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ALGORITHMIC ASPECTS OF A LOCALIZED BRIDGING SCALE METHOD

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ABSTRACT

In this paper, we present a modified version of the bridging scale method (BSM), recently proposed by Liu *et al*. The major purpose of this work is to propose a consistent computational BSM algorithm to maintain of a greate advantage of the element to global assembling scheme in the finite element method.

In BSM, the total displacement $\mathbf{u}(\mathbf{x})$ in a domain Ω may be decomposed into coarse scale part $\bar{\mathbf{u}}(\mathbf{X})$ and fine scale part $\check{\mathbf{u}}(\mathbf{X})$:

$$\mathbf{u}(\mathbf{X}) = \bar{\mathbf{u}}(\mathbf{X}) + \check{\mathbf{u}}(\mathbf{X}).$$

The coarse scale displacement at α-th atom in e-th element $\bar{\mathbf{u}}^e(\mathbf{X}_\alpha)$ may be interpolated by the finite element nodal displacements $\mathring{\mathbf{u}}^e$:

$$\bar{\mathbf{u}}^e(\mathbf{X}_\alpha) = \mathbf{N}^e_\alpha \, \mathring{\mathbf{u}}^e.$$

We may define the difference between the total displacement and the coase scale displacement at $\mathbf{X}_\alpha$:

$$\Delta^e_\alpha = \mathbf{u}^e_\alpha - \mathbf{N}^e_\alpha \, \mathring{\mathbf{u}}^e.$$

To obtain the optimal approximation $\mathbf{u}$, we may define the weighted residual functional in each finite element region Ω^e :

$$\begin{aligned}\mathcal{E}^e &= \sum_{\alpha=1}^{n\alpha_e} m^e_\alpha (\Delta^e_\alpha \cdot \Delta^e_\alpha) = \sum_{\alpha=1}^{n\alpha_e} m^e_\alpha (\mathbf{u}^e_\alpha - \mathbf{N}^e_\alpha \, \mathring{\mathbf{u}}^e)^{\mathrm{T}} (\mathbf{u}^e_\alpha - \mathbf{N}^e_\alpha \, \mathring{\mathbf{u}}^e) \\ &= \left(\mathbf{u}^e - \mathbf{N}^e \, \mathring{\mathbf{u}}^e\right)^{\mathrm{T}} \mathbf{m}^e \left(\mathbf{u}^e - \mathbf{N}^e \, \mathring{\mathbf{u}}^e\right).\end{aligned}$$

where $n\alpha_e$ is the number of atoms in the e-th element, $\mathbf{u}^e$ and $\mathbf{m}^e$ are the total displacement and mass arrays of all atoms in the element respectively, and $\mathbf{N}^e$ is the interpolation operator from the element

nodal displacements to displacements at all atoms in the element. The minimization of the element based weighted residual functional may yeilds following:

$$\frac{\partial \mathcal{E}^e}{\partial \overset{\circ}{\mathbf{u}}{}^e} = 0 \quad \rightarrow \quad \overset{\circ}{\mathbf{m}}{}^e \overset{\circ}{\mathbf{u}}{}^e = (\mathbf{N}^e)^{\mathrm{T}} \mathbf{m}^e \mathbf{u}^e, \qquad \overset{\circ}{\mathbf{m}}{}^e = (\mathbf{N}^e)^{\mathrm{T}} \mathbf{m}^e \mathbf{N}^e$$

The coarse and fine scale parts of the displacement in the element are defined as

$$\bar{\mathbf{u}}^e = \mathbf{N}^e \overset{\circ}{\mathbf{u}}{}^e = \mathbf{N}^e (\overset{\circ}{\mathbf{m}}{}^e)^{-1} (\mathbf{N}^e)^{\mathrm{T}} \mathbf{m}^e \mathbf{u}^e = \mathbf{p}^e \mathbf{u}^e$$
$$\check{\mathbf{u}}^e = \mathbf{u}^e - \bar{\mathbf{u}}^e = (\mathbf{I}^e - \mathbf{p}^e)\mathbf{u}^e = \mathbf{q}^e \mathbf{u}^e$$

Then the total displacement is presented as:

$$\mathbf{u}^e = \bar{\mathbf{u}}^e + \check{\mathbf{u}}^e = \mathbf{N}^e \overset{\circ}{\mathbf{u}}{}^e + \mathbf{u}^e - \mathbf{p}^e \mathbf{u}^e = \mathbf{N}^e \overset{\circ}{\mathbf{u}}{}^e + \mathbf{q}^e \mathbf{u}^e$$

To bridge the scale, the total displacement in the right hand side in the above equation can be presented by the the displacement from the molecular dynamics solution $\overset{\bullet}{\mathbf{u}}{}^e$.

$$\mathbf{u}^e = \mathbf{N}^e \overset{\circ}{\mathbf{u}}{}^e + \overset{\bullet}{\mathbf{u}}{}^e - \mathbf{p}^e \overset{\bullet}{\mathbf{u}}{}^e$$

Differentiating the total displacement $\mathbf{u}^e$ with respect to time gives

$$\dot{\mathbf{u}}^e = \mathbf{N}^e \overset{\circ}{\dot{\mathbf{u}}}{}^e + \mathbf{q}^e \overset{\bullet}{\dot{\mathbf{u}}}{}^e$$

The Lagrangian $\mathcal{L}$ of the bridging scale method can be written as:

$$\mathcal{L} = \sum_{e=1}^{m} \frac{1}{2} (\overset{\circ}{\dot{\mathbf{u}}}{}^e)^{\mathrm{T}} \overset{\circ}{\mathbf{m}}{}^e \overset{\circ}{\dot{\mathbf{u}}}{}^e + \sum_{e=1}^{m} \frac{1}{2} (\overset{\bullet}{\dot{\mathbf{u}}}{}^e)^{\mathrm{T}} \overset{\bullet}{\mathbf{m}}{}^e \overset{\bullet}{\dot{\mathbf{u}}}{}^e - \sum_{e=1}^{m} \mathcal{U}^e (\overset{\circ}{\mathbf{u}}{}^e, \overset{\bullet}{\mathbf{u}}{}^e)$$

where m is the number of finite elements, $\mathcal{U}$ is the interatomic potential energy and the fine scale mass matrix $\overset{\bullet}{\mathbf{m}}{}^e$ is defined to be $\overset{\bullet}{\mathbf{m}}{}^e = (\mathbf{q}^e)^{\mathrm{T}} \mathbf{m}^e$. The element nodal and atomic variables can be presented by the corresponding global value:

$$\overset{\circ}{\dot{\mathbf{u}}}{}^e = \overset{\circ}{\mathcal{A}}{}^e \overset{\circ}{\dot{\mathbf{U}}}, \qquad \overset{\bullet}{\dot{\mathbf{u}}}{}^e = \overset{\bullet}{\mathcal{A}}{}^e \overset{\bullet}{\dot{\mathbf{U}}}$$

where $\overset{\circ}{\dot{\mathbf{U}}}$ and $\overset{\bullet}{\dot{\mathbf{U}}}$ are the global nodal and the global atomic velocity arrays respectively, $\overset{\circ}{\mathcal{A}}{}^e$ and $\overset{\bullet}{\mathcal{A}}{}^e$ are operators which map global value to corresponding element value. The Lagrangian can be written in the global form as:

$$\mathcal{L} = \frac{1}{2} (\overset{\circ}{\dot{\mathbf{U}}})^{\mathrm{T}} \overset{\circ}{\mathbf{M}} \overset{\circ}{\dot{\mathbf{U}}} + \frac{1}{2} (\overset{\bullet}{\dot{\mathbf{U}}})^{\mathrm{T}} \overset{\bullet}{\mathbf{M}} \overset{\bullet}{\dot{\mathbf{U}}} - \mathcal{U} (\overset{\circ}{\mathbf{U}}, \overset{\bullet}{\mathbf{U}})$$

where

$$\overset{\circ}{\mathbf{M}} = \sum_{e=1}^{m} \left(\overset{\circ}{\mathcal{A}}{}^e \right)^{\mathrm{T}} \overset{\circ}{\mathbf{m}}{}^e \overset{\circ}{\mathcal{A}}{}^e, \qquad \overset{\bullet}{\mathbf{M}} = \sum_{e=1}^{m} \left(\overset{\bullet}{\mathcal{A}}{}^e \right)^{\mathrm{T}} \overset{\bullet}{\mathbf{m}}{}^e \overset{\bullet}{\mathcal{A}}{}^e$$

Finally the coupled bridging scale equations of motion have been derived as:

$$\overset{\bullet}{\mathbf{M}} \overset{\bullet}{\ddot{\mathbf{U}}} = \overset{\bullet}{\mathbf{F}} (\overset{\bullet}{\mathbf{U}}), \qquad \overset{\circ}{\mathbf{M}} \overset{\circ}{\ddot{\mathbf{U}}} = \overset{\circ}{\mathbf{F}} (\overset{\circ}{\mathbf{U}}, \overset{\bullet}{\mathbf{U}})$$

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