Bridging methods for coupling atomistic and continuum models

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Abstract. We review some recent developments in the coupling of atomistic and continuum models based on the blending of the two models in a bridge region connecting the other two regions in which the models are separately applied. We define four such models and subject them to patch and consistency tests. We also discuss important implementation issues such as: the enforcement of displacement continuity constraints in the bridge region; and how one defines, in two and three dimensions, the blending function that is a basic ingredient in the methods.

Key words: atomistic to continuum coupling; blended coupling; molecular statics

1 Coupling atomistic and continuum models

For us, continuum models are PDE models that are derived by invoking a (physical) continuum hypothesis. In most situations, these models are *local* in nature, e.g., forces at any point and time depend only on the state at that point. Atomistic models are discrete models. In particular, we consider molecular statics models; these are particle models in which the position of the particles are determined through the minimization of an energy, or, equivalently, by Newton's laws expressing force balances. These models are, in general, *nonlocal* in nature, e.g., particles other than its nearest neighbors exert a force on a particle.

There are two types of situations in which the coupling of atomistic and continuum models arise. In the *concurrent domain* setting, the atomistic model is used to determine information, e.g., parameters such as diffusion coefficients, viscosities, conductivities, equations of state, etc., or stress fields, etc., that are needed by the continuum model. Both models are assumed to hold over the same domain. Typically, these parameters are determined by taking statistical averages of the atomistic solution at points in the domain and, in this setting, usually, only one-way coupling is needed, e.g., the atomistic model is used to

determine the continuum parameters. However, in more realistic situations, two-way coupling is needed, e.g., the atomistic model may need the macroscopic temperature as an input.

In the *domain decomposition* setting (which is the one we consider in this paper), the atomistic and continuum models are applied in different subdomains. The atomistic model is valid everywhere but is computationally expensive to use everywhere. So, it is applied only in regions where "singularities" occur, e.g., cracks, dislocations, plastic behavior, etc., and a continuum model is applied in regions where, e.g., ordinary elastic behavior occurs. There remains the question of how one couples the atomistic to the continuum model; there are two approaches to effect this coupling. For *non-overlapping* coupling, the atomistic and continuum models are posed on disjoint domains that share a common interface. For *overlapping* coupling, the regions in which the atomistic and continuum model are applied are connected by a *bridge* region in which both models are applied. See the sketches in Fig. 1.

Fig. 1. Non-overlapping (left) and overlapping (right) coupling of atomistic and continuum models.

Atomistic-to-continuum (AtC) coupling is distinct from most continuum-to-continuum couplings due to the *non-local nature of atomistic models.* Although the are no "active" particles in the region in which only the continuum model is applied, in a setting in which particles interact nonlocally, the forces exerted by the missing particles on the active particles are not accounted for; this discrepancy gives rise to what is known as *ghost force* phenomena.

In this paper, we consider AtC coupling methods that use overlapping regions because, in that case, it is easier to mitigate the ghost force effect. Note that one should not simply superimpose the two models in the bridge region since this leads to a non-physical "doubling" of the energy in Ω_b. Instead, the two models must be properly *blended* in this region. Such models are considered in [1–4, 6]; here, we review the results of [1, 2, 6].

2 Blended AtC coupled models

We assume that the atomistic model is valid in the *atomistic* and *bridge* regions, Ω_a and Ω_b, respectively; see Fig. 1. The continuum model is valid in the *continuum region* Ω_c and the bridge region Ω_b but is not valid in the atomistic region Ω_a. We want to "seamlessly" blend the two models together using

the bridge region Ω_b according to the following principles: the atomistic model "dominates" the continuum model near the interface surface between the atomistic and bridge regions and the continuum model "dominates" the atomistic model near the interface surface between the continuum and bridge regions.

In the atomistic region Ω_a, we assume that the force on the particle α located at the position $\mathbf{x}_\alpha$ is due to *externally applied force* $\mathbf{f}_{e;\alpha}$ and the *forces exerted by other particles* $\mathbf{f}_{\alpha,\beta}$ within the ball $\mathcal{B}_\alpha = \{\mathbf{x} \in \Omega : |\mathbf{x} - \mathbf{x}_\alpha| \leq \delta\}$ for some given δ. See the sketch in Figure 2.

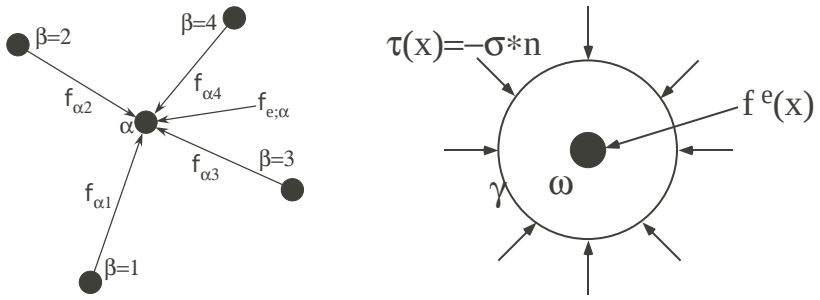

Fig. 2. Left: forces acting on the particle located at $\mathbf{x}_\alpha$. Right: forces acting on a point $\mathbf{x}$ in the continuum region.

The inter-particle forces are determined from a potential function, e.g., if $\mathbf{x}_\alpha$ and $\mathbf{x}_\beta$ denote the positions of the particles α and β, then $\mathbf{f}_{\alpha,\beta} = -\nabla\Phi\big(|\mathbf{x}_\alpha - \mathbf{x}_\beta|\big)$, where $\Phi(\cdot)$ is a prescribed potential function. Instead of using the particle positions $\mathbf{x}_\alpha$, one instead often uses the displacements $\mathbf{u}_\alpha$ from a reference configuration.

Let $\mathcal{N}_\alpha = \{\beta \mid \mathbf{x}_\beta \in \mathcal{B}_\alpha,\, \beta \neq \alpha\}$, i.e., $\mathcal{N}_\alpha$ is the set of the indices of the particles[4] located within $\mathcal{B}_\alpha$, other than the particle located at $\mathbf{x}_\alpha$ itself. Then, for any particle α, force equilibrium gives

$$\mathbf{f}_\alpha + \mathbf{f}_{e;\alpha} = \mathbf{0},$$

where $\mathbf{f}_\alpha = \sum_{\beta\in\mathcal{N}_\alpha} \mathbf{f}_{\alpha,\beta}$. We assume that in Ω_a there are two kinds of particles: particles whose positions are specified in advance and particles whose positions are determined by the force balance equations. The set of indices of the second kind of particles is denoted by $\mathcal{N}_a$. It is convenient to recast the force balance equation for the remaining particles in an equivalent variational form

$$\sum_{\alpha\in\mathcal{N}_a} \mathbf{v}_\alpha \cdot \mathbf{f}_\alpha = -\sum_{\alpha\in\mathcal{N}_a} \mathbf{v}_\alpha \cdot \mathbf{f}_{e;\alpha} \qquad \forall\, \mathbf{v}_\alpha \in \mathbb{R}^d\,, \alpha \in \mathcal{N}_a.$$

[4] Note that for some α, the set $\mathcal{N}_\alpha$ may include the indices of some particles whose positions are specified.

In the continuum region Ω_c, the Cauchy hypothesis implies that the forces acting on any continuum volume ω enclosing the point $\mathbf{x}$ are given by the *externally applied volumetric force* $\mathbf{f}^e$ and the *force exerted by the surrounding material* $\mathbf{f}_c = -\int_\gamma \sigma \cdot \mathbf{n}\, d\gamma$, where γ denotes the boundary of ω and σ denotes the stress tensor. See the sketch in Fig. 2. Note that $-\sigma \cdot \mathbf{n}$ is the stress force acting on a point on γ.

We assume that $\sigma(\mathbf{x}) = \sigma\big(\mathbf{x}, \nabla \mathbf{u}(\mathbf{x})\big)$ and is possibly nonlinear in both its arguments. Here, $\mathbf{u}(\mathbf{x})$ denotes the continuous displacement at the point $\mathbf{x}$. For a homogeneous material, $\sigma(\mathbf{x}) = \sigma\big(\nabla \mathbf{u}(\mathbf{x})\big)$, i.e., the stress does not explicitly depend on position. In the equilibrium state, we have that

$$-\int_\gamma \sigma \cdot \mathbf{n}\, d\gamma + \int_\omega \mathbf{f}^e\, d\omega = \mathbf{0}, \qquad \text{so that} \qquad \int_\omega \big(\nabla \cdot \sigma + \mathbf{f}^e\big)\, d\omega = \mathbf{0}.$$

Then, since ω is arbitrary, we conclude that at any point $\mathbf{x}$ in the continuum region, we have the force balance

$$\nabla \cdot \sigma + \mathbf{f}^e = \mathbf{0}.$$

For simplicity, we assume that we only have displacement boundary conditions.

Again, it will be convenient if we recast the continuum force balance equations in the equivalent variational form

$$\int_{\Omega_c} \sigma(\mathbf{u}) \colon \varepsilon(\mathbf{v})\, d\Omega = \int_{\Omega_c} \mathbf{f}^e \cdot \mathbf{v}\, d\Omega \qquad \forall\, \mathbf{v} \in \mathbf{H}_0^1(\Omega_c),$$

where we have the strain tensor $\varepsilon(\mathbf{v}) = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$ and the homogeneous displacement test space $\mathbf{H}_0^1(\Omega_c)$.

2.1 Blended models in the bridge region

We introduce the blending functions $\theta_a(\mathbf{x})$ and $\theta_c(\mathbf{x})$ satisfying $\theta_a + \theta_c = 1$ in Ω with $0 \le \theta_a, \theta_c \le 1$, $\theta_c = 1$ in Ω_c and $\theta_a = 1$ in Ω_a. Let $\theta_\alpha = \theta_a(\mathbf{x}_\alpha)$ and $\theta_{\alpha,\beta} = \theta_a\left(\frac{\mathbf{x}_\alpha + \mathbf{x}_\beta}{2}\right)$ or $\theta_{\alpha,\beta} = \frac{\theta_\alpha + \theta_\beta}{2}$.

We introduce four ways to blend the atomistic and continuum models. Let $\mathcal{N}_b$ denote the set of indices of the particles in Ω_b whose positions are not fixed by the boundary conditions.

Blended model I

$$-\int_{\Omega_b} \theta_c \sigma(\mathbf{u}) : \varepsilon(\mathbf{v})\, d\Omega + \sum_{\alpha \in \mathcal{N}_b} \theta_\alpha \mathbf{v}_\alpha \cdot \mathbf{f}_\alpha = -\int_{\Omega_b} \theta_c \mathbf{f}^e \cdot \mathbf{v}\, d\Omega - \sum_{\alpha \in \mathcal{N}_b} \theta_\alpha \mathbf{v}_\alpha \cdot \mathbf{f}_{e;\alpha}$$

$$\forall\, \mathbf{v} \in \mathbf{H}_0^1(\Omega_c) \text{ and } \mathbf{v}_\alpha \in \mathbb{R}^d, \alpha \in \mathcal{N}_b.$$

Blended model II

$$-\int_{\Omega_b} \theta_c \sigma(\mathbf{u}) : \varepsilon(\mathbf{v})\, d\Omega + \sum_{\alpha \in \mathcal{N}_b} \mathbf{v}_\alpha \cdot \sum_{\beta \in \mathcal{N}_\alpha} \theta_{\alpha,\beta} \mathbf{f}_{\alpha,\beta} = -\int_{\Omega_b} \theta_c \mathbf{f}^e \cdot \mathbf{v}\, d\Omega$$

$$- \sum_{\alpha \in \mathcal{N}_b} \theta_\alpha \mathbf{v}_\alpha \cdot \mathbf{f}_{e;\alpha} \qquad \forall\, \mathbf{v} \in \mathbf{H}_0^1(\Omega_c) \text{ and } \mathbf{v}_\alpha \in \mathbb{R}^d, \alpha \in \mathcal{N}_b.$$

Blended model III

$$-\int_{\Omega_b} \sigma(\mathbf{u}) : \varepsilon(\theta_c \mathbf{v})\, d\Omega + \sum_{\alpha\in\mathcal{N}_b} \theta_\alpha \mathbf{v}_\alpha \cdot \mathbf{f}_\alpha = -\int_{\Omega_b} \theta_c \mathbf{f}^e \cdot \mathbf{v}\, d\Omega$$
$$- \sum_{\alpha\in\mathcal{N}_b} \theta_\alpha \mathbf{v}_\alpha \cdot \mathbf{f}_{e;\alpha} \qquad \forall\, \mathbf{v} \in \mathbf{H}^1_0(\Omega_c) \text{ and } \mathbf{v}_\alpha \in \mathbb{R}^d, \alpha \in \mathcal{N}_b.$$

Blended model IV

$$-\int_{\Omega_b} \sigma(\mathbf{u}) : \varepsilon(\theta_c \mathbf{v})\, d\Omega + \sum_{\alpha\in\mathcal{N}_b} \mathbf{v}_\alpha \cdot \sum_{\beta\in\mathcal{N}_\alpha} \theta_{\alpha,\beta} \mathbf{f}_{\alpha,\beta} = -\int_{\Omega_b} \theta_c \mathbf{f}^e \cdot \mathbf{v}\, d\Omega$$
$$- \sum_{\alpha\in\mathcal{N}_b} \theta_\alpha \mathbf{v}_\alpha \cdot \mathbf{f}_{e;\alpha} \qquad \forall\, \mathbf{v} \in \mathbf{H}^1_0(\Omega_c) \text{ and } \mathbf{v}_\alpha \in \mathbb{R}^d, \alpha \in \mathcal{N}_b.$$

Methods I and II were introduced in [1, 6] while Method III and IV were introduced in [2]. An important observation is that in the bridge region Ω_b, near the continuum region Ω_c, we have that θ_a is small so that $\theta_{\alpha,\beta}$ and θ_α are small as well. Thus, blended models of the type discussed here automatically mitigate any ghost force effects, i.e., any ghost force will be multiplied by a small quantity such as $\theta_{\alpha,\beta}$ or θ_α.

2.2 Displacement matching conditions in the bridge region

In order to complete the definition of the blended model, one must impose constraints that tie the atomistic displacements $\mathbf{u}_\alpha$ and the continuum displacements $\mathbf{u}(\mathbf{x})$ in the bridge region Ω_b. These take the form of

$$\mathcal{C}\big(\mathbf{u}_\alpha, \mathbf{u}(\mathbf{x})\big) = 0 \qquad \text{for } \alpha \in \mathcal{N}_b \text{ and } \mathbf{x} \in \Omega_b$$

for some specified constraint operator $\mathcal{C}(\cdot,\cdot)$.

One could slave all the atomistic displacements in the bridge region to the continuum displacements, i.e., set

$$\mathbf{u}_\alpha = \mathbf{u}(\mathbf{x}_\alpha) \qquad \forall\, \alpha \in \mathcal{N}_b.$$

We refer to such constraints as *strong constraints.* Alternatively, the atomistic and continuum displacements can be matched in an average sense to define *loose constraints*. For example, one can define a triangulation $\mathcal{T}^H = \{\Delta_t\}_{t=1}^{T_b}$ of the bridge region Ω_b; this triangulation need not be the same as that used to effect a finite element discretization of the continuum model. Let $\mathcal{N}_t \neq \emptyset$ denote indices of the particles in Δ_t. One can then match the atomistic and continuum displacements in an average sense over each triangle Δ_t:

$$\sum_{\alpha\in\mathcal{N}_t} \mathbf{u}(\mathbf{x}_\alpha) = \sum_{\alpha\in\mathcal{N}_t} \mathbf{u}_\alpha \qquad \text{for } t = 1, \ldots, T_b.$$

Once a set of constraints has been chosen, one also has to choose a means for enforcing them. One possibility is to enforce them *weakly* through the use of

the Lagrange multiplier rule. In this case, the test functions $\mathbf{v}_\alpha$ and $\mathbf{v}(\mathbf{x})$ and trial functions $\mathbf{u}_\alpha$ and $\mathbf{u}(\mathbf{x})$ in the variational formulations are not constrained; one ends up with saddle-point type discrete systems

$$\begin{pmatrix} \mathcal{A}_{a,\theta_a} & 0 & \mathcal{C}_a \\ 0 & \mathcal{A}_{c,\theta_c} & \mathcal{C}_c \\ \mathcal{C}_a^* & \mathcal{C}_c^* & 0 \end{pmatrix} \cdot \begin{pmatrix} \text{atomistic unknowns} \\ \text{continuum unknowns} \\ \text{Lagrange multipliers} \end{pmatrix} = \text{RHS}.$$

Note that the coupling of the atomistic and continuum variables is effected only through the Lagrange multipliers.

A second possibility is to enforce the constraints *strongly*, i.e., require that all candidate atomistic and continuum displacements satisfy the constraints. In this case, the test functions $\mathbf{v}_\alpha$ and $\mathbf{v}(\mathbf{x})$ in the variational formulations should be similarly constrained. One ends up with simpler discrete systems of the form

$$\widetilde{\mathcal{A}}_{a,\theta_a,\theta_c} \cdot \big(\text{atomistic unknowns}\big) + \widetilde{\mathcal{A}}_{c,\theta_c,\theta_a} \cdot \big(\text{continuum unknowns}\big) = \text{RHS}.$$

Note that the atomistic and continuum variables are now tightly coupled. The second approach involves fewer degrees of freedom and results in better behaved discrete systems but may be more cumbersome to apply in some settings.

2.3 Consistency and patch tests

To define an AtC coupled problem, one must specify the following data sets:

- $F = \left\{\mathbf{f}_\alpha^e\right\}_{\alpha\in\mathcal{N}_a\cup\mathcal{N}_b}$ (external forces applied to the particles);
- $P = \left\{\mathbf{u}_\alpha\right\}_{\alpha\notin\mathcal{N}_a\cup\mathcal{N}_b}$ (displacements of the particles whose positions are fixed)
- $B = \left\{\mathbf{f}^e(\mathbf{x})\right\}_{\mathbf{x}\in\Omega_c\cup\Omega_b}$ (external forces applied in the continuum region);
- $D = \left\{\mathbf{u}(\mathbf{x})\right\}_{\mathbf{x}\in\partial(\Omega_c\cup\Omega_b)}$ (continuum displacements on the boundary).

We subject the AtC blending methods we have defined to two tests whose passage is crucial to their mathematical and physical well posedness. To this end, we define two types of test problems. The set $\{F, P, B, D\}$ defines a *consistency test problem* if the pure atomistic solution $\mathbf{u}_\alpha$ and the pure continuum solution $\mathbf{u}(\mathbf{x})$ are such that the constraint equations, i.e, $C\big(\mathbf{u}_\alpha, \mathbf{u}(\mathbf{x})\big) = 0$, are satisfied on Ω. Further, a consistency test problem defines a *patch test problem* if the pure continuum solution $\mathbf{u}(\mathbf{x})$ is such that $\varepsilon(\mathbf{u}) =$ constant, i.e., it is a solution with constant strain.

If we assume that $\{F, P, B, D\}$ defines a patch test problem with atomistic solution $\mathbf{u}_\alpha$ and continuum solution $\mathbf{u}(\mathbf{x})$, then, an AtC coupling method *passes the patch test* if $\{\mathbf{u}_\alpha, \mathbf{u}(\mathbf{x})\}$ satisfies the AtC model equations. Similarly, an AtC coupling method *passes the consistency test* if $\{\mathbf{u}_\alpha, \mathbf{u}(\mathbf{x})\}$ satisfies the AtC model equations for any consistency test problem. Note that passing the consistency test implies passage of the patch test, but not conversely.

Our analyses of the four blending methods (see [2]) have shown that Methods I and IV are not consistent and do not pass patch test problems; Method III is consistent and thus also passes any patch test problem; and Method II is conditionally consistent: it is consistent if, for a pair of atomistic and continuum solutions $\mathbf{u}_\alpha$ and $\mathbf{u}$, respectively

$$-\int_\Omega \theta_c \sigma(\mathbf{u}) : \varepsilon(\mathbf{v})\, d\Omega + \int_\Omega \sigma(\mathbf{u}) : \varepsilon(\theta_c \mathbf{v})\, d\Omega + \sum_{\alpha \in \mathcal{N}_a \cup \mathcal{N}_b} \mathbf{v}_\alpha \cdot \sum_{\beta \in \mathcal{N}_\alpha} \theta_{\alpha,\beta} \mathbf{f}_{\alpha,\beta} - \sum_{\alpha \in \mathcal{N}_a \cup \mathcal{N}_b} \theta_\alpha \mathbf{v}_\alpha \cdot \sum_{\beta \in \mathcal{N}_\alpha} \mathbf{f}_{\alpha,\beta} = 0$$

and passes patch tests if this condition is met for patch test solutions .

From these results, we can forget about Methods I and IV and it seems that Method III is better than Method II. The first conclusion is valid but there are additional considerations that enter into the relative merits of Methods II and III. Most notably, Method II is the only one of the four blended models that satisfies[5] Newton's third law. In addition, the violation of patch and consistency tests for Method II is tolerable, i.e., the error introduced can be made smaller by proper choices for the model parameters, e.g., in a 1D setting, we have shown (see [1]) that the patch test error is proportional to $\frac{s^2}{L_b h}$, where s = particle lattice spacing (a material property), h = finite element grid size, and L_b = width of the bridge region Ω_b. While we cannot control the size of s, it is clear that in realistic models this parameter is small. Also, the patch test error for Method II can be made smaller by making L_b larger (widening the bridge region) and/or making h larger (having more particles in each finite element).

2.4 Fully discrete systems in higher dimensions

We now discuss how the fully discrete system can be defined in 2D; we only consider Method II for which we have

$$-\int_{\Omega_b \cup \Omega_c} \theta_c \sigma(\mathbf{u}) : \varepsilon(\mathbf{v})\, d\Omega + \sum_{\alpha \in \mathcal{N}_b \cup \mathcal{N}_a} \mathbf{v}_\alpha \cdot \sum_{\beta \in \mathcal{N}_\alpha} \theta_{\alpha,\beta} \mathbf{f}_{\alpha,\beta} = -\int_{\Omega_b \cup \Omega_c} \theta_c \mathbf{f}^e \cdot \mathbf{v}\, d\Omega - \sum_{\alpha \in \mathcal{N}_b \cup \mathcal{N}_a} \theta_\alpha \mathbf{v}_\alpha \cdot \mathbf{f}_{e;\alpha}$$

$$\forall\, \mathbf{v} \in \mathbf{H}_0^1(\Omega_b \cup \Omega_c) \text{ and } \mathbf{v}_\alpha \in \mathbb{R}^d, \alpha \in \mathcal{N}_b \cup \mathcal{N}_a.$$

We also consider the case of the strong enforcement of the hard constraints

$$\mathbf{u}_\alpha = \mathbf{u}(\mathbf{x}_\alpha) \qquad \forall \alpha \in \mathcal{N}_b.$$

The other methods and looser constraints handled using the Lagrange multiplier rule can be handled in a similar manner.

[5] Related to this observation is the fact that Method II is the only blended method that has symmetric weak form provided the weak forms of the pure atomistic and continuum problems are also symmetric.

To discretize the continuum contributions to the blended model, we use a finite element method. Let $W^h \subset \mathbf{H}^1_0(\Omega_b \cup \Omega_c)$ be a nodal finite element space and let $\{\mathbf{w}^h_j(\mathbf{x})\}_{j=1}^J$ denote a basis for W^h. Then, the continuum displacement $\mathbf{u}(\mathbf{x})$ is approximated by

$$\mathbf{u}(\mathbf{x}) \approx \mathbf{u}^h(\mathbf{x}) = \sum_{j=1}^{J} c_j \mathbf{w}^h_j(\mathbf{x}).$$

Let $\mathcal{S}_c = \Big\{ j \in \{1,\dots,J\} \mid \mathbf{x}_j \in \Omega_c \Big\}$ and $\mathcal{S}_b = \Big\{ j \in \{1,\dots,J\} \mid \mathbf{x}_j \in \Omega_b \Big\}$ denote the set of indices of the nodes in Ω_c and Ω_b, respectively. We use continuous, piecewise linear finite element spaces with respect to partition of $\Omega_b \cup \Omega_c$ into a set of T triangles $\mathcal{T}^h = \{\Delta_t\}_{t=1}^T$; higher-order finite element spaces can also be used.

For $j = 1,\dots,J$, we let $\mathcal{T}^h_j = \{t : \Delta_t \in \operatorname{supp}(\mathbf{w}_j)\}$, i.e., $\mathcal{T}^h_j$ is the set of indices of the triangles sharing the finite element node $\mathbf{x}_j$ as a vertex. Thus, we have that

$$\int_{\operatorname{supp}(\mathbf{w}^h_j)} F(\mathbf{x})\, d\Omega = \sum_{t \in \mathcal{T}^h_j} \int_{\Delta_t} F(\mathbf{x})\, d\Omega.$$

The standard choice for the quadrature rule, since we are using piecewise linear finite element functions, is the mid-side rule for triangles. Thus, if $\widehat{\mathbf{x}}_{\Delta;k}$, $k = 1,\dots,3$, are the vertices of a triangle Δ, we have the quadrature rule $\int_\Delta F(\mathbf{x})\, d\Omega \approx \frac{V_\Delta}{3} \sum_{q=1}^3 F(\mathbf{x}_{\Delta;q})$, where V_Δ denotes the volume of the triangle Δ, $\mathbf{x}_{\Delta;1} = \frac{\widehat{\mathbf{x}}_{\Delta;1}+\widehat{\mathbf{x}}_{\Delta;2}}{2}$, $\mathbf{x}_{\Delta;2} = \frac{\widehat{\mathbf{x}}_{\Delta;2}+\widehat{\mathbf{x}}_{\Delta;3}}{2}$, and $\mathbf{x}_{\Delta;3} = \frac{\widehat{\mathbf{x}}_{\Delta;3}+\widehat{\mathbf{x}}_{\Delta;1}}{2}$.

In the continuum region Ω_c, we have the discretized continuum model

$$\begin{aligned} -\sum_{t \in \mathcal{T}^h_j} \frac{V_{\Delta_t}}{3} \sum_{q=1}^{3} \sigma\Big((\mathbf{x}_{\Delta_t;q}), \nabla \mathbf{u}^h(\mathbf{x}_{\Delta_t;q})\Big) : \nabla \mathbf{w}^h_j(\mathbf{x}_{\Delta_t;q}) \\ = -\sum_{t \in \mathcal{T}^h_j} \frac{V_{\Delta_t}}{3} \sum_{q=1}^{3} \mathbf{f}^e(\mathbf{x}_{\Delta_t;q}) \cdot \mathbf{w}^h_j(\mathbf{x}_{\Delta_t;q}) \qquad \text{for } j \in \mathcal{S}_c. \end{aligned}$$

Of course, in the atomistic region Ω_a, we have that

$$\sum_{\beta \in \mathcal{N}_\alpha} \mathbf{f}_{\alpha,\beta} = -\mathbf{f}^e_\alpha \qquad \text{for } \alpha \in \mathcal{N}_a.$$

Due to the way we are handling the constraints, we have that the atomistic test and trial functions in the bridge region Ω_b are slaved to the continuum test and trial functions, i.e., $\mathbf{u}_\alpha = \mathbf{u}^h(\mathbf{x}_\alpha)$ and $\mathbf{v}_\alpha = \mathbf{w}^h_j(\mathbf{x}_\alpha)$.

For $j \in \mathcal{S}_b$, let $\mathcal{N}_j = \{\alpha \mid \mathbf{x}_\alpha \in \operatorname{supp}(\mathbf{w}^h_j)\}$ denote the set of particle indices such that the particles are located within the support of the finite element basis

function $\mathbf{w}_j^h$. Then, in the bridge region Ω_b, we have that

$$\begin{aligned}
-\sum_{t\in\mathcal{T}_j^h}\frac{V_{\Delta_t}}{3}\sum_{q=1}^{3}\theta_c(\mathbf{x}_{\Delta_t;q})\sigma\Big((\mathbf{x}_{\Delta_t;q}),\nabla\mathbf{u}^h(\mathbf{x}_{\Delta_t;q})\Big):\nabla\mathbf{w}_j^h(\mathbf{x}_{\Delta_t;q})\\
+\sum_{\alpha\in\mathcal{N}_j}\sum_{\beta\in\mathcal{N}_\alpha}\theta_{\alpha,\beta}\mathbf{f}_{\alpha,\beta}\cdot\mathbf{w}_j^h(\mathbf{x}_\alpha)\\
=-\sum_{t\in\mathcal{T}_j^h}\frac{V_{\Delta_t}}{3}\sum_{q=1}^{3}\theta_c(\mathbf{x}_{\Delta_t;q})\mathbf{f}^e(\mathbf{x}_{\Delta_t;q})\cdot\mathbf{w}_j^h(\mathbf{x}_{\Delta_t;q})\\
-\sum_{\alpha\in\mathcal{N}_j}\theta_\alpha\mathbf{f}_\alpha^e\cdot\mathbf{w}_j^h(\mathbf{x}_\alpha)\qquad\text{for } j\in\mathcal{S}_b.
\end{aligned}$$

In 3D, one cannot use mid-face or mid-edge quadrature rules as one can in 1D and 2D, even for uncoupled continuum problems. Instead, one must use rules for which at least some of the quadrature points are in the interior of tetrahedra. Other than this, the development of a fully discretized method follows the same process as in the 2D case.

2.5 Choosing the blending function in 2D and 3D

For the blending function $\theta_c(\mathbf{x})$ for $\mathbf{x}\in\Omega_b$, we of course have that $\theta_a(\mathbf{x}) = 1-\theta_c(\mathbf{x})$, $\theta_a(\mathbf{x})=1$, $\theta_c(\mathbf{x})=0$ in Ω_a, $\theta_a(\mathbf{x})=0$. and $\theta_c(\mathbf{x})=1$ in Ω_c.

In many practical settings, the domain Ω_b is a rectangle in 2D or is a rectangular parallelepiped in 3D. In such cases, one may simply choose $\theta_c(\mathbf{x})$ in the bridge region to be the tensor product of global 1D polynomials connecting the atomistic and continuum regions across the bridge region. One could choose linear polynomials in each direction such that their values are zero at the bridge/atomistic region interface and one at the bridge/continuum region interface. If one wishes to have a smoother transition from the atomistic to the bridge to the continuum regions, one can choose cubic polynomials in each direction such that they have zero value and zero derivative at the bridge/atomisitic region interface and value one and zero derivative at the bridge/continuum region interface.

For the general case in 2D, we triangulate the bridge region Ω_b into the set of triangles having vertices $\{\mathbf{x}_{b;i}\}_{i=1}^{l}$. In practice, this triangulation is the same as that used for the finite element approximation of the continuum model in the bridge region but, in general, it may be different. For the two triangulations to be the same, we must have that the finite element triangulation is conforming with the interfaces between the bridge region and the atomistic and continuum regions, i.e., those interfaces have to be made up of edges of triangles of the finite element triangulation. The simplest blending function is then determined by setting $\theta_c(\mathbf{x})=\xi^h(\mathbf{x})$, where $\xi^h(\mathbf{x})$ is a continuous, piecewise linear function with respect to this triangulation. The nodal values of $\xi^h(\mathbf{x})$ are chosen as follows. Set $\xi^h(\mathbf{x}_{b;i})=0$ at all nodes $\mathbf{x}_{b;i}\in\overline{\Omega}_a\cap\overline{\Omega}_b$, i.e., on the interface between the atomistic and bridge regions. Then, set $\xi^h(\mathbf{x}_{b;i})=1$ at all nodes $\mathbf{x}_{b;i}\in$

$\overline{\Omega}_b \cap \overline{\Omega}_c$, i.e., on the interface between the continuum and bridge regions. For the remaining nodes $\mathbf{x}_{b;i} \in \Omega_b$, there are several ways to choose the values of ξ^h. One way is to choose them according to the relative distances to the interfaces. A more convenient way is to let ξ^h be a finite element approximation, with respect to the grid, of the solution of Laplace's equation in Ω_b that satisfies the specified values at the interfaces. Once $\xi^h(\mathbf{x})$ is chosen, we set $\theta_a(\mathbf{x}) = 1 - \xi^h(\mathbf{x})$ for all $\mathbf{x} \in \Omega_b$ and choose $\theta_\alpha = \theta_a(\mathbf{x}_\alpha) = 1 - \xi^h(\mathbf{x}_\alpha)$ so that

$$\theta_{\alpha,\beta} = 1 - \frac{\xi^h(\mathbf{x}_\alpha) + \xi^h(\mathbf{x}_\beta)}{2} \qquad \text{or} \qquad \theta_{\alpha,\beta} = 1 - \xi^h\Big(\frac{\mathbf{x}_\alpha + \mathbf{x}_\beta}{2}\Big).$$

This recipe can be extended to 3D settings.

One may want $\theta_c(\mathbf{x})$ to have a smoother transition from the atomistic to the bridge to the continuum regions. To this end, one can choose $\xi^h(\mathbf{x})$ to not only be continuous, but to be continuously differentiable in the bridge region and across the interfaces. Note that in 2D, this requires the use of the fifth-degree piecewise polynomial Argyris element or the cubic Clough-Tocher macro-element; see [5]. Such elements present difficulties in a finite element approximation setting, but are less problematical in an interpolatory setting.

3 Simple computational examples in 1D

For $0 < a < c < 1$, let $\Omega = (0,1)$, $\Omega_a = (0,a)$, $\Omega_b = (a,c)$, and $\Omega_c = (c,1)$. In $\overline{\Omega}_c \cup \overline{\Omega}_b = [a,1]$, we construct the uniform partition $x_j = a + (j-1)h$ for $j = 1, \ldots, J$ having grid size h. We then choose W^h to be the continuous, piecewise linear finite element space with respect to this partition. Without loss of generality, we define the bridge region Ω_b using the finite element grid, i.e., we assume that there are finite element nodes at $x = a$ and $x = c$; this arrangement leads to a more convenient implementation of blending methods in 2D and 3D. In $\overline{\Omega}_a \cup \overline{\Omega}_b = [0,c]$, we have a uniform particle lattice with lattice spacing s given by $x_\alpha = (\alpha - 1)s$, $\alpha = 1, \ldots, N$. Note that the lattice spacing s is a fixed material property so that there is no notion of $s \to 0$. One would think that one can still let $h \to 0$; however, it makes no sense to have $h < s$.

We consider the atomistic model to be a one-dimensional linear mass-spring system with two-nearest neighbor interactions and with elastic moduli K_{a1} and K_{a2} for the nearest-neighbor and second nearest-neighbor interactions; only the two particles to the immediate left and right of a particle exert a force on that particle. The continuum model is one-dimensional linear elasticity with elastic modulus K_c. We set $K_{a1} = 50$, $K_{a2} = 25$, $K_c = K_{a1} + 2K_{a2} = 100$. A unit point force is applied at the finite element node at the end point $x = 1$ and the displacement of the particle located at the end point $x = 0$ is set to zero. Using either the atomistic or finite element models, the resulting solutions are ones having uniform strain 0.01; thus, we want a blended model solution to also recover the uniform strain solution.

We choose $h = 1.5s$ and $s = 1/30$ so that we have $a = 0.3$, $c = 0.6$, 20 particles, and 16 finite element nodes; there are no particles located at either

$x = a$ or $x = c$, the end points of the bridge region Ω_b. For the right-most particle $x_{20} < c$, we have that $\theta_a(x_{20}) \neq 0$. To avoid the ghost forces associated with the missing bond to the right of the 20th particle, a 21st particle is added to the right of $x = c$. Since $x_{21} \in \Omega_c$, we have that $\theta_a(x_{21}) = 0$ so that we need not be concerned with its missing bond to the right; this is a way that blending methods mitigate the ghost force effect. We see from Fig. 3 that Method III passes the patch test but Method II does not. However, the degree of failure for Method II is "small." From Fig. 4, we see that Method I fails the patch test; the figure for that method is for the even simpler case of nearest-neighbor interactions. Similarly, Method IV fails the patch test.

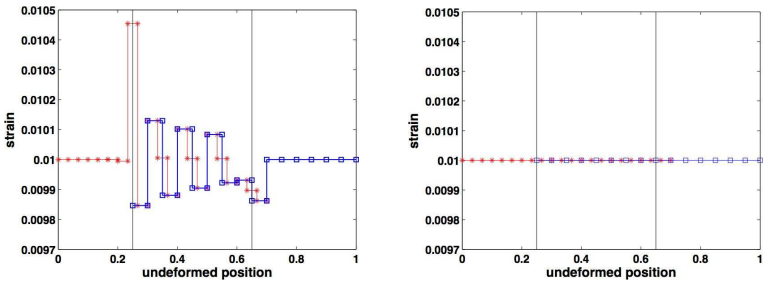

Fig. 3. Strain for Method II (left) and Method III(right).

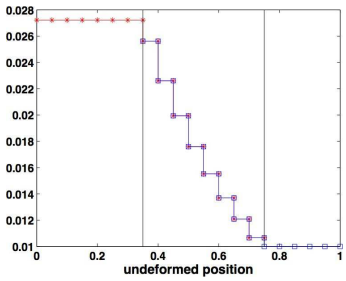

Fig. 4. Strain for Method I.

In Fig. 5, we compare the blended atomistic solutions in the bridge region, obtained using Method III with both strong and loose constraints, with that obtained using the fully atomistic solution. We consider a problem with a uniform load and zero displacements at the two ends; we only consider nearest-neighbor interactions. The loose constraint allows the atomistic solution to be free to reproduce the curvature of the fully atomistic solution, leading to better results. The strong constraint is too restrictive, forcing the atomistic solution to follow

the finite element solution; it results in a substantial reduction in the accuracy in the bridge region.

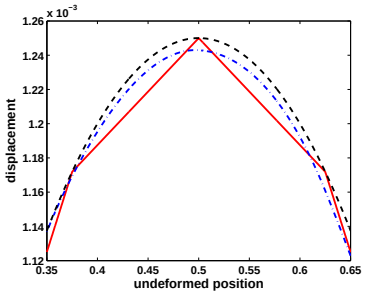

Fig. 5. Fully atomistic solution (dashed line); loose constraints (dash-dotted line); and strong constraints (solid line).

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