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SAND2007-0905

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Printed February, 2007

Blended Atomistic-to-Continuum coupling analyses and methods

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Blended Atomistic-to-Continuum coupling analyses and methods

Santiago Badia * Pavel Bochev * Max Gunzburger †
Richard Lehoucq * Michael Parks *

Abstract

This article considers the blending of atomistic and continuum problems on a bridging subdomain building upon the ideas introduced in [1, 2, 7]. The continuity of the atomistic and continuum solutions is imposed by a constraint operator using Lagrange multipliers. These methods are stated in an abstract form. The consistency of these methods is analyzed. A new blending model is designed using mechanical arguments. The consistency and accuracy of the method is discussed theoretically and confirmed numerically.

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Acknowledgements

The authors acknowledge funding by the DOE Office of Science Advanced Scientific Computing Research Program. Santiago Badia acknowledges the support of the European Community through the Marie Curie contract *NanoSim* (MOIF-CT-2006-039522).

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1 Introduction

Fully atomistic simulation on an entire model domain is computationally infeasible for many applications of interest. In order to alleviate the computational cost, the atomistic problem is approximated by a continuum model on some region for where the solution is sufficiently smooth. These two models must be tied together in an interface region. That is, some kind of continuity of atomistic and continuum position or displacement is required. A seemingly natural approach is to enforce this continuity of solution using Lagrange multipliers. Unfortunately, this approach has some complications.

When coupling two different continuum equations approximated by a finite element analysis in two different domains, we can couple these two problems on the $d - 1$ -dimensional interface manifold via Lagrange multipliers. Unfortunately, the atomistic problem is in general nonlocal, and so the interface atoms are not confined to a $d - 1$ -dimensional manifold. Any desirable AtC coupling method must therefore not rely only on transmission conditions at a surface (in the mathematical sense). We instead consider techniques that glue both models in a d -dimensional domain, which we will call the bridging region.

We cannot naïvely tie together atomistic and continuum solutions in the bridging region because the effective stiffness on this region would be the sum of the stiffnesses of the atomistic and continuum models, which is clearly nonphysical. We must instead account for the material properties of both the atomistic and continuum material in such a way that the coupled model in the bridging region has the correct elastic response.

Blended AtC coupling are motivated by the following two observations:

- the boundary for the atomistic problem is not a $d - 1$ -dimensional manifold;
- naïve coupling does not reproduce the correct stiffness in the bridging region,

These methods couple the atomistic and continuum problems in the bridging domain with a blending model that enforces solution continuity while reproducing the correct stiffness. This blending model is a combination of atomistic and continuum models by (atomistic and continuum) blending functions that are a partition of the unity in the bridging domain.

We explain the difference between a straightforward coupling and a blending approach, let \mathcal{A}^c and \mathcal{A}^a denote continuum and atomistic operators acting on Ω_c and Ω_a , respectively. A Naïve coupling method will tie the two models together by using Lagrange multipliers in some d -dimensional blending region $\Omega_b \subset \Omega_a \cap \Omega_c$. The

resulting AtC operator can be formally stated as

$$\begin{pmatrix} \mathcal{A}^a & 0 & \mathcal{C}_1^t \\ 0 & \mathcal{A}^c & \mathcal{C}_2^t \\ \mathcal{C}_1 & \mathcal{C}_2 & 0 \end{pmatrix} \quad (1.1)$$

In contrast, a blending approach to AtC replaces the original continuum and atomistic operators by *blended* operators \mathcal{A}_θ^c and \mathcal{A}_θ^a such that $\mathcal{A}_\theta^c = \mathcal{A}^c$ on Ω_c/Ω_b and $\mathcal{A}_\theta^a = \mathcal{A}^a$ on Ω_a/Ω_b , and where θ is a partition of unity. The resulting AtC operator has the form

$$\begin{pmatrix} \mathcal{A}_\theta^a & 0 & \mathcal{C}_1^t \\ 0 & \mathcal{A}_\theta^c & \mathcal{C}_2^t \\ \mathcal{C}_1 & \mathcal{C}_2 & 0 \end{pmatrix} \quad (1.2)$$

AtC blended coupling is a relatively recent development. In [1] a blending of energy functionals was considered and Lagrange multipliers used for enforcing a set of constraints in the bridging domain. The extension to the transient case was considered in [2]. A blending method for coupling atomistic and continuum equations without blending energy functionals has recently been proposed in [7]. The last approach is the one we consider herein.

The outline of the paper is the following. Section 2 is devoted to atomistic and continuum models. In Section 3 we state in an abstract manner AtC blended coupling techniques and address the issues of consistency and ghost forces. Four different AtC coupling methods are introduced in Section 4 and their consistency properties analyzed. For one of these methods, in Section 5 we construct a blending model which is consistent when applied to different test problems. We motivate this model using mechanical arguments. Theoretical results are confirmed numerically in Section 6. Some conclusions are drawn in Section 7.

2 The atomistic and continuum models

2.1 The atomistic model

Let us consider an undeformed lattice \mathbf{P} within a given domain Ω . We denote by \mathbf{D} the subset of atoms whose position is fixed. The lattice statics problem consists of finding an equilibrium deformed configuration for an inter-atomic potential (i.e., the Lennard-Jones potential) that defines the internal forces. The space of possible atomistic configurations is denoted by \mathcal{X}^a . An element $W \in \mathcal{X}^a$ can be defined as:

$$W_\alpha^i = (\mathbf{x}_\alpha)_i, \quad \alpha \in \mathbf{P}, \quad i = 1, \dots, d,$$

where d is the space dimension and \mathbf{x}_α the coordinates of the atom α for this corresponding deformed configuration. This space is simply a set of properly ordered $|\mathbf{P}| \times d$ scalar values.¹ We also introduce the affine space of configurations that satisfy the constraints over \mathbf{D} :

$$\mathcal{X}_\mathbf{D}^a := \{V \in \mathcal{X}^a \mid \forall \alpha \in \mathbf{D}, V_\alpha = U_\alpha^\mathbf{D}\}$$

where $U_\alpha^\mathbf{D} = \mathbf{x}_\alpha^\mathbf{D}$ is the array of fixed coordinates for constrained atoms. Analogously, the space $\mathcal{X}_\mathbf{0}^a$ consists of:

$$\mathcal{X}_\mathbf{0}^a := \{V \in \mathcal{X}^a \mid \forall \alpha \in \mathbf{D}, V_\alpha = \mathbf{0}\}.$$

The atomistic statics problem consists of: find $U \in \mathcal{X}_\mathbf{D}^a$ such that,

$$\mathbf{L}(U)_\alpha = F_\alpha \quad \forall \alpha \in \mathbf{P} \setminus \mathbf{D}. \quad (2.1)$$

The operator $\mathbf{L} : \mathcal{X}_\mathbf{D}^a \rightarrow \mathcal{X}^a$ (possibly non-linear) gives the internal forces for a given atomistic configuration U . F is the array of external forces applied over the atoms of the lattice. Therefore, (2.1) is nothing but Newton's second law for a system of particles interacting via \mathbf{L} . Alternatively, we can write the previous problem in *weak form* as: find $U \in \mathcal{X}_\mathbf{D}^a$ such that

$$(\mathbf{L}(U), V) = (F, V) \quad \forall V \in \mathcal{X}_\mathbf{0}^a. \quad (2.2)$$

2.2 The continuum model

The continuum model is defined by a differential operator $\mathcal{L} : \mathcal{X}^c \rightarrow (\mathcal{X}^c)'$, where \mathcal{X}^c is an appropriate function space and $(\mathcal{X}^c)'$ its corresponding dual space. The continuum problem (in strong form) consists of: find $\mathbf{u} \in \mathcal{X}^c$ such that

$$\mathcal{L}\mathbf{u} = \mathbf{f} \quad \text{in } \Omega, \quad (2.3a)$$

$$\mathbf{u} = \mathbf{u}^\mathbf{D} \quad \text{on } \partial\Omega, \quad (2.3b)$$

¹ $|\cdot|$ denotes the cardinality of the set.

where $\mathbf{f} \in (\mathcal{X}^c)'$ is the external force and \mathbf{u}^D the Dirichlet boundary value. We only consider essential boundary conditions for the sake of simplicity. The atomistic problem is usually stated in terms of displacements. Without loss of generality, let us consider \mathbf{u} the continuum displacement.

A basic assumption we will make is that the continuum model is *a good approximation of the atomistic model* under suitable conditions (e.g. smoothness). Therefore, the atomistic problem (2.1) and the continuous problem (2.3) must be related. It does not only imply a link between \mathbf{L} and \mathcal{L} , but also between the external forces \mathbf{f} and F , fixed values \mathbf{u}^D and U^D and $\partial\Omega$ and \mathbf{D} .

In order to state the weak form we introduce the following function spaces:

$$\begin{aligned}\mathcal{X}_{\mathbf{D}}^c &:= \{\mathbf{v} \in \mathcal{X}^c \mid \mathbf{v} = \mathbf{u}^D \text{ on } \partial\Omega\}, \\ \mathcal{X}_{\mathbf{0}}^c &:= \{\mathbf{v} \in \mathcal{X}^c \mid \mathbf{v} = \mathbf{0} \text{ on } \partial\Omega\}.\end{aligned}$$

We define the bilinear form

$$\ell(\mathbf{u}, \mathbf{v}) := \int_{\Omega} \alpha(\mathbf{u})\beta(\mathbf{v})d\Omega$$

for $\mathbf{u} \in \mathcal{X}^c$ and $\mathbf{v} \in \mathcal{X}_{\mathbf{0}}^c$; $\alpha(\cdot)$ and $\beta(\cdot)$ are differential operators obtained after integrating by parts $\langle \mathcal{L}\mathbf{u}, \mathbf{v} \rangle$. The weak form of system (2.3) consists of: find $\mathbf{u} \in \mathcal{X}_{\mathbf{D}}^c$ such that

$$\ell(\mathbf{u}, \mathbf{v}) = \langle \mathbf{f}, \mathbf{v} \rangle \quad \forall \mathbf{v} \in \mathcal{X}_{\mathbf{0}}^c. \quad (2.4)$$

3 An abstract framework for blended AtC coupling

The aim of this section is to state in an abstract setting the family of blended AtC coupling methods. We subdivide the given body Ω into three disjoint regions Ω_a , Ω_b , and Ω_c , with Ω_b sandwiched in some way between the other two (see Figure 3.1). Let us also denote by \mathbf{A} , \mathbf{B} and \mathbf{C} the set of atoms of the overall lattice that belong to Ω_a , Ω_b and Ω_c respectively. We make the following assumptions:

- the atomistic model is valid throughout, and in particular in the atomistic region Ω_a and in the bridge region Ω_b ;
- the continuum model is valid in the continuum region Ω_c and in the bridge region Ω_b .

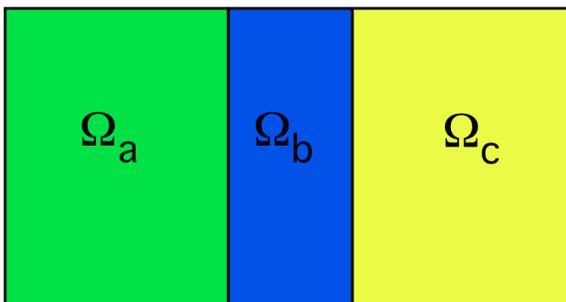


Figure 3.1: The atomistic domain (left), the continuum domain (right), and the bridging domain (center).

This family of methods requires the solution of

- the atomistic problem on Ω_a (which in general will be small in comparison with Ω);
- the continuous problem on Ω_c ;
- a blended model (a weighted average of the atomistic and continuum models) on Ω_b .²

²Let us remark that the blending is basic when considering both atomistic and continuum models on Ω_b ; see (1.1). In case of tying both models without blending, we cannot consider both atomistic and continuum models in the same region. It leads to wrong results because *we are counting two times the strength of the material* (the atomistic and continuous strength). There are two ways to solve this issue: to consider the atomistic problem and slave nodes (of the FEM approximation of the continuous problem) in the bridging region or to consider the continuous problem and slave atoms on Ω_b .

We denote by θ_c and θ_a the continuous and atomistic scalar blending functions such that:

$$\begin{aligned}\theta_c &= 1 && \text{in } \Omega_c, \\ \theta_a &= 1 && \text{in } \Omega_a, \\ \theta_c + \theta_a &= 1 && \text{in } \Omega.\end{aligned}$$

These blending functions define the purely atomistic region Ω_a (where $\theta_a = 1$), the purely continuous region Ω_c (where $\theta_c = 1$), and the bridge domain Ω_b .

The results of this section have been obtained under the following assumptions (unless indicated otherwise):

Asumption 3.1. *The blending functions are such that, given a function $\mathbf{v} \in \mathcal{X}^c$, the weighted function $\theta_a \mathbf{v} \in \mathcal{X}^c$, and subsequently $\theta_c \mathbf{v} \in \mathcal{X}^c$.*

In order to state blending-based methods in an abstract framework, it is useful to introduce some restrictions of global spaces to subdomains.

Given a function (element) $\mathbf{v} \in \mathcal{W}$, where \mathcal{W} is an appropriate function space (set), its restriction $\text{Re}_\omega(\mathbf{v})$ onto ω is a function (element) with support in ω such that

$$\text{Re}_\omega(\mathbf{v}) = \mathbf{v} \quad \text{on } \omega. \tag{3.2}$$

We can also define the restriction of the space $\text{Re}_\omega(\mathcal{W}) := \{\text{Re}_\omega(\mathbf{v})\}_{\mathbf{v} \in \mathcal{W}}$. It allows to introduce the spaces $\mathcal{R}_D^c = \text{Re}_{\Omega_c \cup \Omega_b}(\mathcal{X}_D^c)$ and $\mathcal{B}_D^c = \text{Re}_{\Omega_b}(\mathcal{X}_D^c)$. We also define their atomistic counterparts, $\mathcal{R}_D^a = \text{Re}_{A \cup B}(\mathcal{X}_D^a)$ and $\mathcal{B}_D^a = \text{Re}_B(\mathcal{X}_D^a)$. Analogously, we get \mathcal{R}_0^c and \mathcal{R}_0^a .

Another basic ingredient is the *constraint operator* that enforces *continuity* of the atomistic and continuum solutions in the bridging domain. We denote this operator by $\Lambda(\cdot, \cdot)$, which is a bilinear functional defined over $\mathcal{X}_D^c \times \mathcal{X}_D^a$. For instance, we can define $\Lambda(\cdot, \cdot)$ by introducing a *projection* $\Pi_B : \mathcal{B}_D^c \rightarrow \mathcal{B}_D^a$ as follows:

$$\Lambda(\mathbf{u}, U) = \sum_{\alpha \in \mathbf{B}} \|U_\alpha - \Pi_B(\mathbf{u})_\alpha\|.$$

This particular choice of the constraint operator implies that the atoms *are slaves* of the continuous solution on Ω_b . In Section 5 we consider a natural atom-wise constraint that is given by the following *projection*:

$$\Pi_B(\mathbf{u})_\alpha = \mathbf{u}(\mathbf{x}_\alpha) \quad \forall \alpha \in \mathbf{B}.$$

For this particular choice of $\Pi_B(\cdot)$ the constraint $\Lambda(\mathbf{u}, U) = 0$ simply means:

$$\mathbf{u}(\mathbf{x}_\alpha)_i = U_\alpha^i \quad \forall \alpha \in \mathbf{B}, \quad i = 1, \dots, d.$$

Alternatively, we consider $\Lambda(\mathbf{u}, U) = \|\mathbf{u} - \pi_b(U)\|_{\mathcal{B}^c}$ with a *projection* $\pi_b : \mathcal{B}_D^a \rightarrow \mathcal{B}_D^c$. In this case the bridging problem is stated only in terms of \mathbf{u} . Hybrid situations in which the bridging domain cannot be stated only in terms of atomistic (or continuum) solutions may also be considered.³ Any AtC blended coupling can be written in the following abstract form: find $\mathbf{u} \in \mathcal{R}_D^c$ and $U \in \mathcal{R}_D^a$ such that

$$\mathcal{A}_\theta^c(\mathbf{u}, \mathbf{v}) + \mathcal{A}_\theta^a(U, V) = 0, \quad (3.3a)$$

$$\Lambda(\mathbf{u}, U) = 0, \quad (3.3b)$$

for all $\mathbf{v} \in \mathcal{R}_0^c$ and $V \in \mathcal{R}_0^a$.⁴ $\mathcal{A}_\theta^c(\mathbf{u}, \mathbf{v})$ includes all the terms related to the continuum model whereas $\mathcal{A}_\theta^a(\mathbf{u}, \mathbf{v})$ includes all the atomistic terms. The form of these operators will depend on the blending functions and the blending approach used. In the next section we discuss different choices for these operators.

3.1 Ghost forces

One of the basic features of AtC coupling methods is that the atomistic problem is only solved for a subset of atoms of the lattice. Therefore, $\mathcal{A}_\theta^a(U, V)$ must only involve the equilibrium equations of atoms on $\mathbf{A} \cup \mathbf{B}$. Given the purely atomistic solution $U^a \in \mathcal{X}_D^a$, its restriction $U_{\mathbf{A} \cup \mathbf{B}}^a$ over $\mathbf{A} \cup \mathbf{B}$, and its counterpart U_C^a for \mathbf{C} , we know that the atomistic problem is

$$(\mathbf{L}(U^a), V) = (\mathbf{L}(U_{\mathbf{A} \cup \mathbf{B}}^a + U_C^a), V) = \langle F, V \rangle.$$

In the AtC coupling method U_C^a is approximated by a continuous solution \mathbf{u} . We must account for the force exerted by the atoms in \mathbf{C} upon the atoms in $\mathbf{A} \cup \mathbf{B}$. If not, *ghost forces* (surface effects) appear.

For the numerical approximation of the atomistic problem, only atoms within some distance δ (known as the *cut-off radius*) interact. Therefore, only the set of atoms

$$\mathbf{H} := \{\alpha \in \mathbf{C} \mid \exists \beta \in \mathbf{A} \cup \mathbf{B} \text{ s.t. } \|\mathbf{x}_\alpha - \mathbf{x}_\beta\| \leq \delta\}^5$$

must be considered when evaluating $(\mathbf{L}(\cdot), \cdot)$ ⁶. There are two formal ways to include this effect:

- We can recover an atomistic displacement U_C as:

$$U_C = \Pi_C(\mathbf{u}) := \mathbf{u}(\mathbf{x}_\alpha), \quad \forall \alpha \in \mathbf{C}, \quad (3.4)$$

³These hybrid constraints are not possible for AtC coupling without blending.

⁴The condition $\Lambda(\mathbf{u}, U) = 0$ can be easily imposed via Lagrange multipliers.

⁵Let us remark that the definition of \mathbf{H} is *non-linear* because it depends on the atomistic configuration. In a non-linear iterative procedure, this set must be recalculated.

⁶That is to say, only those atoms belonging to \mathbf{C} in the cut-off radius of some atom in $\mathbf{A} \cup \mathbf{B}$ must be accounted.

and replace $(\mathbf{L}(U_{\mathbf{A} \cup \mathbf{B}}^a + U_{\mathbf{C}}^a), V)$ by an approximate force $(\mathbf{L}(U_{\mathbf{A} \cup \mathbf{B}} + \Pi(\mathbf{u})), V)$, that depends on \mathbf{u} . Obviously, (3.4) only needs to be computed for atoms in \mathbf{H} .

- We can alternatively consider the constraint $\Lambda(\mathbf{u}, U) = 0$ to enforce all the atoms belonging to \mathbf{B} in the cut-off radius of any atom in \mathbf{C} to be slaves of the continuous solution. This is the approach we consider when defining the different AtC coupling methods.⁷

Assumption 3.2. *Given the subset of atoms*

$$\mathbf{H}' := \{\alpha \in \mathbf{B} \mid \exists \beta \in \mathbf{C} \text{ s.t. } \|\mathbf{x}_\alpha - \mathbf{x}_\beta\| \leq \delta\},$$

the constraint $\Lambda(\mathbf{u}, U) = 0$ enforces

$$U = \mathbf{u}(\mathbf{x}_\alpha), \quad \forall \alpha \in \mathbf{H}'.$$

3.2 AtC consistency and the patch test

Numerous AtC coupling methods have been designed based on physical motivations. However, the numerical analysis of AtC coupling methods is in its infancy. Almost nothing is known about basic numerical properties such as consistency, convergence, and stability. Some analysis exists for the quasi-continuum method, in which the model error is basically interpolation error (see [9, 8]).

A preliminary step for analyzing AtC coupling methods is writing these procedures in an abstract mathematical framework. This is one of the goals of our article for blending-based coupling techniques.

The numerical analysis of AtC coupling methods is non-trivial because questions that have a trivial answer in finite element analysis are not at all clear. Because we do not have a global equation on the entire domain, the identification of the exact solution is not obvious. Under the assumption that the atomistic model is valid everywhere, the exact solution is the purely atomistic solution U^a . Unfortunately, it is not straightforward to use this solution in the AtC coupling scheme. The aim of this section is to formulate a well-defined notion of *AtC consistency*. We introduce the following definitions:

Definition 3.1 (Consistency test problem). *We say that a problem is a consistency test problem when the purely atomistic solution U^a of (2.2) and the purely continuous solution \mathbf{u}^c of (2.3) do satisfy the constraint $\Lambda(\mathbf{u}^c, U^a) = 0$ on the bridging domain Ω_b .*

A consistency test problem is characterized by data $F, f, U_\alpha^D, \mathbf{u}^D$ such that solutions of (2.2) and (2.4) match in the bridging domain *modulo* the constraint operator Λ .

⁷Reasonably assuming (for simplicity) that there is not any atom in \mathbf{A} in the cut-off radius of \mathbf{C}

Definition 3.2 (Patch test problem). *A consistency test problem is called patch test problem if the purely continuous solution is such that $\alpha(\mathbf{u}) = \mathbf{c}$ where \mathbf{c} is a constant matrix.*⁸

The following definition formalizes the notion of *passing a patch test* for a coupled AtC formulation.

Definition 3.3 (Passing a patch test problem). *Let $[U^a, \mathbf{u}^c]$ denote a patch test problem. An AtC coupling method passes a patch test if $[U^a, \mathbf{u}^c]$ satisfies the coupled AtC system.*

Definition 3.4 (AtC consistency). *An AtC coupling method is consistent when, for any consistency test problem, the pair of purely atomistic and purely continuous solutions $[U^a, \mathbf{u}^c]$ satisfies the coupled AtC system.*

Atomistic problems with Cauchy-Born solutions (see [6]) are a physical example of consistency test problems.

From the previous definitions we can easily infer that consistency implies passage of the patch test problem. However, the opposite statement is not true.

⁸That is to say, constant stress solutions

4 Some blended AtC coupling methods

In this section we list four blended AtC coupling methods. The first was proposed by [7]. To the best of knowledge, the remaining three methods are new. We refer to Section 5 and [7] for justification of some of these methods by mechanical arguments.

Throughout this section we will assume that for any smooth functions θ and \mathbf{v} the differential operator $\beta(\cdot)$ has the following *product rule* property:

$$\beta(\theta\mathbf{v}) = \theta\beta(\mathbf{v}) + \beta(\theta)\mathbf{v}. \quad (4.1)$$

4.1 Method I

The underlying mechanical motivation of Method I has been recently introduced in [7] with the aim of coupling atomistic and continuum simulations via the *blending of stresses*. Unfortunately, *stress* is not a clear concept at the atomistic level (see [10, 5]). By the definition of the blending functions and Assumption 3.1 we can rewrite (2.4) and (2.2) as:

$$\begin{aligned} \int_{\Omega} \theta_c \alpha(\mathbf{u}) \beta(\mathbf{v}) d\Omega + \int_{\Omega} \theta_a \alpha(\mathbf{u}) \beta(\mathbf{v}) d\Omega &= \langle \mathbf{f}, \theta_c \mathbf{v} \rangle + \langle \mathbf{f}, \theta_a \mathbf{v} \rangle, \\ (\mathbf{L}(U), \Theta_c V) + (\mathbf{L}(U), \Theta_a V) &= \langle F, \Theta_c V \rangle + \langle F, \Theta_a V \rangle, \end{aligned}$$

where Θ_a is a diagonal weighting matrix whose diagonal values are equal to θ_a evaluated at the corresponding atoms:

$$(\Theta_a)_{\alpha\beta}^{ij} = \delta_{ij} \delta_{\alpha\beta} \theta_a(\mathbf{x}_\alpha), \quad i, j = 1, \dots, d, \quad \alpha, \beta \in \mathbf{P},$$

and similarly for Θ_c . In order to couple both equations, we merge the continuous terms weighted with θ_c and the atomistic terms weighted with θ_a . Furthermore, the continuous and atomistic solution are tied together on Ω_b via the constraint operator. The resulting AtC bridging method consists of: find $\mathbf{u} \in \mathcal{R}_D^c$ and $U \in \mathcal{R}_D^a$ such that

$$\int_{\Omega} \theta_c \alpha(\mathbf{u}) \beta(\mathbf{v}) d\Omega + (\mathbf{L}(U), \Theta_a V) = \langle \mathbf{f}, \theta_c \mathbf{v} \rangle + \langle F, \Theta_a V \rangle, \quad (4.2a)$$

$$\Lambda(\mathbf{u}, U) = 0, \quad (4.2b)$$

for all $\mathbf{v} \in \mathcal{R}_D^c$ and $V \in \mathcal{R}_D^a$.

We can write (4.2a) in the fashion of (3.3) with:

$$\begin{aligned} \mathcal{A}_\theta^c(\mathbf{u}, \mathbf{v}) &:= \int_{\Omega} \theta_c \alpha(\mathbf{u}) \beta(\mathbf{v}) d\Omega - \langle \mathbf{f}, \theta_c \mathbf{v} \rangle, \\ \mathcal{A}_\theta^a(U, V) &:= (\mathbf{L}(U), \Theta_a V) - \langle F, \Theta_a V \rangle. \end{aligned}$$

In the following theorem, we analyze the consistency of Method I.

Theorem 4.1. *Method (4.2) is not consistent and does not pass a patch test problem.*

Proof. Let $[U^a, \mathbf{u}^c]$ be a solution of a consistency test problem. The purely atomistic part U^a is such that $\mathcal{A}_\theta^a(U^a, V) = 0$ for any θ_a . However, using (4.1) we see that for the purely continuous solution \mathbf{u}^c of (2.3)

$$\begin{aligned} \mathcal{A}_\theta^c(\mathbf{u}^c, \mathbf{v}) &= \int_{\Omega} \theta_c \alpha(\mathbf{u}^c) \beta(\mathbf{v}) d\Omega - \ell(\mathbf{u}^c, \theta_c \mathbf{v}) = \int_{\Omega} \alpha(\mathbf{u}^c) \beta(\theta_c) \mathbf{v} d\Omega \\ &:= \epsilon(\theta_c, \mathbf{u}^c, \mathbf{v}), \end{aligned}$$

The last term is zero if and only if

$$\alpha(\mathbf{u}^c) \beta(\theta_c) = 0, \quad (4.3)$$

which is not true in general. In particular, for a patch test problem, (4.3) is only true if $\beta(\theta_c) = 0$.⁹ \square

Remark 1. Let us consider a discrete version of system (4.2) where a finite element approximation of the continuous problem and a discretized expression of the blending parameters are considered: find $\mathbf{u}_h \in \mathcal{R}_{\mathbf{D},h}^c$ and $U \in \mathcal{R}_{\mathbf{D}}^a$ such that

$$\int_{\Omega} \theta_c^h \alpha(\mathbf{u}_h) \beta(\mathbf{v}_h) d\Omega + (\mathbf{L}(U), V_{\theta_c^h}) = \langle \mathbf{f}, \theta_c^h \mathbf{v}_h \rangle + \langle F, V_{\theta_c^h} \rangle, \quad (4.4a)$$

$$\Lambda_h(\mathbf{u}_h, U) = 0 \quad (4.4b)$$

for all $\mathbf{v}_h \in \mathcal{R}_{\mathbf{D},h}^c$ and $V_{\theta_c^h} \in \mathcal{R}_{\mathbf{D}}^a$. In [7] the blending parameters have been considered element-wise constant. It is easy to check that also for this particular choice method (4.4) is not consistent and does not pass a patch test problem. For a discrete consistency test, such that \mathbf{u}_h^c (the solution of the finite element discretization of problem (2.4)) and U^a (purely atomistic problem) satisfy $\Lambda_h(\mathbf{u}_h^c, U^a) = 0$, the atomistic terms cancel. Due to the fact that $\theta_c^h \mathbf{v}_h$ does not belong to $\mathcal{X}_{\mathbf{D},h}^c$ (we do not make Assumption 3.1), we have to modify the way we treat the continuous terms. Again, we know that

$$\ell(\mathbf{u}_h^c, \mathbf{v}_h) = \int_{\Omega} \alpha(\mathbf{u}_h^c) \beta(\mathbf{v}_h) d\Omega = \langle \mathbf{f}, \mathbf{v}_h \rangle.$$

⁹For instance, let us consider one-dimensional linear elasticity for the continuous problem. We can easily see that:

$$\epsilon(\theta_c, \mathbf{u}^c, \mathbf{v}) = \int_{\Omega} \nabla \mathbf{u}^c \cdot \mathbf{v} \cdot \nabla \theta_c d\Omega.$$

In order for method (4.2) to pass the patch test, the following relation should be satisfied:

$$\nabla \mathbf{u}^c \cdot \nabla \theta_c = 0.$$

The only situation in which (4.3) holds is when $\theta_a = \theta_c = 1/2$, computationally infeasible. The original motivation of the method is to activate the atomistic problem in a small part of the domain.

Let us denote with Ω_e the domain for a finite element e and \sum_e the sum over all the finite elements. The consistency condition

$$\sum_e \int_{\Omega_e} \theta_c^h \alpha(\mathbf{u}_h) \beta(\mathbf{v}_h) d\Omega = \langle \mathbf{f}, \theta_c^h \mathbf{v}_h \rangle$$

holds for arbitrary element-wise constant blending functions only if:

$$\int_{\Omega_e} \alpha(\mathbf{u}_h^c) \beta(\mathbf{v}_h) d\Omega = \int_{\Omega_e} \mathbf{f} \mathbf{v}_h,$$

which is not true in general.

4.2 Method II

The previous method fails (in terms of consistency) because, whereas the atomistic blending operator \mathcal{A}_θ^a vanishes for the purely atomistic solution, its continuous counterpart \mathcal{A}_θ^c does not vanish for the purely continuous solution. As a result, equation (3.3) can never be satisfied exactly by this coupling scheme. One possible solution is to relax \mathcal{A}_θ^a so that consistency could be proved. The idea is to define \mathcal{A}_θ^a in such a way that $\mathcal{A}_\theta^a(U^a, V) = -\mathcal{A}_\theta^c(\mathbf{u}^c, \mathbf{v})$, i.e., to have (3.3) satisfied by relaxing the atomistic operator over the blending region.

A modification that can be mechanically justified as a *blended force balance*, and that achieves this goal, will be presented in Section 5 (see also Figure 5.2). The atomistic part that results from this approach can be expressed as

$$\mathcal{A}_\theta^a(U, V) := (\mathbf{L}_{\theta_a} U, V) - \langle F, \Theta_a V \rangle,$$

where \mathbf{L}_{θ_a} is an appropriate modification of \mathbf{L} via the blending functions. Section 5 is devoted to the construction of this operator. Therefore, the AtC coupling procedure consists of: find $\mathbf{u} \in \mathcal{R}_D^c$ and $U \in \mathcal{R}_D^a$ such that

$$(\mathbf{L}_{\theta_a} U, V) + \int_{\Omega} \theta_c \alpha(\mathbf{u}) \beta(\mathbf{v}) d\Omega = \langle \mathbf{f}, \theta_c \mathbf{v} \rangle + \langle F, \Theta_a V \rangle \quad (4.5a)$$

$$\Lambda(\mathbf{u}, U) = 0 \quad (4.5b)$$

for all $\mathbf{v} \in \mathcal{R}_D^c$ and $V \in \mathcal{R}_D^a$.

The consistency of the method depends on the definition of the operator \mathbf{L}_θ . In Section 5 we obtain the condition that must be satisfied by this operator when considering finite elements for the numerical approximation of the continuum problem.

4.3 Method III

One of the assumptions used for the design of AtC coupling algorithms is that the continuous model is a good approximation of the atomistic model in Ω_b and Ω_c . This

assumption implies that the continuous differential operator \mathcal{L} is a good representation of \mathbf{L} under suitable conditions (e.g., smoothness). A reasonable approach is to blend both models in a pointwise sense. Roughly speaking, blend the operators \mathcal{L} and \mathbf{L} .¹⁰ This approach leads to the following AtC coupling system: find $\mathbf{u} \in \mathcal{R}_{\mathbf{D}}^c$ and $U \in \mathcal{R}_{\mathbf{D}}^a$ such that

$$\ell(\mathbf{u}, \theta_c \mathbf{v}) + (\mathbf{L}(U), \Theta_a V) = \langle \mathbf{f}, \theta_c \mathbf{v} \rangle + \langle F, \Theta_a V \rangle, \quad (4.6a)$$

$$\Lambda(\mathbf{u}, U) = 0, \quad (4.6b)$$

for all $\mathbf{v} \in \mathcal{R}_{\mathbf{D}}^c$ and $V \in \mathcal{R}_{\mathbf{D}}^a$.¹¹

Again, we can write (4.6a) as

$$\mathcal{A}_{\theta}^c(\mathbf{u}, \mathbf{v}) + \mathcal{A}_{\theta}^a(U, V) = 0.$$

A positive feature of this approach, which is not shared by the previous methods, is that the purely atomistic and continuous solutions cancel $\mathcal{A}_{\theta}^a(U, V)$ and $\mathcal{A}_{\theta}^c(\mathbf{u}, \mathbf{v})$ for any AtC bridging problem. The following theorem is a direct consequence of this observation.

Theorem 4.2. *The AtC system (4.6) is consistent and, subsequently, passes any patch test problem.*

The consistency of this method makes its use appealing and will be the subject of future work.

4.4 Method IV

Our fourth method can be viewed as a *dual* of Method I.

$$\begin{aligned} (\mathbf{L}_{\theta_a} U, V) + \ell(\mathbf{u}, \theta_c \mathbf{v}) &= \langle \mathbf{f}, \theta_c \mathbf{v} \rangle + \langle F, \Theta_a V \rangle \\ \Lambda(\mathbf{u}, U) &= 0 \end{aligned}$$

for all $\mathbf{v} \in \mathcal{R}_{\mathbf{D}}^c$ and $V \in \mathcal{R}_{\mathbf{D}}^a$. In this case, the purely continuous solution cancels the continuous operator \mathcal{A}_{θ}^c , while $\mathcal{A}_{\theta}^a(U^a, V) \neq 0$. As a result, this method is not consistent and so does not pass the patch test.

4.5 Summary of the four methods

Table 4.1 summarizes the consistency of the different methods.

¹⁰In [7] a similar blending method has been discarded for not passing the patch test. The reason seems to be the fact that ghost forces were not accounted for.

¹¹This method can be understood as a *blending of forces* (instead of stresses), because it is $\mathcal{L}\mathbf{u}$ and $\mathbf{L}(U)$ that are blended. Mechanically, the unconditional consistency of the method is related to the fact that *force* is well-defined both for the atomistic and continuous problem.

Table 4.1: Values of the atomistic and continuous operators of AtC blending methods evaluated at $[U^a, \mathbf{u}^c]$.

Method	$\mathcal{A}_\theta^c(\mathbf{u}^c, \mathbf{v})$	$\mathcal{A}_\theta^a(U^a, V)$	Consistent
I	$\neq 0$	$= 0$	No
II	$\neq 0$	$\neq 0$	Depending on \mathbf{L}_{θ_a}
III	$= 0$	$= 0$	Yes
IV	$= 0$	$\neq 0$	No

5 On a consistent method based on the blending of stresses

Let us consider a family of *quasi-uniform* finite element partitions $\mathcal{T}_h(t)$ of $\Omega_c \cup \Omega_b$. As usual, h represents the maximum size of the elements of \mathcal{T}_h . Let \mathcal{R}_h^c be a nodal-based finite element space approximating \mathcal{R}^c . Analogously, we define $(\mathcal{R}_0^c)_h$ and $(\mathcal{R}_D^c)_h$. We introduce the Lagrange basis $\{\phi_j\}_{j \in \mathcal{N}}$ associated to \mathcal{R}_h^c , where \mathcal{N} is the set of finite element nodes. The approximation to the continuous displacement is denoted by \mathbf{u}_h and we let $\sigma_h = \sigma(\mathbf{u}_h)$. We denote by $\{\mathbf{v}_h^j\}_{j \in \mathcal{N}}$ a basis for \mathcal{R}_h^c . Then, we can write the finite element discretization of the AtC coupling method (4.5) as: find $\mathbf{u}_h \in (\mathcal{R}_D^c)_h$ and $U \in \mathcal{R}_D^a$ such that

$$(\mathbf{L}_{\theta_a} U, V) + \int_{\Omega} \theta_c \alpha(\mathbf{u}_h) \beta(\mathbf{v}_h) d\Omega = \langle \mathbf{f}, \theta_c \mathbf{v}_h \rangle + \langle F, \Theta_a V \rangle \quad (5.1a)$$

$$\Lambda(\mathbf{u}_h, U) = 0 \quad (5.1b)$$

for all $\mathbf{v}_h \in (\mathcal{R}_D^c)_h$ and $V \in \mathcal{R}_D^a$.

Theorem 5.1. *When the constraint operator enforces slave atoms, system (5.1) can be written in the following equivalent way: find $\mathbf{u}_h \in (\mathcal{R}_D^c)_h$ and $U \in \mathcal{R}_D^a$ such that*

$$(\mathbf{L}_{\theta_a} U, V) + \int_{\Omega} \theta_c \alpha(\mathbf{u}_h) \beta(\mathbf{v}_h) d\Omega = \langle \mathbf{f}, \theta_c \mathbf{v}_h \rangle + \langle F, \Theta_a V \rangle \quad (5.2a)$$

$$\Lambda(\mathbf{u}_h, U) = 0 \quad (5.2b)$$

for all $\mathbf{v}_h \in \mathcal{R}_0^c$ and $V \in \mathcal{R}_0^a$ satisfying $\Lambda(\mathbf{v}_h, V) = 0$.

Proof. Let us introduce the following finite element matrix:

$$K^{jk} = \ell(\phi_j, \phi_k), \quad j, k \in \mathcal{N}. \quad (5.3)$$

We denote by \mathbf{U} the array of nodal values for \mathbf{u}_h . On the other hand, the constraint

$$\mathbf{u}(\mathbf{x}_\alpha)_i = (U_\alpha)_i \quad \forall \alpha \in \mathbf{B}, \quad i = 1, \dots, d.$$

can be written as

$$C_u \mathbf{U} + C_U U_{\mathbf{B}} = \mathbf{0}, \quad (5.4)$$

where

$$\begin{aligned} C_u^{\alpha k} &= \phi_b(\mathbf{x}_\alpha), \quad \alpha \in \mathbf{B}, \quad k \in \mathcal{N}_k, \\ C_U^{\alpha\beta} &= \delta_{\alpha\beta} := I_{\mathbf{B}}^{\alpha\beta}, \quad \alpha, \beta \in \mathbf{B}. \end{aligned} \quad (5.5)$$

We can write this problem as:

$$\begin{aligned} L(U)_\mathbf{A} &= F_\mathbf{A} \\ L(U)_\mathbf{B} + I_\mathbf{B}\boldsymbol{\lambda} &= F_\mathbf{B} \\ K\mathbf{U} - C_u^t\boldsymbol{\lambda} &= \mathbf{F} \\ -C_u\mathbf{U} + I_\mathbf{B}U_\mathbf{B} &= \mathbf{0}. \end{aligned}$$

where $L(U)_\mathbf{A}$ and $L(U)_\mathbf{B}$ represent the sub-systems (non-linear) equilibrium equations for atoms in \mathbf{A} and \mathbf{B} respectively. These equations imply that

$$K\mathbf{U} + C_u^tL(U)_\mathbf{B} = \mathbf{F} + C_u^tF_\mathbf{B}. \quad (5.6)$$

Now, we can multiply (5.6) by the set $\{\mathbf{V}^j\}_{j \in \mathcal{N}}$, arrays of nodal values of $\{\mathbf{v}_h^j\}_{j \in \mathcal{N}}$: Idem for F . We define $V_\mathbf{B}^j = C_u^t\mathbf{V}^j$ for $j \in \mathcal{N}$. Thus, the set of test function V such that $\Lambda(\mathbf{v}_h, V) = 0$ can be written as $V = V_\mathbf{A} + C_u^t\mathbf{V}$, for $V_\mathbf{A}$ arbitrary. With these ingredients, we get the form of the statement. \square

We will use this expression in the following theorem and subsection. In the next theorem we analyze the conditions under which this method is consistent.

Theorem 5.2. *Method (4.5) is consistent if the operator \mathbf{L}_θ is constructed in such a way that, for any consistency test problem, the appropriate restrictions of the pair $[\mathbf{u}_h^c, U^a]$ satisfy*

$$(\mathbf{L}_{\theta_a}U^a, V) - (\mathbf{L}(U^a), V\Theta_a) = - \left[\int_\Omega \theta_c \alpha(\mathbf{u}_h^c) \beta(\mathbf{v}_h) d\Omega - \ell(\mathbf{u}_h^c, \theta_c \mathbf{v}_h) \right] \quad (5.7)$$

for all $\mathbf{v}_h \in \mathcal{R}_\mathbf{D}^c$ and $V \in \mathcal{R}_\mathbf{D}^a$ holding $\Lambda(\mathbf{v}, V) = 0$. A method passes the patch test if (5.7) is only satisfied for patch test solutions.

Proof. In order to have a consistent method, the consistency error

$$\epsilon(\theta_c, \mathbf{u}_h^c, \mathbf{v}_h) := \mathcal{A}_\theta^a(U, V) + \mathcal{A}_\theta^c(\mathbf{u}, \mathbf{v}) \quad (5.8)$$

must be equal to zero. We know that $[\mathbf{u}^c, U^a]$ satisfies:

$$\begin{aligned} (\mathbf{L}(U), \Theta_a V) &= (F, \Theta_a V), \\ \ell(\mathbf{u}, \theta_a \mathbf{v}) &= \langle \mathbf{f}, \theta_a \mathbf{v} \rangle, \\ \Lambda(\mathbf{u}, U) &= 0. \end{aligned}$$

Invoking this system of equalities in (5.8) we prove the theorem. \square

The remaining point is how to build an operator \mathbf{L}_θ for which condition (5.7) is satisfied for every consistent (or, less demanding, patch) test problem. We construct this operator below and prove condition (5.7) for some particular patch test problems.

5.1 Mechanical motivation and some test problems

For the numerical solution of the atomistic problem we consider that, in addition to an externally applied force, the force on the particle α located at the position \mathbf{x}_α is due only to the set of particles $\mathfrak{B}_\alpha = \{\beta \in \mathbf{P} : |\mathbf{x}_\beta - \mathbf{x}_\alpha| \leq \delta\}$ within the ball of radius δ (the cut-off distance). Here, we consider interatomic potentials such that the force at atom α due to its interactions with all other atoms can be written as

$$\mathbf{f}_\alpha = \sum_{\beta \in \mathfrak{B}_\alpha} \mathbf{f}_{\alpha,\beta} \quad (5.9)$$

where $\mathbf{f}_{\alpha,\beta}$ is the force on atom α due to its interaction with atom β . See Figure 5.1. This model clearly applies to all pairwise interatomic potentials, such as Lennard-Jones, as well as models such as the embedded atom method (EAM) [3, 4]. In the case of EAM, the energy associated with atom α can be written as

$$E_\alpha = \sum_{\beta \neq \alpha} E_{pair}(r_{\alpha\beta}) + E_{embed} \left(\sum_{\beta \neq \alpha} \rho(r_{\alpha\beta}) \right),$$

where $r_{\alpha\beta} = \|\mathbf{r}_\alpha - \mathbf{r}_\beta\|$. We see that the negative gradient of the previous expression has the form (5.9). In the atomistic region, force equilibrium requires that, for any particle α , we have the force balance

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

or

$$\sum_{\beta \in \mathfrak{B}_\alpha} \mathbf{f}_{\alpha,\beta} + \mathbf{f}_\alpha^e = \mathbf{0} \quad (5.10)$$

where \mathbf{f}_α^e denotes the external force applied to the particle α .

According to Cauchy, if we take any continuum volume ω enclosing the point \mathbf{x} , the force acting on that volume by the material surrounding it is given by

$$\mathbf{f}_\gamma = - \int_\gamma \boldsymbol{\sigma} \cdot \mathbf{n} \, d\gamma \quad (5.11)$$

where γ denotes the boundary of ω and $\boldsymbol{\sigma}$ denotes the stress tensor. See Figure 5.1. We assume that $\boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x}, \nabla \mathbf{u}(\mathbf{x}))$ 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, $\boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{\sigma}(\nabla \mathbf{u}(\mathbf{x}))$, i.e., it does not explicitly depend on position. This is due to the observation that $-\boldsymbol{\sigma} \cdot \mathbf{n}$ is the stress force acting on a point on γ . In the equilibrium state, we have that

$$- \int_\gamma \boldsymbol{\sigma} \cdot \mathbf{n} \, d\gamma + \int_\omega \mathbf{f} \, d\omega = \mathbf{0}$$

where \mathbf{f} is the externally applied volumetric force. We then have that

$$\int_\omega (\nabla \cdot \boldsymbol{\sigma} + \mathbf{f}) \, d\omega = \mathbf{0}.$$

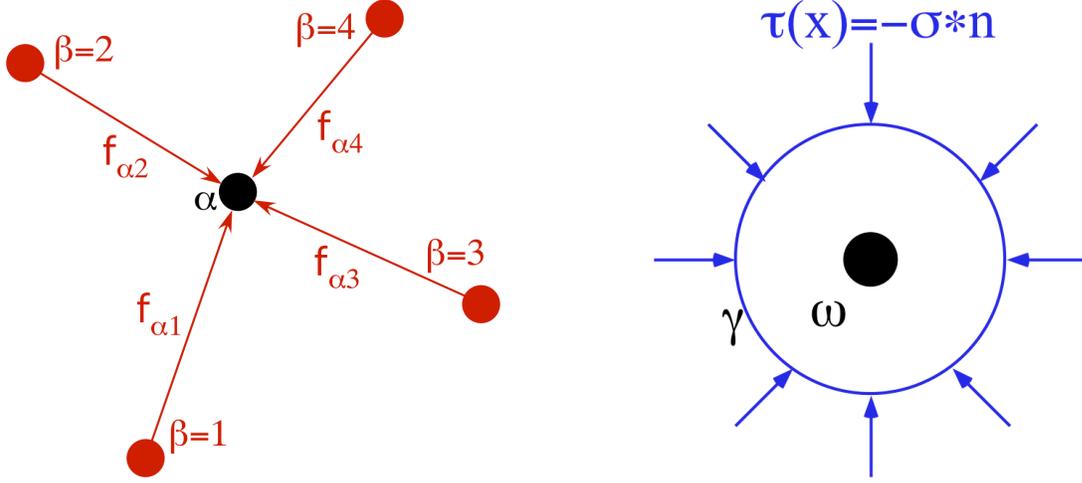


Figure 5.1: Force balance at a particle for the atomistic model (left) and at a point for the continuum model (right).

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

$$\nabla \cdot \sigma + \mathbf{f} = \mathbf{0}. \quad (5.12)$$

In the bridge region Ω_b , we have assumed that both the atomistic and continuum model are valid. We want to “blend” the two models to create a single model for that region that transitions, across the bridge region, from the atomistic model to the continuum model. *We choose to blend the two models at the level of forces acting at points.*

We have that (5.10) and (5.12) hold in the bridge region. The most straightforward blending of forces produces the blended model

$$\begin{aligned} & - \int_{\Omega} \theta_c \sigma : \nabla \mathbf{w} \, d\omega + \sum_{\alpha \in \mathbf{P}} \theta_a^\alpha \sum_{\beta \in \mathfrak{B}_\alpha} \mathbf{f}_{\alpha,\beta} \cdot \mathbf{w}(\mathbf{x}_\alpha) \\ & = - \int_{\Omega} \theta_c \mathbf{f} \cdot \mathbf{w} \, d\omega - \int_{\Gamma_t} \theta_c \mathbf{t} \cdot \mathbf{w} \, d\gamma - \sum_{\alpha \in \mathbf{P}} \theta_a^\alpha \mathbf{f}_\alpha^e \cdot \mathbf{w}(\mathbf{x}_\alpha). \end{aligned} \quad (5.13)$$

We claim that the blended model (5.13) violates Newton’s third law of motion.¹² Consider the atomistic term in (5.13); it implies that the force on particle α due to particle β is given by $\theta_a^\alpha \mathbf{f}_{\alpha,\beta}$. But, if we reverse the roles of α and β , the force on particle β due to particle α would be $\theta_a^\beta \mathbf{f}_{\beta,\alpha} = -\theta_a^\beta \mathbf{f}_{\alpha,\beta}$. Since, in general, $\theta_a^\beta \neq \theta_a^\alpha$, we have a violation of Newton’s third law that requires the force on particle α due to particle β to be equal and opposite to the force on particle β due to particle α . A similar argument can be presented to show that the continuum part of (5.13) also violates Newton’s third law.¹³

¹²This may account why this method fails the patch test.

¹³Another problem with (5.13) is that it is not a symmetric formulation, even when each of the

To obtain a blended model that satisfies Newton's third law we have to start with the more "basic" force definitions. We now define the force on particle α due to the other particles in its cut-off region \mathfrak{B}_α by¹⁴

$$\mathbf{f}_\alpha = \sum_{\beta \in \mathfrak{B}_\alpha} \theta_a^{\alpha\beta} \mathbf{f}_{\alpha,\beta}. \quad (5.14)$$

See Figure 5.2. If we require that

$$\theta_a^{\alpha\beta} = \theta_a^{\beta\alpha} \quad (5.15)$$

then Newton's third law is satisfied, i.e., $\theta_a^{\alpha\beta} \mathbf{f}_{\alpha,\beta} = -\theta_a^{\beta\alpha} \mathbf{f}_{\beta,\alpha}$.¹⁵ Then, the atomistic contribution to the blended model is given by

$$\sum_{\beta \in \mathfrak{B}_\alpha} \theta_a^{\alpha\beta} \mathbf{f}_{\alpha,\beta} + \theta_a^\alpha \mathbf{f}_\alpha^e = \mathbf{0}. \quad (5.16)$$

Note that if $\theta_a(\mathbf{x}) = 1$, then (5.16) reduces to the atomistic model (5.10).

A similar approach can be followed to determine the continuum contribution to the blended model. We replace (5.11) by

$$\mathbf{f}_c = - \int_\gamma \theta_c \boldsymbol{\sigma} \cdot \mathbf{n} \, d\gamma \quad (5.17)$$

where $\theta_c(\mathbf{x})$ will be defined later. See Figure 5.2. This leads to the force balance

$$- \int_\gamma \theta_c \boldsymbol{\sigma} \cdot \mathbf{n} \, d\gamma + \int_\omega \theta_c \mathbf{f} \, d\omega = \mathbf{0}$$

which in turn leads to, instead of (5.12),

$$\nabla \cdot (\theta_c \boldsymbol{\sigma}) + \theta_c \mathbf{f} = \mathbf{0}. \quad (5.18)$$

Note that if $\theta_c(\mathbf{x}) = 1$, then (5.18) reduces to the atomistic model (5.12).

atomistic and continuum models are symmetric as is the case, e.g., for linear spring-mass systems coupled to the equations of linear elasticity.

¹⁴The definition in (5.14) should be contrasted with what is used in (5.13) where that force is defined as

$$\theta_a^\alpha \sum_{\beta \in \mathfrak{B}_\alpha} \mathbf{f}_{\alpha,\beta}.$$

¹⁵One way to define $\theta_a^{\alpha\beta}$ is to first define a function $\theta_a(\mathbf{x})$ over the bridge region and then define $\theta_a^{\alpha\beta}$ from θ_a . The obvious choices are

$$\theta_a^{\alpha\beta} = \theta_a \left(\frac{\mathbf{x}_\alpha + \mathbf{x}_\beta}{2} \right) \quad \text{or} \quad \theta_a^{\alpha\beta} = \frac{\theta_a^\alpha + \theta_a^\beta}{2}$$

where $\theta_a^\alpha = \theta_a(\mathbf{x}_\alpha)$.

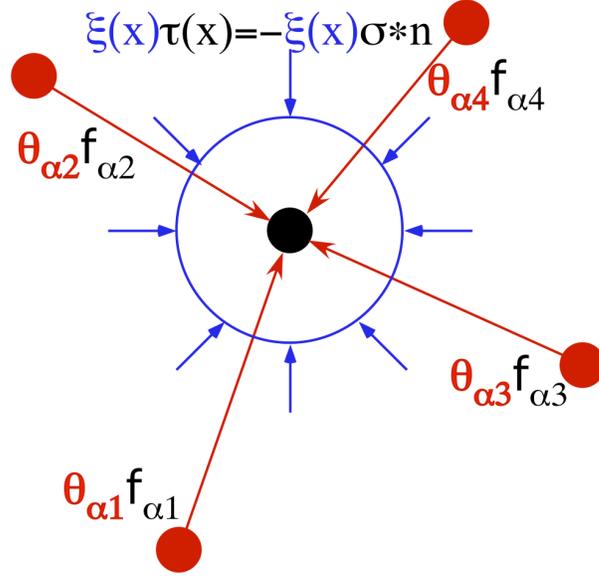


Figure 5.2: Blended force balance at a particle in the bridge region.

The blended model is then the force balance given by the sum of the weak forms of (5.16) and (5.18), i.e.,

$$\begin{aligned}
& - \int_{\Omega} \theta_c \boldsymbol{\sigma} : \nabla \mathbf{w} \, d\omega + \sum_{\alpha \in \mathbf{P}} \sum_{\beta \in \mathfrak{B}_{\alpha}} \theta_a^{\alpha, \beta} \mathbf{f}_{\alpha, \beta} \cdot \mathbf{w}(\mathbf{x}_{\alpha}) \\
& = - \int_{\Omega} \theta_c \mathbf{f} \cdot \mathbf{w} \, d\omega - \int_{\Gamma_t} \theta_c \mathbf{t} \cdot \mathbf{w} \, d\gamma - \sum_{\alpha \in \mathbf{P}} \theta_a^{\alpha} \mathbf{f}_{\alpha}^c \cdot \mathbf{w}(\mathbf{x}_{\alpha})
\end{aligned} \tag{5.19}$$

where Γ_t that part of the boundary of $\Omega_c \cup \Omega_b$ on which traction force \mathbf{t} is specified. In (5.19), \mathbf{w} is a test function chosen from a suitable class of functions.

In addition to (5.19), we will pose additional constraints in the blended region. These will be discussed in the next section.

5.2 The discrete equations

In order to get a first set of discrete equations, we test (5.19) with $\mathbf{w} = \mathbf{w}_j^h$, $j \in \mathcal{N}$, to obtain the first set of discrete equations

$$\begin{aligned}
& - \int_{\text{supp}(\mathbf{w}_j^h)} \theta_c \sigma^h : \nabla \mathbf{w}_j^h \, d\omega + \sum_{\substack{\alpha \text{ such that} \\ \mathbf{x}_\alpha \in \text{supp}(\mathbf{w}_j^h)}} \sum_{\beta \in \mathfrak{B}_\alpha} \theta_a^{\alpha, \beta} \mathbf{f}_{\alpha, \beta} \cdot \mathbf{w}_j^h(\mathbf{x}_\alpha) \\
& = - \int_{\text{supp}(\mathbf{w}_j^h)} \theta_c \mathbf{f} \cdot \mathbf{w}_j^h \, d\omega - \int_{\Gamma_t \cap \text{supp}(\mathbf{w}_j^h)} \theta_c \mathbf{t} \cdot \mathbf{w}_j^h \, d\gamma \\
& \quad - \sum_{\substack{\alpha \text{ such that} \\ \mathbf{x}_\alpha \in \text{supp}(\mathbf{w}_j^h)}} \theta_a^\alpha \mathbf{f}_\alpha^e \cdot \mathbf{w}_j^h(\mathbf{x}_\alpha) \quad \text{for } j = 1, \dots, J.
\end{aligned} \tag{5.20}$$

Note that, in (5.20), test functions are defined with respect to finite element nodes in both Ω_c and Ω_b .

As commented in the previous section, we impose the following constraints on the particle displacements in Ω_b :

$$\mathbf{u}_\alpha = \mathbf{u}^h(\mathbf{x}_\alpha) \quad \alpha \in \mathbf{B} \tag{5.21}$$

i.e., the particle displacements are determined by evaluating the finite element displacement at the position of the particle.¹⁶ If we view (5.21) as a set of *essential* constraints for the discrete system (5.20)–(5.23) that are to be enforced strongly, we should not include¹⁷ in that system those equations that correspond to test functions that are associated with particles in Ω_b , i.e., we do not include (5.23).¹⁸ Thus, the discrete system reduces to (5.20)–(5.22) and (5.21). Note that the constraints (5.21) can be explicitly substituted into (5.20) in which case (5.20)–(5.22) reduces to a system of $|\mathbf{A}| + |\mathcal{N}|$ equations in the same number of unknowns.

Remark 2. Instead of using slave atoms, we would consider test functions that correspond to the particles. We define these test functions by

$$\mathbf{w}_\alpha(\mathbf{x}) = \mathbf{e}_i \chi(|\mathbf{x} - \mathbf{x}_\alpha|) \quad \alpha \in \mathbf{A}, \quad i = 1, \dots, d$$

¹⁶This is reminiscent of the quasi-continuum method for which the displacement of slave atoms are determined from the displacement of a few master atoms.

¹⁷This is entirely analogous to the Dirichlet problem for the Poisson equation for which the equations corresponding to test function associated with nodes on the boundary are not included in the discrete system.

¹⁸This is not the only possibility for improving the system (5.20)–(5.22). For example, all of the equations of that system could be retained and the essential constraints (5.21) applied via the Lagrange multiplier rule or by penalization. Again, these choices are entirely analogous to what is possible for the Poisson equation.

where $\chi(r)$ is an integrable function with support in a small neighborhood¹⁹ of $r = 0$ and such that $\chi(0) = 1$; here, \mathbf{e}_i is the unit vector in the i -th direction.

We then have from (5.19) with $\mathbf{w} = \mathbf{w}_\alpha$ that

$$\sum_{\beta \in \mathfrak{B}_\alpha} \theta_a^{\alpha\beta} \mathbf{f}_{\alpha,\beta} = -\theta_a^\alpha \mathbf{f}_\alpha^e \quad \alpha \in \mathbf{A} \cup \mathbf{B}^{20} \quad (5.22)$$

and

$$\begin{aligned} \sum_{\beta \in \mathfrak{B}_\alpha} \theta_a^{\alpha\beta} \mathbf{w}_\alpha(0) \cdot \mathbf{f}_{\alpha,\beta} - \int_{\text{supp}(\mathbf{w}_\alpha)} \theta_c \sigma^h : \nabla \mathbf{w}_\alpha \, d\omega &= -\theta_a^\alpha \mathbf{w}_\alpha(0) \cdot \mathbf{f}_\alpha^e \\ - \int_{\text{supp}(\mathbf{w}_\alpha)} \theta_c \mathbf{b} \cdot \mathbf{w}_\alpha \, d\omega - \int_{\Gamma_t \cap \overline{\text{supp}(\mathbf{w}_\alpha)}} \theta_c \mathbf{t} \cdot \mathbf{w}_\alpha \, d\gamma &\quad \alpha \in \mathbf{B}. \end{aligned} \quad (5.23)$$

The (nonlinear) system of discrete equations (5.20)–(5.23) consists of $|\mathbf{A} \cup \mathbf{B}| + |\mathcal{N}|$ equations in $|\mathbf{A} \cup \mathbf{B}| + |\mathcal{N}|$ unknowns. However, it may not be a “nice” system. For one thing, it may be singular²¹ and for another, the appearance of the derivative of the test function \mathbf{w}_α in (5.23) can lead to serious ill-conditioning.²²

5.3 A simple 1D example and the patch test

5.3.1 A simple, linear 1D example

We let $\Omega_a = (0, a)$, $\Omega_b = (a, c)$, and $\Omega_c = (c, 1)$. In $\overline{\Omega_c} \cup \overline{\Omega_b} = [a, 1]$, we have a uniform finite element triangulation with grid size h given by $x_j = a + (j - 1)h$, $j = 1, \dots, J$. We choose the space \mathcal{R}_h^c to be the continuous, piecewise linear finite element space with respect to the triangulation. We let $u_j^h = u^h(x_j)$, i.e., the nodal value of the finite element approximation to the continuum displacement evaluated at the node x_j . We also assume only nearest-neighbor atomistic interactions. In $\overline{\Omega_a} \cup \overline{\Omega_b} = [0, c]$, we have a uniform particle lattice²³ with lattice spacing s given by $x_\alpha = (\alpha - 1)s$, $\alpha = 0, \dots, N$. The displacement of particle α is denoted by u_α . Without loss of generality,²⁴ we assume that there exists a particle α such that $x_\alpha = a$, i.e., there is a particle positioned at the interface between the atomistic and bridge regions $\overline{\Omega_a} \cap \overline{\Omega_b}$.

¹⁹In fact, the support neighborhood should be small enough so that it encloses only one particle. Moreover, the support of $\chi(r)$ should be small enough so that for all particles α located in Ω_a , $\text{supp} \chi(|\mathbf{x} - \mathbf{x}_\alpha|) \in \Omega_a$. This last assumption guarantees that the integral terms in (5.19) vanish whenever the test function \mathbf{w}_α corresponds to a particle in Ω_a .

²⁰In case of $\alpha \in \mathbf{A}$ without “neighbors” belonging to \mathbf{B} , $\theta_a^{\alpha\beta} = 1$.

²¹The situation is entirely analogous to the Neumann problem for the Poisson equation. The lack of essential boundary condition results in a discrete problem with a singular coefficient matrix.

²²The fact that the support of \mathbf{w}_α is small, i.e., less than the inter-particle spacing, means that its derivative is large relative to size of the function itself.

²³Recall that here x denotes positions in the reference, or undeformed configuration.

²⁴A simple redefinition of the bridge region, i.e., of a and c may be necessary.

Likewise, we assume that there is a finite element node located at $x = c$, i.e., at the interface between the continuum and bridge regions $\bar{\Omega}_c \cap \bar{\Omega}_b$. Again without loss of generality, we assume that $h = Ms$ for some integer $M > 0$, i.e., that the finite element grid spacing is an integer multiple of the particle lattice spacing. See Figure 5.3.

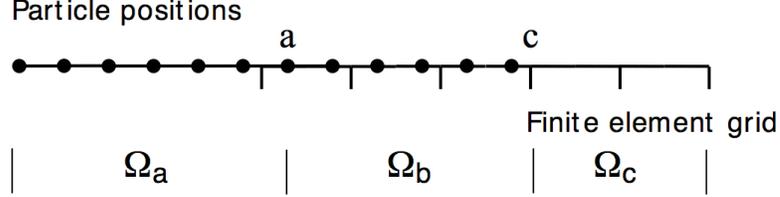


Figure 5.3: Particle positions and finite element nodes for the 1D example problem.

We assume that $u_1 = A$ and $u_j^h = B$ for given A and B , i.e., the atomistic displacement is specified for the particle located at $x = 0$ and the continuum displacement is specified at $x = 1$.

We consider the example of the linear elasticity/linear spring-mass model in 1D for which we have the constitutive relations

$$\sigma(u) = K_c \frac{du}{dx} \quad \text{and} \quad f_{\alpha,\beta} = K_a \left(\frac{u_\beta - u_\alpha}{s} \right)$$

where K_a and K_c respectively denote the spring constant and the elastic modulus which we assume are constants.

Since $\theta_c = 1$, $\theta_a^\alpha = 0$, and $\theta_a^{\alpha\beta} = 0$ in $\bar{\Omega}_c = [c, 1]$, (5.20) reduces to

$$-K_c \left(\frac{u_{j+1}^h - 2u_j^h + u_{j-1}^h}{h} \right) = \int_{x_{j-1}}^{x_{j+1}} bw_j^h dx \quad \text{for } j \text{ such that } x_j \in \Omega_c = (c, 1). \quad (5.24)$$

In the bridge region $\bar{\Omega}_b$, we have

$$\begin{aligned} & -K_c \left\{ \left(\int_{x_j}^{x_{j+1}} \theta_c dx \right) \left(\frac{u_{j+1}^h - u_j^h}{h^2} \right) + \left(\int_{x_{j-1}}^{x_j} \theta_c dx \right) \left(\frac{u_{j-1}^h - u_j^h}{h^2} \right) \right\} \\ & -K_a \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) \left\{ \theta_a^{\alpha,\alpha+1} \left(\frac{u_{\alpha+1} - u_\alpha}{s} \right) + \theta_a^{\alpha,\alpha-1} \left(\frac{u_{\alpha-1} - u_\alpha}{s} \right) \right\} \\ & = \int_{x_{j-1}}^{x_{j+1}} \theta_c bw_j^h dx + \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) \theta_a^\alpha f_\alpha \quad \text{for } j \text{ such that } x_j \in \bar{\Omega}_b = [a, c]. \end{aligned} \quad (5.25)$$

Since $\theta_c = 0$, $\theta_a^\alpha = 1$, and $\theta_a^{\alpha\beta} = 1$ in $\bar{\Omega}_a = [0, a]$, (5.22) reduces to

$$-K_a \left(\frac{u_{\alpha+1} - 2u_\alpha + u_{\alpha-1}}{s} \right) = f_\alpha \quad \text{for } \alpha \text{ such that } x_\alpha \in \Omega_a = (0, a). \quad (5.26)$$

At this point we have to choose a quadrature rule for the finite element method and we have to choose a definition for $\theta_a^{\alpha\beta}$. These are not to be chosen independently. First, we choose $\theta_c(x)$ in $\bar{\Omega}_b = [a, c]$ such that $\theta_c(a) = 0$ and $\theta_c(c) = 1$. We then apply a trapezoidal rule approximation to the integrals appearing in (5.25), e.g., if $\theta_c^j = \theta_c(x_j)$, we have

$$\int_{x_j}^{x_{j+1}} \theta_c dx \approx \frac{h}{2} (\theta_c(x_j) + \theta_c(x_{j+1})) = \frac{h}{2} (\theta_c^j + \theta_c^{j+1}).$$

Next, we let $\theta_a = 1 - \theta_c$ in $\bar{\Omega}_b = [a, c]$ and, if $\theta_a^\alpha = \theta_a(x_\alpha)$, we define

$$\theta_a^{\alpha\beta} = \frac{\theta_a(x_\alpha) + \theta_a(x_\beta)}{2} = \frac{\theta_a^\alpha + \theta_a^\beta}{2}.$$

Then, (5.25) reduces to

$$\begin{aligned} & -K_c \left\{ \left(\frac{\theta_c^{j+1} + \theta_c^j}{2} \right) \left(\frac{u_{j+1}^h - u_j^h}{h} \right) + \left(\frac{\theta_c^j + \theta_c^{j-1}}{2} \right) \left(\frac{u_{j-1}^h - u_j^h}{h} \right) \right\} \\ & -K_a \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) \left\{ \left(\frac{\theta_a^{\alpha+1} + \theta_a^\alpha}{2} \right) \left(\frac{u_{\alpha+1} - u_\alpha}{s} \right) + \left(\frac{\theta_a^\alpha + \theta_a^{\alpha-1}}{2} \right) \left(\frac{u_{\alpha-1} - u_\alpha}{s} \right) \right\} \\ & = \theta_c^j b(x_j) + \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) \theta_a^\alpha f_\alpha \quad \text{for } j \text{ such that } x_j \in \bar{\Omega}_b = [a, c]. \end{aligned} \quad (5.27)$$

Finally, we have that (5.21) reduces to

$$u_\alpha = u^h(x_\alpha) \quad \text{for } \alpha \text{ such that } x_\alpha \in \bar{\Omega}_b = [a, c].$$

Of course, $u^h(x_\alpha)$ is determined from the nodal values of u^h at the vertices of the elements that contains x_α . Specifically, since we are using continuous piecewise linear finite element spaces, we have that

$$u_\alpha = \left(\frac{x_\alpha - x_j}{h} \right) u_{j+1}^h - \left(\frac{x_\alpha - x_{j+1}}{h} \right) u_j^h \quad \text{if } x_\alpha \in [x_j, x_{j+1}] \subset \bar{\Omega}_b = [a, c]. \quad (5.28)$$

The fully discrete system is given by (5.24), (5.26), (5.27), and (5.28).²⁵

²⁵Other choices for the quadrature rule and for $\theta_a^{\alpha\beta}$ are possible. For example, we could use the

5.3.2 A patch test for the 1D example

Now, let us look at the patch test. We choose $K_a = K_c$, $b = 0$, and $f_\alpha = 0$. We test whether or not the uniform strain solution satisfies the discrete system (5.24), (5.26), (5.27), and (5.28). For the uniform strain solution we have that, for some constant Q ,

$$\frac{u_{j+1}^h - u_j^h}{h} = Q \quad \text{for } j = 1, \dots, J-1 \quad (5.30)$$

and

$$\frac{u_{\alpha+1} - u_\alpha}{s} = Q \quad \text{for } \alpha = 1, \dots, N-1. \quad (5.31)$$

In fact, we have that $Q = B - A$ where $u_1 = A$ and $u_j^h = B$. Note that (5.30) and (5.31) are consistent with (5.28) in the bridge region, i.e., the (5.28) and (5.30) imply (5.31). For example, using (5.28) and (5.30),

$$\begin{aligned} \frac{u_{\alpha+1} - u_\alpha}{s} &= \frac{1}{s} \left\{ \left(\frac{x_\alpha + s - x_j}{h} \right) u_{j+1}^h - \left(\frac{x_\alpha + s - x_{j+1}}{h} \right) u_j^h \right. \\ &\quad \left. - \left(\frac{x_\alpha - x_j}{h} \right) u_{j+1}^h + \left(\frac{x_\alpha - x_{j+1}}{h} \right) u_j^h \right\} = \frac{u_{j+1} - u_j}{h} = Q \end{aligned}$$

for $x_\alpha \in [x_j, x_j + 1) \subset [a, c)$.

With $b = 0$ and $f_\alpha = 0$, we clearly have that the uniform strain solution (5.30)–(5.31) satisfies (5.24) and (5.26), respectively. We have also shown that they satisfy (5.28).

Now, let us examine (5.27). We assume that the particle lattice is commensurate with the finite element grid, i.e., that $h = Ms$, where $M > 0$ is an integer, i.e., the midpoint rule so that

$$\int_{x_j}^{x_{j+1}} \theta_c dx \approx h\theta_c \left(\frac{x_j + x_{j+1}}{2} \right) = h\theta_c^{j+\frac{1}{2}}$$

and then define

$$\theta_a^{\alpha\beta} = \theta_a \left(\frac{x_\alpha + x_\beta}{2} \right).$$

Then, instead of (5.27), we would obtain

$$\begin{aligned} &-K_c \left\{ \theta_c^{j+\frac{1}{2}} \left(\frac{u_{j+1}^h - u_j^h}{h} \right) + \theta_c^{j-\frac{1}{2}} \left(\frac{u_{j-1}^h - u_j^h}{h} \right) \right\} \\ &-K_a \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) \left\{ \theta_a^{\alpha+\frac{1}{2}} \left(\frac{u_{\alpha+1} - u_\alpha}{s} \right) + \theta_{\alpha-\frac{1}{2}} \left(\frac{u_{\alpha-1} - u_\alpha}{s} \right) \right\} \\ &= \frac{1}{2} \left(\theta_c^{j+\frac{1}{2}} b(x_{j+\frac{1}{2}}) + \theta_c^{j-\frac{1}{2}} b(x_{j-\frac{1}{2}}) \right) + \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) \theta_a^\alpha f_\alpha \quad \text{for } j \text{ such that } x_j \in \bar{\Omega}_b = [a, c] \end{aligned} \quad (5.29)$$

where $\theta_a^{\alpha+\frac{1}{2}} = \theta_a \left(\frac{x_{\alpha+1} + x_\alpha}{2} \right)$ and $x_{j+\frac{1}{2}} = x \left(\frac{x_{j+1} + x_j}{2} \right)$.

finite element grid size is an integer multiple of the particle spacing s , and we also assume that every finite element node is occupied by a particle. See Figure 5.4.

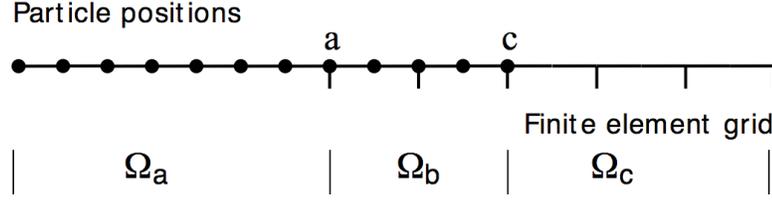


Figure 5.4: Particle positions and finite element for commensurate grids with $h = 2s$.

Substituting (5.30) and (5.31) into the left-hand side of (5.27), we obtain, with $b = 0$, $f_\alpha = 0$, and $K_a = K_c = K$,

$$\begin{aligned}
\text{LHS}(5.27) &= -\frac{KQ}{2} \left\{ (\theta_c^{j+1} - \theta_c^{j-1}) + \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) (\theta_a^{\alpha+1} - \theta_a^{\alpha-1}) \right\} \\
&= -\frac{KQ}{2} \left\{ (\theta_c(x_{j+1}) - \theta_c(x_{j-1})) + \sum_{\substack{\alpha \text{ such that} \\ x_\alpha \in (x_{j-1}, x_{j+1})}} w_j(x_\alpha) (\theta_a(x_{\alpha+1}) - \theta_a(x_{\alpha-1})) \right\} \\
&\quad \text{for } j \text{ such that } x_j \in \bar{\Omega}_b = [a, c]
\end{aligned} \tag{5.32}$$

where we have recalled that $\theta_c^j = \theta_c(x_j)$ and $\theta_a^\alpha = \theta_a(x_\alpha)$.

Note that if $M = 1$ so that $h = s$, then the only particle in the support of $w_j(x)$, i.e., in (x_{j-1}, x_{j+1}) , is the particle located at $x_\alpha = x_j$. Then, since $w_j(x_\alpha) = w_j(x_j) = 1$, (5.32) reduces to

$$\text{LHS}(5.27) = -\frac{KQ}{2} \left\{ (\theta_c(x_{j+1}) + \theta_a(x_{j+1})) - (\theta_c(x_{j-1}) + \theta_a(x_{j-1})) \right\} = -\frac{KQ}{2}(1-1) = 0$$

where we have recalled that $\theta_c(x) + \theta_a(x) = 1$ everywhere. Thus, if in the bridge region, every particle occupies a finite element node, the uniform strain solution also satisfies (5.27) and thus the discrete system (5.24), (5.26), (5.27), and (5.28) passes our patch test.

For the more general case of commensurate grids with $M > 1$, we choose in (5.32) $\theta_a(x)$ and $\theta_c(x)$ that are linear in the bridge region $\bar{\Omega}_b = [a, c]$, i.e.,

$$\theta_c(x) = \frac{x-a}{c-a} \quad \text{and} \quad \theta_a(x) = 1 - \theta_c(x) = \frac{c-x}{c-a} \quad \text{for } x \in \bar{\Omega}_b = [a, c].$$

Then,

$$\theta_c(x_{j+1}) - \theta_c(x_{j-1}) = \frac{2h}{c-a} \quad \text{and} \quad \theta_a(x_{\alpha+1}) - \theta_a(x_{\alpha-1}) = -\frac{2s}{c-a}$$

so that, from (5.32), we obtain

$$\text{LHS(5.27)} = -\frac{KQ}{c-a} \left\{ h - s \sum_{m=1}^{2M-1} w_j(x_j - h + ms) \right\} \quad (5.33)$$

where we have used the fact that in the open interval (x_{j-1}, x_{j+1}) , we have that the particles are located at the points $x_j - h + ms$, $m = 1, \dots, 2M - 1$. Note that since $w_j(x_{j-1}) = w_j(x_{j+1}) = 0$, we have that

$$\begin{aligned} & \sum_{m=1}^{2M-1} w_j(x_j - h + ms) \\ &= \frac{1}{2} \left(w_j(x_{j-1}) + 2 \sum_{m=1}^{M-1} w_j(x_j - h + ms) + w(x_j) \right) \\ & \quad + \frac{1}{2} \left(w(x_j) + 2 \sum_{m=1}^{M-1} w_j(x_j + ms) + w_j(x_{j+1}) \right) \\ &= \frac{1}{s} \left\{ \int_{x_{j-1}}^{x_j} w_j(x) dx + \int_{x_j}^{x_{j+1}} w_j(x) dx \right\} = \frac{h}{s} \end{aligned} \quad (5.34)$$

where we have used the fact that for the piecewise linear function $w_j(x)$, the trapezoidal rule is exact.²⁶ Substituting (5.34) into (5.33), we obtain that $\text{LHS(5.27)} = 0$. Thus, if, in the bridge region, the finite element grid is commensurate with the lattice spacing and the blending functions $\theta_c(x)$ and $\theta_a(x)$ are linear polynomials, then the uniform strain solution also satisfies (5.27) and thus the discrete system (5.24), (5.26), (5.27), and (5.28) passes our patch test.²⁷

Let us now explore what happens with the patch test if the finite element grid is not commensurate with the lattice spacing. We again assume that the blending functions $\theta_c(x)$ and $\theta_a(x)$ are linear in the bridge region and that the particle spacing is denoted by s and the finite element grid size is denoted by h . Furthermore, we consider that there are nodes and atoms positioned at a and c . But, now we assume that (for some finite elements) the particles are offset by a distance s_0 with respect to the finite element grid and we denote by \widetilde{M} the number of particles in each finite element interval. We assume that $h = \widetilde{M}s$ See Figure 5.5

If we follow the same process that led to (5.33), we are instead led to

$$\text{LHS(5.27)} = -\frac{KQ}{c-a} \left\{ h - s \sum_{m=1}^{2\widetilde{M}} w_j(x_j - h + s_0 + (m-1)s) \right\}. \quad (5.35)$$

²⁶The commensurate nature of the lattice spacing and the finite element grid is needed so that the locations of the particles become equally spaced quadrature points for the integrals in (5.34).

²⁷In the same way, it can be shown that the discrete scheme (5.24), (5.26), (5.28), and (5.29) that results from using the midpoint quadrature rule also passes the patch test in the two cases discussed.

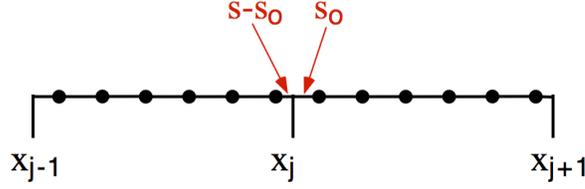


Figure 5.5: Non-commensurate particle lattice and finite element grid with $\widetilde{M} = 6$ and offset s_0 .

Now,

$$\sum_{m=1}^{\widetilde{M}} w_j(x_j - h + s_0 + (m-1)s) = \frac{\widetilde{M}}{h} \left(s_0 + \frac{s}{2}(\widetilde{M} - 1) \right) = \frac{1}{s} \left(s_0 + \frac{s}{2}(\widetilde{M} - 1) \right)$$

and

$$\sum_{m=\widetilde{M}+1}^{2\widetilde{M}} w_j(x_j - h + s_0 + (m-1)s) = \frac{\widetilde{M}}{h} \left(s - s_0 + \frac{s}{2}(\widetilde{M} - 1) \right) = \frac{1}{s} \left(s - s_0 + \frac{s}{2}(\widetilde{M} - 1) \right)$$

so that, substituting in (5.35) we obtain that

$$\text{LHS}(5.27) = -\frac{KQ}{c-a} (h - \widetilde{M}s) = -\frac{KQ}{c-a} (h - h) = 0$$

so that again the uniform strain solution satisfies (5.27) and thus the discrete system (5.24), (5.26), (5.27), and (5.28) passes our patch test even when the particle spacing is offset from the finite element grid.

We can easily infer that, for a general case in which \widetilde{M} is not an integer, and no assumptions over the position of nodes and atoms are made, we can easily prove:

$$\text{LHS}(5.27) \leq Cs^2h$$

C being uniform with respect to h .

5.4 Quadrature rules and blending functions

5.4.1 Choosing the quadrature rule

We now consider the two-dimensional case. The one-dimensional case was discussed in Section 5.3.

We use continuous, piecewise linear finite element spaces with respect to a partition of $\Omega_b \cup \Omega_c$ into a set of T triangles $\mathcal{T}^h = \{\Delta_t\}_{t=1}^T$. For $j = 1, \dots, J$, we let

$\mathcal{T}_j^h = \{\Delta_t : \Delta_t \in \text{supp}(\mathbf{w}_j)\} \subset \mathcal{T}^h$, i.e., the set of triangles sharing the finite element node \mathbf{x}_j as a vertex. Thus, we have that

$$\int_{\text{supp}(\mathbf{w}_j^h)} F(\mathbf{x}) \, d\omega = \sum_{\substack{t \text{ such that} \\ \Delta_t \in \mathcal{T}_j^h}} \int_{\Delta_t} F(\mathbf{x}) \, d\omega. \quad (5.36)$$

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

$$\int_{\Delta} F(\mathbf{x}) \, d\omega \approx \frac{V_{\Delta}}{3} \sum_{q=1}^3 F(\mathbf{x}_{\Delta;q}) \quad (5.37)$$

where V_{Δ} denotes the volume of the triangle Δ and

$$\mathbf{x}_{\Delta;1} = \frac{\widehat{\mathbf{x}}_{\Delta;1} + \widehat{\mathbf{x}}_{\Delta;2}}{2}, \quad \mathbf{x}_{\Delta;2} = \frac{\widehat{\mathbf{x}}_{\Delta;2} + \widehat{\mathbf{x}}_{\Delta;3}}{2}, \quad \text{and} \quad \mathbf{x}_{\Delta;3} = \frac{\widehat{\mathbf{x}}_{\Delta;3} + \widehat{\mathbf{x}}_{\Delta;1}}{2}.$$

We also need a quadrature rule for the boundary integral appearing in (5.20). Let $\mathcal{I}_j^h = \{\overline{\Delta}_t \cap \Gamma_t : \Delta_t \subset \text{supp}(\mathbf{w}_j^h) \text{ and } \text{length}(\overline{\Delta}_t \cap \Gamma_t) > 0\}$, i.e., \mathcal{I}_j^h is the set of sides of the triangles Δ_t in the support of \mathbf{w}_j^h that intersect with the boundary Γ_t . We then have that

$$\int_{\Gamma_t \cap \text{supp}(\mathbf{w}_j^h)} F(\mathbf{x}) \, d\gamma = \sum_{\substack{t \text{ such that} \\ \overline{\Delta}_t \cap \Gamma_t \in \mathcal{I}_j^h}} \int_{\overline{\Delta}_t \cap \Gamma_t} F(\mathbf{x}) \, d\gamma. \quad (5.38)$$

Integrals over individual line segments are approximated using the trapezoidal rule. Without loss of generality, assume that $\widehat{\mathbf{x}}_{\Delta;1}$ and $\widehat{\mathbf{x}}_{\Delta;2}$ are the two boundary vertices of a triangle Δ .²⁸ We then have that

$$\int_{\overline{\Delta}_t \cap \Gamma_t} F(\mathbf{x}) \, d\gamma \approx \frac{L_{\Delta}}{2} \sum_{q=1}^2 F(\widehat{\mathbf{x}}_{\Delta;q}) \quad (5.39)$$

where L_{Δ} denotes the length of the boundary segment $\overline{\Delta}_t \cap \Gamma_t$.

²⁸By triangulating into corners, we can guarantee that no triangle has three vertices on the boundary.

Using (5.36)–(5.39) in (5.20) results in

$$\begin{aligned}
& - \sum_{\substack{t \text{ such that} \\ \Delta_t \in \mathcal{T}_j^h}} \left\{ \frac{V_{\Delta_t}}{3} \sum_{q=1}^3 \left(\theta_c(\mathbf{x}_{\Delta_t;q}) \sigma \left((\mathbf{x}_{\Delta_t;q}), \nabla \mathbf{u}^h(\mathbf{x}_{\Delta_t;q}) \right) : \nabla \mathbf{w}_j^h(\mathbf{x}_{\Delta_t;q}) \right) \right\} \\
& \quad + \sum_{\substack{\alpha \text{ such that} \\ \mathbf{x}_\alpha \in \text{supp}(\mathbf{w}_j^h)}} \sum_{\beta \in \mathfrak{B}_\alpha} \theta_a^{\alpha,\beta} \mathbf{f}_{\alpha,\beta} \cdot \mathbf{w}_j^h(\mathbf{x}_\alpha) \\
& = - \sum_{\substack{t \text{ such that} \\ \Delta_t \in \mathcal{T}_j^h}} \left\{ \frac{V_{\Delta_t}}{3} \sum_{q=1}^3 \left(\theta_c(\mathbf{x}_{\Delta_t;q}) \mathbf{f}(\mathbf{x}_{\Delta_t;q}) \cdot \mathbf{w}_j^h(\mathbf{x}_{\Delta_t;q}) \right) \right\} \\
& \quad - \sum_{\substack{t \text{ such that} \\ \bar{\Delta}_t \cap \Gamma_t \in \mathcal{T}_j^h}} \frac{L_{\Delta_t}}{2} \left\{ \sum_{q=1}^2 \left(\theta_c(\bar{\mathbf{x}}_{\Delta_t;q}) \mathbf{t}(\bar{\mathbf{x}}_{\Delta_t;q}) \cdot \mathbf{w}_j^h(\bar{\mathbf{x}}_{\Delta_t;q}) \right) \right\} \\
& \quad - \sum_{\substack{\alpha \text{ such that} \\ \mathbf{x}_\alpha \in \text{supp}(\mathbf{w}_j^h)}} \theta_a^\alpha \mathbf{f}_\alpha^e \cdot \mathbf{w}_j^h(\mathbf{x}_\alpha) \quad \text{for } j = 1, \dots, J.
\end{aligned} \tag{5.40}$$

Thus, in two dimensions, the fully discretized system is given by (5.22), (5.22), (5.21), and (5.40).²⁹

In three dimensions, one cannot use mid-face or mid-edge rules as we can in one and two dimensions, 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 that led to (5.40) in the two-dimensional case.

5.4.2 Choosing the blending functions

We now want to give a recipe for choosing the blending functions $\theta_c(x)$ for $\mathbf{x} \in \Omega_b$ and $\theta_a^{\alpha,\beta}$ and θ_a^α for $\mathbf{x}_\alpha \in \Omega_b$ that appear in (5.20).³⁰ In two dimensions, we triangulate the

²⁹We note that if the continuum material is homogeneous, then $\sigma = \sigma(\nabla \mathbf{u})$. Then, since both \mathbf{u}^h and \mathbf{w}_j^h are linear functions in any triangle, the first term of (5.40) simplifies to

$$\sum_{\substack{t \text{ such that} \\ \Delta_t \in \mathcal{T}_j^h}} \left\{ \frac{V_{\Delta_t}}{3} \sum_{q=1}^3 \left(\theta_c(\mathbf{x}_{\Delta_t;q}) \right) \sigma \left(\nabla \mathbf{u}^h(\tilde{\mathbf{x}}_{\Delta_t}) \right) : \nabla \mathbf{w}_j^h(\tilde{\mathbf{x}}_{\Delta_t}) \right\}$$

where $\tilde{\mathbf{x}}_{\Delta_t}$ is any point in Δ_t .

³⁰Of course, in Ω_a we have that $\theta_c = 0$, $\theta_a^{\alpha,\beta} = 1$, and $\theta_a^\alpha = 1$ and in Ω_c we have that $\theta_c = 1$, $\theta_a^{\alpha,\beta} = 0$, and $\theta_a^\alpha = 0$.

bridge region Ω_a into the set of triangles having vertices $\{\mathbf{x}_{b;i}\}_{i=1}^l$. In practice, this triangulation would be 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.³¹ We then choose $\theta_c(\mathbf{x}) = \theta_c^h(\mathbf{x})$, where $\theta_c^h(\mathbf{x})$ is a continuous, piecewise linear function with respect to this triangulation. The nodal values of $\theta_c^h(\mathbf{x})$ are chosen as follows. First, set $\theta_c^h(\mathbf{x}_{b;i}) = 0$ 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 and $\theta_c^h(\mathbf{x}_{b;i}) = 1$ 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 value of θ_c^h . One way is to choose

$$\theta_c^h(\mathbf{x}_{b;i}) = \frac{\text{dist}(\mathbf{x}_{b;i}, \overline{\Omega_a} \cap \overline{\Omega_b})}{\text{dist}(\mathbf{x}_{b;i}, \overline{\Omega_a} \cap \overline{\Omega_b}) + \text{dist}(\mathbf{x}_{b;i}, \overline{\Omega_b} \cap \overline{\Omega_c})} \quad \text{for } \mathbf{x}_{b;i} \in \Omega_b.$$

Once $\theta_c^h(\mathbf{x})$ is chosen, we choose $\theta_a(\mathbf{x}) = \theta_a^h(\mathbf{x}) = 1 - \theta_c^h(\mathbf{x})$ for all $\mathbf{x} \in \Omega_b$. Then, we can choose

$$\theta_a^\alpha = \theta_a^h(\mathbf{x}_\alpha) \quad \text{and} \quad \theta_a^{\alpha,\beta} = \frac{\theta_a^h(\mathbf{x}_\alpha) + \theta_a^h(\mathbf{x}_\beta)}{2}.$$

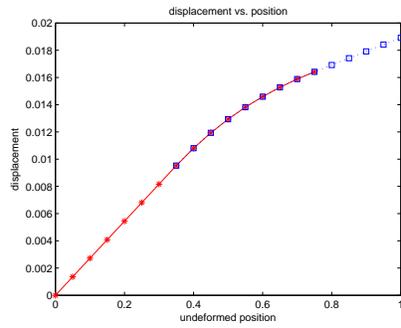
³¹For the two triangulations to be the same, we must have that the finite element triangulation is conforming with the interfaces between the bridge region and the atomistic and continuum regions, i.e., those interfaces have to be made up of edges of triangles of the finite element triangulation.

6 Numerical Experiments

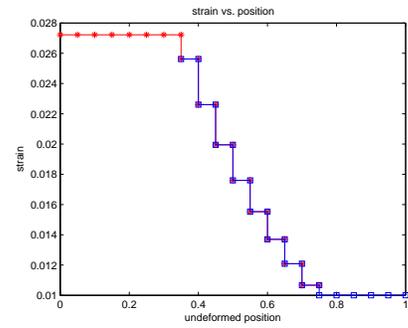
In this section we conduct simple experiments to numerically demonstrate the results of Theorem 4.1 regarding Method I, and also the discussion of Method II in Section 5.3. In all cases, we construct our discrete system as described in Section 5.1. All examples are one-dimensional, and consist of an atomistic domain and finite element domain joined by a bridging domain. A unit point force will be applied to the end finite element node, and the end atom will be constrained at the origin. For our atomistic or finite element models, the resulting solution is one of uniform strain. We thus desire that our blended models also recover this solution.

The first numerical example we will consider is the simplest case possible, where the lattice constant s is equal to the mesh width h ($M = 1$). In this situation, we constrain the atoms in the blend region to move with the finite element nodes. In Figure 6.1, we show computed displacements and strains for a case of 16 atoms and 14 nodes for Methods I and II. Method I is unable to recover the patch test solution. Even for this simple test problem the solution obtained with this method is very inaccurate. On the contrary, Method II recovers the patch test solution.

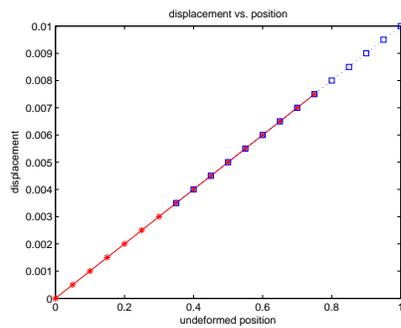
In our second numerical example, we set the mesh width h to twice the lattice constant s ($M = 2$). For the atoms in the blend region, we constrain the atoms coincident with finite element nodes to move with the nodes, and atoms in the interior of an element to move in accordance with the corresponding shape functions. In Figure 6.2, we show computed displacements and strains for a case of 15 atoms and 8 nodes for Methods I and II. Again, whereas Method II pass the patch test problem, the results obtained with Method I are extremely inaccurate.



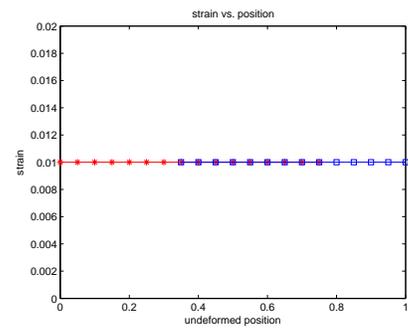
(a) Displacement, Method I



(b) Strain, Method I

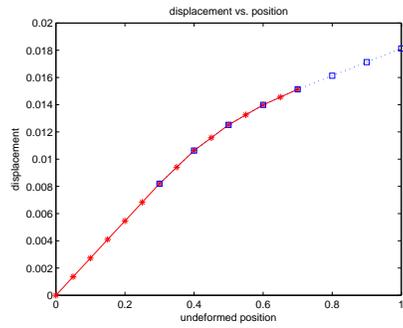


(c) Displacement, Method II

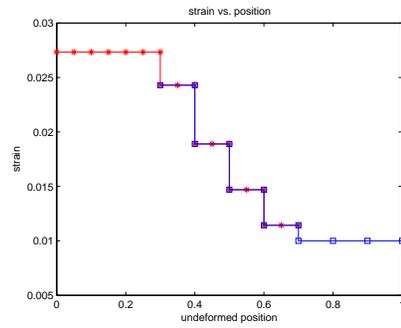


(d) Strain, Method II

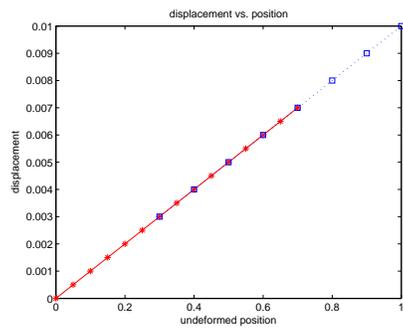
Figure 6.1: Plots for example 1. Atoms are represented in red, and finite element nodes in blue.



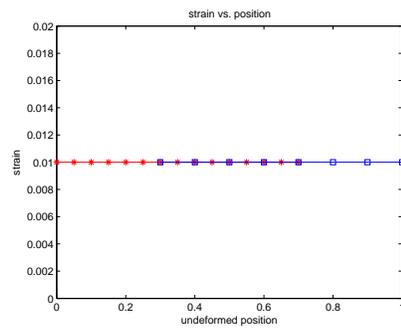
(a) Displacement, Method I



(b) Strain, Method I



(c) Displacement, Method II



(d) Strain, Method II

Figure 6.2: Plots for example 2. Atoms are represented in red, and finite element nodes in blue.

7 Conclusions

In this article we have analyzed blended AtC coupling techniques. This family of methods has been stated in an abstract form, and a well-defined concept of consistency has been suggested. We have considered how to design these methods without being affected by ghost forces. Four different methods have been listed.

Based on the consistency properties of the methods, we have chosen one, for which an accurate AtC blending model for the bridging region which pass some patch test problems has been constructed. This model has been motivated using mechanical arguments, based on the blending of forces on points.

Numerical experimentation supports the accuracy of the method in comparison with the method proposed in [7] based on the blending of stresses.

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