# CONTINUUM-BASED SENSITIVITY ANALYSIS FOR ATOMISTIC/CONTINUUM COUPLING USING TWO-DIMENSIONAL BRIDGING SCALE DECOMPOSITION

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*Summary* This paper presents a sensitivity analysis method for two dimensional coupled atomistic and continuum problems using the bridging scale decomposition. We established a generalized variational formulation for the bridging scale and derived the continuum-based sensitivity analysis expressions. Two numerical examples are employed to demonstrate the accuracy of the sensitivity coefficients with respect to both material and sizing design variables.

## INTRODUCTION

The bridging scale method is recently proposed by Liu et al. [1] as an alternative approach of multi-scale simulation, in which the total displacement is decomposed into orthogonal coarse and fine scales. In bridging scale method, the continuum presentation exists everywhere while the molecular dynamics (MD) simulation is confined into a small region. The equations of motion describing the evolution of the MD system and the continuum can be separated. The unwanted fine scale degrees of freedom outside the MD region can be eliminated and mathematically accounted for in the form of an impedance force acting upon the boundary of the MD simulation.
The bridging scale method has been developed in a fully generalized three-dimensional setting. The design sensitivity analysis for bridging scale problems has been studied by Cho et al. [2] using semi-analytical method. The originality of our work lies in the energy based variational formulation developed for the bridging scale. The variational formulation provides a uniform and generalized system of equations from which the differential equations can be obtained naturally. Another benefit is that the sensitivity expressions can be developed in a continuum setting, avoiding many of the issues hampering the discrete approaches. Two numerical examples are presented to demonstrate the feasibility and accuracy of the sensitivity analysis method.

## VARIATINAL FORMULATION FOR BRIDGING SCALE DECOMPOSITION

The basic idea of the bridging scale method is to decompose the total solution **z** into coarse scale **u** and fine scale **v**.

$$\mathbf{z}(\mathbf{X}) = \mathbf{u}(\mathbf{X}) + \mathbf{v}(\mathbf{X}) = \mathbf{N}\mathbf{d} + \mathbf{Q}\mathbf{q} \tag{1}$$

The coarse scale can be represented using finite element (FE) shape functions. The fine scale is defined to be the projection of the MD displacements **q** onto the FE basis functions subtracted from the total solution **z**, which is equivalent to the MD displacements **q**. The equations of motion describing the MD and FE simulations can be separated as following

$$\mathbf{M}_A\ddot{\mathbf{q}} = \mathbf{f}(\mathbf{q}) \quad \text{and} \quad \mathbf{M}\ddot{\mathbf{d}} = \mathbf{N}^T\mathbf{f}(\mathbf{z}) \tag{2}$$

Using variational method, we developed the variational formulation for the bridging scale approach; that is

$$\int_0^{t_T} \bar{\mathbf{z}}_a^T \mathbf{M}_A \ddot{\mathbf{z}}_a\, dt = \int_0^{t_T} \bar{\mathbf{z}}_a^T \left[\mathbf{f}(\mathbf{z}_a, \mathbf{u}_h) + \mathbf{F}^{imp}\right] dt \quad \text{and} \quad \int_0^{t_T} \iint_\Omega \rho(\mathbf{X}) \bar{\boldsymbol{u}}^T \ddot{\boldsymbol{u}}\, d\Omega dt = \int_0^{t_T} \left[\bar{\mathbf{u}}^T \mathbf{f}(\mathbf{z}) - \iint_{\Omega_2} \bar{\boldsymbol{\varepsilon}}^T(\bar{\boldsymbol{u}}) \boldsymbol{\sigma}(\boldsymbol{u}) d\Omega_2\right] dt \tag{3}$$

where the coarse scale is treated as a continuous function $\boldsymbol{u}$, in order to achieve a general energy formulation. $\mathbf{F}^{imp}$ is the impedance boundary force which mimics the effect of the fine scale degrees of freedom outside the MD region. We demonstrated that the complete set of differential equations for the bridging scale method can be naturally derived from these variational equations. The displacement fields belong to a space $Z$ defined as

$$Z = \left\{\mathbf{z} = \mathbf{u} + \mathbf{v}, \boldsymbol{u} \in \left[H^m(\Omega)\right]^2 \mid \mathbf{u}, \mathbf{v} = 0 \text{ on } \mathbf{X} \in \Gamma^h,\ \boldsymbol{u}(\mathbf{X},0) = \boldsymbol{u}(\mathbf{X},t_T) = \mathbf{v}(\mathbf{X},0) = \mathbf{v}(\mathbf{X},t_T) = 0\right\} \tag{4}$$

## CONTINUUM-BASED SENSITIVITY ANALYSIS

The continuum sensitivity analysis is carried out using direct differentiation method. The sensitivity expressions are obtained by taking variation of the energy-based variational formulation with respect to design variables. After discretization, the resulting expressions can be used to solve for the sensitivity coefficients of the coarse and fine scale displacements, velocities and accelerations. The sensitivity differential equations obtained for material design variables $b_m$ and sizing design variables $b_s$ are shown in Eqs. 5 and 6, respectively.

$$\mathbf{M}_{A_{,b_m}} \ddot{\mathbf{z}}_a \delta b_m + \mathbf{M}_A \ddot{\mathbf{z}}'_a = \mathbf{f}_{,b_m}(\mathbf{z}_a, \mathbf{u}_h)\delta b_m + \mathbf{f}(\mathbf{z}'_a, \mathbf{u}'_h) + \mathbf{F}^{imp\,\prime} \quad \text{and} \quad \mathbf{M}_{,b_m}\ddot{\mathbf{d}}\delta b_m + \mathbf{M}\ddot{\mathbf{d}}' = \begin{bmatrix} \mathbf{N}^T\left[\mathbf{f}_{,b_m}(\mathbf{N}\mathbf{d} + \mathbf{Q}\mathbf{q})\delta b_m + \mathbf{f}(\mathbf{N}\mathbf{d}' + \mathbf{Q}\mathbf{q}')\right] \\ \mathbf{F}^{CB\,\prime} \end{bmatrix} \tag{5}$$

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$$\mathbf{M}_A\ddot{\mathbf{z}}'_a = \mathbf{f}\left(\mathbf{z}'_a,\mathbf{u}'_h\right)+\mathbf{F}^{imp\,\prime} \quad \text{and} \quad \hat{\mathbf{M}}_{,b_s}\ddot{\mathbf{d}}\delta b_s + \hat{\mathbf{M}}\ddot{\mathbf{d}}' = \begin{bmatrix} \mathbf{N}_{R1}^T\left(\mathrm{t}_{a_{,b_s}}\mathbf{f}(\mathbf{z})\delta b_s + \mathrm{t}_a\mathbf{f}(\mathbf{z}')\right) \\ \left(\mathrm{t}_{b_{,b_s}}\mathbf{F}^{CB}\delta b_s + \mathrm{t}_b\mathbf{F}^{CB\,\prime}\right) \end{bmatrix} \tag{6}$$

## NUMERICAL EXAMPLES

In this section, two example problems will be presented to show the feasibility and accuracy of the sensitivity analysis methods. In the 2-D circular type wave propagation example, the design change is through varying the material used. The design variables are atomic mass $m_A$ and potential function parameter $\varepsilon$. Figure 1 shows the cross section view of the simulation result after 15 time steps and its sensitivity with respect to $m_A$, which implies that the wave will travel slower with a larger atomic mass. Also demonstrated in this example is the accuracy of the variation of the time history kernel computed using numerical procedures.

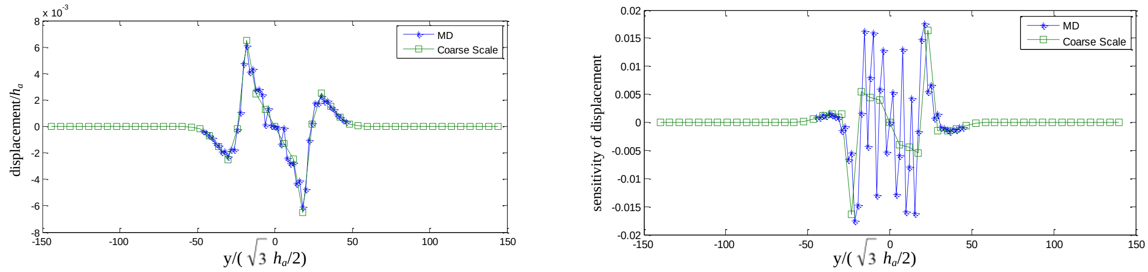
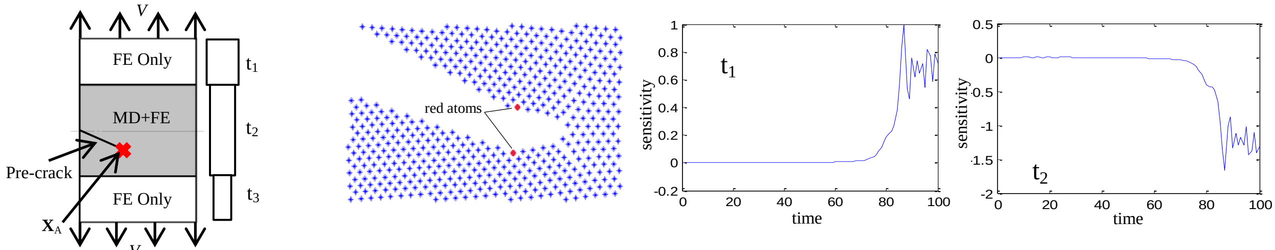



Figure 1 Cross section of the circular type wave and its sensitivity with respect to $m_A$

In the crack propagation example, the design variables are the thicknesses of individual sections of a 2-D plate. The plate with an initial crack in the MD region is pulled at the top and bottom boundaries by a ramped velocity (Fig. 2(a)). The sensitivity results accurately predict the impact of thickness changes on dynamic crack propagation speed (Fig. 2(b)). For example, the crack propagation will slow down when $t_2$ is increased.




(a) (b)

Figure 2 (a) Schematic model of the crack propagation example, (b) Sensitivity of *y* direction distance between the red atoms with respect to thicknesses $t_1$ and $t_2$

The sensitivity coefficients calculated for both two examples are verified by comparing with overall finite difference results, showing excellent accuracy. The accuracy of the sensitivity coefficients for the atom $\mathbf{X}_A$ in Fig. 2(a) with respect to $t_1$ is demonstrated in the table below.

| Time Step $\Delta t$ | Current Design | | | Perturbed Design | | | Overall Finite Difference | | | Sensitivity Prediction | | | Accuracy Comparison | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | q(b) | p(b) | s(b) | q(b+db) | p(b+db) | s(b+db) | del q | del p | del s | DSA q | DSA p | DSA s | %q | %p | %s |
| 50 | -6.73E-02 | -1.31E-02 | -1.72E-04 | -6.73E-02 | -1.31E-02 | -1.72E-04 | 1.48E-07 | 9.98E-08 | 3.31E-08 | 1.48E-02 | 9.98E-03 | 3.31E-03 | 100.00% | 99.98% | 100.02% |
| 70 | -1.16E-01 | 3.35E-03 | 8.36E-03 | -1.16E-01 | 3.35E-03 | 8.36E-03 | 1.51E-06 | 4.26E-07 | 1.17E-07 | 1.51E-01 | 4.26E-02 | 1.17E-02 | 100.00% | 99.96% | 99.85% |
| 90 | 2.04E-01 | 6.75E-02 | -1.19E-01 | 2.04E-01 | 6.75E-02 | -1.19E-01 | 5.16E-06 | -1.74E-06 | 3.54E-05 | 5.16E-01 | -1.74E-01 | 3.54E+00 | 99.99% | 100.19% | 100.17% |
| 110 | 1.07E+00 | 2.54E-01 | 4.12E-02 | 1.07E+00 | 2.54E-01 | 4.11E-02 | 1.16E-05 | 1.15E-06 | -1.01E-04 | 1.16E+00 | 1.15E-01 | -1.01E+01 | 100.02% | 100.21% | 100.16% |

## CONCLUSIONS

In this paper, a continuum-based sensitivity analysis method for two dimensional coupled atomistic and continuum problems have been presented. The variational formulation for the bridging scale method was developed and the continuum sensitivity analysis expressions were derived. Accuracy of the sensitivity results has been verified.

### References

[1] Liu W.K., Park H.: Bridging Scale Methods for Computational Nanotechnology. American Scientific Publishers, CA 2005.

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[3] Choi K.K., Kim N.: Structural Sensitivity Analysis and Optimization 1. Springer, CA 2004.