 1733-1772, (2004).