On Atomistic-to-Continuum Couplings without Ghost Forces in Three Dimensions

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In this paper, we construct energy-based numerical methods free of ghost forces in three-dimensional lattices arising in crystalline materials modeled by pair interaction potentials. The analysis hinges on establishing a connection of the coupled system to conforming finite elements. Key ingredients are: (i) a new representation of discrete derivatives related to long range interactions of atoms as volume integrals of gradients of piecewise linear functions over bond volumes, and (ii) the construction of an underlying globally continuous function representing the coupled modeling method.

1 Introduction

In recent years, substantial progress has been made in the multiscale modeling of materials; see, for example, [4, 11]. A class of important problems concerns atomistic-to-continuum coupling in crystals, for example, the quasicontinuum method [22] and its variants. Since continuum models often fail to provide accurate predictions in the vicinity of defects and singularities, coupled atomistic/continuum (A/C) methods have become popular as an adaptive modeling approach; see, for example, the references in [13, 16, 20, 21]. The main issue that arises in these methods is the proper matching of information across scales. Initial attempts in this direction employed ad hoc coupling of atomistic and continuum energies. This resulted in numerical artifacts at the
interface between the atomistic and continuum regions, known as ghost forces; see, for example, [5]. In view of this, the construction of ghost-force consistent A/C couplings—that are free of ghost forces—is crucial in the numerical modeling of crystalline materials. Further, since this problem is one of the better identified mathematical problems related to matching of information across scales in materials, it might provide useful insight into the study of multi-scale computational methods of a more general nature.

This paper is devoted to the construction of energy-based methods free of ghost forces in three-dimensional crystal lattices. The problem of constructing consistent energies in two-dimensional lattices was recently resolved for pair potentials by Shapeev [20]; see also [9]. Our work considers pair potentials as well, allowing interactions of finite but otherwise arbitrarily long range. A key idea in [20] is to express differences (discrete derivatives) related to long-range interactions of atoms as appropriate line integrals over bonds. In two space dimensions it is then possible to transform the assembly of line integrals over all possible interactions into an area integral, through a counting argument known as the bond density lemma [20]. This lemma fails to hold in three space dimensions; thus this approach for construction of energy-based consistent couplings does not seem to be extendable to this case. We note that in [21] an interesting attempt to circumvent this problem is made; see Section 4.2 for further discussion. Other papers dealing with similar problems include [2, 6, 10, 12, 19, 23].

Our work adopts a different approach, based on control volumes associated with bonds, which we call bond volumes, and on the construction of an underlying globally continuous function representing the coupled modeling method. The three-dimensional coupled energies constructed in this way are free of ghost forces. Moreover, they can be combined in a consistent way with coarse-mesh and high-order finite element discretizations of the continuum region.

The paper is organized as follows. In Section 1, we introduce necessary notation. In Section 2, we define suitable finite element spaces; we then introduce the atomistic Cauchy–Born (A-CB) models used in the construction of the coupled methods. In Section 3, we state and prove a key result, Lemma 3.1, that establishes a connection between long range differences and volume integrals of piecewise linear functions defined over appropriate decompositions of bond volumes into tetrahedra. In Section 4, we present a conforming coupling method based on bond volumes. We note that in the continuum region we use the A-CB models as in [16]. In Section 5, we show that it is possible to introduce discontinuities at the interface, thus allowing greater flexibility in the design of underlying meshes, while still obtaining a consistent method free of ghost forces. The analysis in this section may lead to the design of more general A/C
coupled methods based on discontinuous finite elements. Finally, in Section 6, we show that one can use finite elements of high order over general decompositions to discretize the continuum region, thus reducing significantly the number of degrees of freedom. All methods presented here are free of ghost forces; they provide a framework that facilitates the design of several alternative formulations.

**Notation.** Lattice, discrete domain, continuum domain. We let $e_i$ be the standard basis vectors for $\mathbb{R}^3$, and choose $\mathbb{Z}^3$ as the three-dimensional lattice. The extension to lattices generated by any three linearly independent vectors of $\mathbb{R}^3$ is straightforward since it merely involves compositions with a fixed affine map. The *scaled lattice* is $\varepsilon \mathbb{Z}^3 = \{x_\ell = (x_{\ell_1}, x_{\ell_2}, x_{\ell_3}) = \varepsilon \ell, \ \ell \in \mathbb{Z}^3\}$, with lattice distance $\varepsilon = 1/k, k \in \mathbb{Z}_+$. We will consider discrete periodic functions on $\mathbb{Z}^3$ defined over a “periodic domain” $\mathcal{L}$. More precisely, let $M_i \in \mathbb{Z}_+, i = 1, 2, 3$, and define

$$\Omega := (0, M_1] \times (0, M_2] \times (0, M_3].$$

$$\Omega_{\text{discr}} := \varepsilon \mathbb{Z}^3 \cap \Omega, \ \mathcal{L} := \mathbb{Z}^3 \cap \frac{1}{\varepsilon} \Omega.$$

Here $\Omega$ is the continuum domain; the actual configuration of the atoms is $\Omega_{\text{discr}}$, the set of atoms of the scaled lattice contained in $\Omega$. In particular, the convex hull of $\Omega_{\text{discr}}$ is $\Omega$. Also $\mathcal{L}$ is the basic lattice period in the unscaled lattice $\mathbb{Z}^3$.

**Functions and spaces.** The atomistic deformations are defined

$$y_\ell = y(x_\ell), \ x_\ell = \varepsilon \ell, \ \ell \in \mathcal{L} \ \text{where}$$

$$y_\ell = Fx_\ell + v_\ell, \ \text{with } v_\ell = v(x_\ell) \ \text{periodic with respect to } \mathcal{L}.$$

Here $F$ is a constant $3 \times 3$ matrix with $\det F > 0$. The corresponding spaces for $y$ and $v$ are denoted by $\mathcal{X}$ and $\mathcal{Y}$ and are defined, respectively, as follows:

$$\mathcal{X} := \{y : \mathcal{L} \rightarrow \mathbb{R}^3, \ y_\ell = Fx_\ell + v_\ell, \ v \in \mathcal{Y}, \ \ell \in \mathcal{L}\},$$

$$\mathcal{Y} := \{u : \mathcal{L} \rightarrow \mathbb{R}^3, \ u_\ell = u(x_\ell) \ \text{periodic with zero average with respect to } \mathcal{L}\}.$$

For functions $y, v : \mathcal{L} \rightarrow \mathbb{R}^3$ we define the inner product

$$\langle y, v \rangle_\ell := \varepsilon^3 \sum_{\ell \in \mathcal{L}} y_\ell \cdot v_\ell.$$

For a positive real number $s$ and $1 \leq p \leq \infty$ we denote by $W^{s,p}(\Omega, \mathbb{R}^3)$ the usual Sobolev space of functions $y : \Omega \rightarrow \mathbb{R}^3$. By $W^{s,p}_\#(\Omega, \mathbb{R}^3)$ we denote the corresponding Sobolev space of periodic functions with basic period $\Omega$. By $\langle \cdot, \cdot \rangle$, we denote the standard $L^2(\Omega)$ inner product; for a given nonlinear operator $A$, we shall denote as well by $\langle DA, v \rangle$ the action...
of its derivative $DA$ as a linear operator applied to $v$. The space corresponding to $X$ in which the minimizers of the continuum problem are sought is

$$X := \{ y: \Omega \to \mathbb{R}^3, \ y(x) = Fx + v(x), \ v \in V \},$$

where

$$V := \left\{ u: \Omega \to \mathbb{R}^3, \ u \in W^{k,p}(\Omega, \mathbb{R}^3) \cap W^{1,p}_0(\Omega, \mathbb{R}^3), \int_{\Omega} u \, dx = 0 \right\}.$$

**Difference quotients and derivatives.** The following notation will be used throughout:

$$\bar{D}_\eta y_\ell := \frac{y_{\ell+\eta} - y_\ell}{\varepsilon}, \ \ell, \ell + \eta \in \mathcal{L}, \ (1.1)$$

denotes the difference quotient (discrete derivative) in the direction of the vector $\eta$. Also,

$$\partial_\zeta \phi(\zeta) := \frac{\partial \phi(\zeta_1, \zeta_2, \zeta_3)}{\partial \zeta_i}, \ \zeta = (\zeta_1, \zeta_2, \zeta_3),$$

$$\nabla_{\zeta} \phi(\zeta) := \{ \partial_{\zeta_1} \phi(\zeta) \}_i,$$  \quad (1.2)

$$\partial_{\alpha} v(x) := \frac{\partial v(x)}{\partial x_\alpha}, \ \nabla u(x) := \left\{ \frac{\partial u^i(\mathbf{x})}{\partial x_\alpha} \right\}_{i\alpha}.$$  

**Atomistic and Cauchy–Born potential.** We consider the atomistic energy

$$\Phi^a(y) := \varepsilon^3 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \phi_\eta(\bar{D}_\eta y_\ell), \ (1.3)$$

where $R \subset \mathbb{Z}^3$ is a given finite set of interaction vectors, and the interatomic potential $\phi_\eta(\cdot)$ may vary with the type of bond, that is, $\phi_\eta$ may depend explicitly on $\eta$. Further, $\phi_\eta(\cdot)$ is assumed to be sufficiently smooth.

For a given field of external forces $f: \mathcal{L} \to \mathbb{R}^3$, where $f_\ell = f(x_\ell)$, the atomistic problem reads as follows:

$$\text{find a local minimizer } y^a \text{ in } X \text{ of: } \Phi^a(y) - \langle f, y \rangle_\varepsilon. \ (1.4)$$

If such a minimizer exists, then

$$\langle D\Phi^a(y^a), v \rangle_\varepsilon = \langle f, v \rangle_\varepsilon \quad \text{for all } v \in \mathcal{Y},$$

where

$$\langle D\Phi^a(y), v \rangle_\varepsilon := \varepsilon^3 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \partial_{\zeta} \phi_\eta(\bar{D}_\eta y_\ell) [\bar{D}_\eta v_\ell]_i = \varepsilon^3 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \nabla_{\zeta} \phi_\eta(\bar{D}_\eta y_\ell) \cdot \bar{D}_\eta v_\ell. \quad (1.5)$$

We employ the summation convention for repeated indices.
The corresponding Cauchy–Born stored energy function is \[ W(F) = W_{CB}(F) := \sum_{\eta \in R} \phi_{\eta}(F_{\eta}). \]

Then the continuum Cauchy–Born model is stated as follows:

\[
\text{find a local minimizer } y^{CB} \text{ in } X \text{ of : } \Phi_{CB}(y) - \langle f, y \rangle, \quad (1.6)
\]

where the external forces \( f \) are appropriately related to the discrete external forces and

\[
\Phi_{CB}(y) := \int_{\Omega} W_{CB}(\nabla y(x)) \, dx.
\]

If such a minimizer exists, (and is a diffeomorphism on \( \Omega \)), then

\[
\langle D\Phi_{CB}(y^{CB}), v \rangle = \langle f, v \rangle \quad \text{for all } v \in V, \quad (1.7)
\]

where

\[
\langle D\Phi_{CB}(y), v \rangle = \int_{\Omega} S_{\alpha}(\nabla y(x)) \frac{\partial v^i(x)}{\partial x_\alpha} \, dx = \int_{\Omega} S_{\alpha}(\nabla y(x)) \partial_\alpha v^i(x) \, dx, \quad v \in V.
\]

Here the stress tensor \( S \) is defined, as usual, by

\[
S := \left\{ \frac{\partial W(F)}{\partial F_{i\alpha}} \right\}_{i\alpha}.
\]

The stress tensor and the atomistic potential are related through

\[
S_{\alpha\beta}(F) = \frac{\partial W(F)}{\partial F_{i\alpha}} = \sum_{\eta \in R} \partial_{\alpha} \phi_{\eta}(F_{\eta}) \eta_{\beta}. \quad (1.8)
\]

### 2 Finite Element Spaces and A-CB Models

In the sequel, we introduce the finite element spaces used in the rest of the paper. In addition, we introduce an intermediate model connecting the continuum and atomistic models. We call this the A-CB model.

**Trilinear finite elements on the lattice.** Let \( V_{\epsilon, Q} \) be the linear space of all periodic functions that are continuous and piecewise trilinear on \( \Omega \). More precisely, let

\[
T_Q := \{ K \subset \Omega : K = (x_{\ell_1}, x_{\ell_1+1}) \times (x_{\ell_2}, x_{\ell_2+1}) \times (x_{\ell_3}, x_{\ell_3+1}), \ x_\ell = (x_{\ell_1}, x_{\ell_2}, x_{\ell_3}) \in \Omega_{\text{discr}} \},
\]

\[
V_{\epsilon, Q} := \{ v : \Omega \rightarrow \mathbb{R}^3, \ v \in C(\Omega), \ v|_K \in Q_1(K) \text{ and } v_\ell = v(x_\ell) \text{ periodic with respect to } \mathcal{L} \},
\]

where \( Q_1(K) \) denotes the set of all trilinear functions on \( K \). Whenever we wish to emphasize that we work on the specific cell \( K = (x_{\ell_1}, x_{\ell_1+1}) \times (x_{\ell_2}, x_{\ell_2+1}) \times (x_{\ell_3}, x_{\ell_3+1}) \), we shall
denote it by $K_{\ell}$. The elements of $V_{\varepsilon, \Omega}$ can be expressed in terms of the nodal basis functions $\Psi_{\ell} = \Psi_{\ell}(x)$ as

$$v(x) = \sum_{\ell \in \Sigma} v_{\ell} \Psi_{\ell_1}(x_1) \Psi_{\ell_2}(x_2) \Psi_{\ell_3}(x_3), \quad v_{\ell} = v(x_\ell),$$

where we have used the fact that $\Psi_{\ell}(x)$ can be written as the tensor product of the standard one-dimensional piecewise linear hat functions $\Psi_{\ell_i}(x_i)$. Here $\Psi_{\ell_i}(x_\ell_i) = \delta_{\ell_i \ell_i}$.

For any connected set $\mathcal{O}$ such that $\bar{\mathcal{O}} = \bigcup_{K \in S_{\Omega}} Q_k$, $S_{\Omega}$ being a subset of $T_{\Omega}$, we denote by $V_{\varepsilon, \Omega}(\mathcal{O})$ the natural restriction of $V_{\varepsilon, \Omega}$ on $\mathcal{O}$.

**Linear finite elements on lattice tetrahedra.** Let $V_{\varepsilon, T}$ be the space of continuous periodic functions that are piecewise linear on lattice tetrahedra. A crucial observation is that there are more than one ways to subdivide a given lattice cell $K$ into lattice tetrahedra. Our analysis is sensitive to the choice of such a subdivision. At this point we assume that the lattice tetrahedra in the following definition are all of the same type, that is, they have been obtained via a type A decomposition of each lattice cell; see Section 2.1 for a precise definition. With this in mind, we define

$$T_T = \{ T \subset \Omega : T \text{ is a tetrahedron whose vertices are lattice vertices of } K_{\ell}, \ x_\ell \in \Omega_{\text{discr}} \},$$

$$V_{\varepsilon, T} := \{ v: \Omega \to \mathbb{R}^2, v \in C(\Omega), \ v|_T \in P_1(T) \text{ and } v_{\ell} = v(x_\ell) \text{ periodic with respect to } \Sigma \},$$

where $P_1(T)$ denotes the set of affine functions on $T$. As above, for any connected set $\mathcal{O}$ such that $\bar{\mathcal{O}} = \bigcup_{T \in S_T} T$, $S_T$ being a subset of $T_T$, we denote by $V_{\varepsilon, T}(\mathcal{O})$ the natural restriction of $V_{\varepsilon, T}$ on $\mathcal{O}$.

### 2.1 Atomistic Cauchy-Born models on cells and tetrahedra

A decomposition of the cell $K_{\ell}$ with a vertex at $x_\ell$ into six tetrahedra is called a type A decomposition if the diagonals $(x_\ell, x_\ell + e_1 + e_2)$ and $(x_\ell + e_2, x_\ell + e_1 + e_2 + e_3)$ are edges of the resulting tetrahedra; see Figure 1. In other words, the main diagonal $(x_\ell, x_\ell + e_1 + e_2)$, the three face diagonals starting at $x_\ell$, the three face diagonals starting at $x_\ell + e_1 + e_2 + e_3$, and the edges of $K_{\ell}$, together comprise the edges of the six tetrahedra. Note that in each tetrahedron originating from a type A decomposition of a cell, exactly three edges are edges of the original cell; these are depicted with black solid lines in Figure 2. To define the
A-CB model on tetrahedra, we need to define first discrete gradients at each tetrahedron $T$. To this end, we assume that all cells are divided into tetrahedra from a type A decomposition. Let $v \in V_{\epsilon,T}$. Define $\tilde{\nabla} v$ as

$$\{\tilde{\nabla} v|_{T}\}_\alpha := \tilde{D}_{e_\alpha} v^i_{\ell},$$

where the discrete derivatives $\tilde{D}_{e_\alpha} v^i_{\ell}$ on the tetrahedron $T$ are just the difference quotients of $v$ along the edges of $T$ with directions $e_\alpha$. These are the edges shared with those of $K_\ell$, shown in black solid lines in Figure 2. For example, for the tetrahedron of Figure 2, $\tilde{D}_{e_3} v^i_{\ell} = \tilde{D}_{e_3} v^i_{\ell}$ (see (1.1)) whereas $\tilde{D}_{e_2} v^i_{\ell} = \tilde{D}_{e_2} v^i_{\ell + e_1 + e_3}$. Note that the definition of
these discrete derivatives can be extended to any smooth function. Then, for \( v \in V_{\varepsilon, T} \) and for each tetrahedron \( T \), there holds \( \nabla v = \nabla' v \) and thus it follows that

\[
\int_T W_{CB}(\nabla v) \, dx = \frac{\varepsilon^3}{6} W_{CB}(\nabla' v);
\]

compare with [6, Section II.A].

Further, let \( y \) be a sufficiently smooth deformation. We define the corresponding A-CB energy

\[
\tilde{\Phi}^{a,\text{CB}}(y) := \frac{\varepsilon^3}{6} \sum_{\ell \in \mathcal{L}} \sum_{T \in K_{\ell}(T)} \sum_{\eta \in \mathcal{R}} \phi'_{\eta}(\nabla' y_{\eta}) = \frac{\varepsilon^3}{6} \sum_{\ell \in \mathcal{L}} \sum_{T \in K_{\ell}(T)} W_{CB}(\nabla y).
\]  

(2.4)

Now, for a given field of external forces \( f : \mathcal{L} \to \mathbb{R}^3 \) the tetrahedral A-CB problem reads as follows:

find a local minimizer \( y^{a,\text{CB}} \) in \( X \) of : \( \tilde{\Phi}^{a,\text{CB}}(y^{a,\text{CB}}) - \langle f, y^{a,\text{CB}} \rangle_{\varepsilon} \).

If such a minimizer exists, then

\[
\langle D\tilde{\Phi}^{a,\text{CB}}(y^{a,\text{CB}}), v \rangle_{\varepsilon} = \langle f, v \rangle_{\varepsilon} \quad \text{for all } v \in \mathcal{V}.
\]

This atomistic model is consistent, in the sense that the above is satisfied for homogeneous deformations \( y_{F}(x) = Fx, x \in \Omega \):

\[
\langle D\tilde{\Phi}^{a,\text{CB}}(y_{F}), v \rangle = 0, \quad y_{F}(x) = Fx,
\]  

(2.5)

for all \( v \in V_{\varepsilon, T} \). To show that, it suffices to observe

\[
\langle D\tilde{\Phi}^{a,\text{CB}}(y_{F}), v \rangle = \frac{\varepsilon^3}{6} \sum_{\ell \in \mathcal{L}} \sum_{T \in K_{\ell}(T)} \sum_{\eta \in \mathcal{R}} \phi'_{\eta}(\nabla y_{F_{\eta}}) \cdot \nabla' v_{\eta}
\]

\[
= \sum_{\eta \in \mathcal{R}} \phi'_{\eta}(F_{\eta}) \cdot \sum_{\ell \in \mathcal{L}} \frac{\varepsilon^3}{6} \sum_{T \in K_{\ell}(T)} \nabla' v_{\eta}
\]

\[
= \sum_{\eta \in \mathcal{R}} \phi'_{\eta}(F_{\eta}) \cdot \sum_{\ell \in \mathcal{L}} \sum_{T \in K_{\ell}(T)} \int_T \nabla v_{\eta} \, dx
\]

\[
= \sum_{\eta \in \mathcal{R}} \phi'_{\eta}(F_{\eta}) \cdot \int_{\Omega} \nabla v_{\eta} \, dx = 0.
\]  

(2.6)

An alternative discrete model defined over cells was introduced in [16]. The average discrete derivatives were defined, for example, as

\[
\bar{D}_{e_{\ell}} v_{\ell} = \frac{1}{4} \{ \bar{D}_{e_{\ell}} v_{\ell} + \bar{D}_{e_{\ell}} v_{\ell+e_{2}} + \bar{D}_{e_{\ell}} v_{\ell+e_{3}} + \bar{D}_{e_{\ell}} v_{\ell+e_{2}+e_{3}} \}.
\]  

(2.7)
This leads to a discrete gradient $\bar{\nabla} y|_{K,\ell}$ in analogy to (2.3); see [16] for details. The corresponding cell A-CB energy is then defined by

$$\Phi_{a,CB}(y) := \varepsilon^3 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in \mathbb{R}} \phi_{\eta}(\bar{\nabla} y \eta) = \varepsilon^3 \sum_{\ell \in \mathcal{L}} W_{CB}(\bar{\nabla} y).$$

The corresponding cell A-CB problem is

find a local minimizer $y_{a,CB}^{*}$ in $X$ of: $\Phi_{a,CB}(y_{a,CB}^{*}) - \langle f, y_{a,CB}^{*} \rangle_{\varepsilon}$. This atomistic model is consistent as well, in the sense that

$$\langle D \Phi_{a,CB}(y_{F}), v \rangle = 0, \quad y_{F}(x) = F_{x}, \quad (2.8)$$

for all $v \in V_{\varepsilon,Q}$. Indeed, for elements of $V_{\varepsilon,Q}$ we have $\varepsilon^3 \bar{\nabla} v|_{K,\ell} \eta = \int_{K,\ell} \nabla v \eta \, dx$, hence

$$\langle D \Phi_{a,CB}(y_{F}), v \rangle = \varepsilon^3 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in \mathbb{R}} \phi'_{\eta}(\bar{\nabla} y_{F} \eta) \cdot \bar{\nabla} v \eta$$

$$= \sum_{\eta \in \mathbb{R}} \phi'_{\eta}(F_{\eta}) \cdot \varepsilon^3 \bar{\nabla} v \eta$$

$$= \sum_{\eta \in \mathbb{R}} \phi'_{\eta}(F_{\eta}) \cdot \sum_{\ell \in \mathcal{L}} \int_{K,\ell} \nabla v \eta \, dx$$

$$= \sum_{\eta \in \mathbb{R}} \phi'_{\eta}(F_{\eta}) \cdot \int_{\Omega} \nabla v \eta \, dx = 0. \quad (2.9)$$

It was shown in [16] that this model is both energy- and variationally consistent to second order in $\varepsilon$, approximating the exact atomistic model as well as the continuum Cauchy–Born model.

3 Bond Volumes and Long Range Differences

To construct methods that couple the atomistic and continuum descriptions, we need to relate long range differences and derivatives of functions defined over bond volumes. To fix ideas, let $\eta \in \mathbb{R}$, and define the bond as the line segment $b_{\ell} = \{ x \in \mathbb{R}^3 : x = x_{\ell} + t \eta, \, 0 < t < 1 \}$ with endpoints $x_{\ell}$ and $x_{\ell + \eta}$. The set of all bonds $B_{\eta}$ consists of all $b = b_{\ell}$ for $\ell \in \mathcal{L}$ (but for $\eta$ fixed). For given $\ell$ and $\eta \in \mathbb{Z}^3$ with $\eta_{1} \eta_{2} \eta_{3} \neq 0$, the corresponding bond volume $B_{\ell,\eta}$ is the interior of the rectangular parallelepiped with edges parallel to the standard basis vectors $e_{\ell}$ and main diagonal $b_{\ell}$; see Figure 3. Next we shall establish a connection between long range differences and piecewise linear functions defined over type A decompositions of bond volumes $B_{\ell,\eta}$ into tetrahedra, which is defined in analogy to type A decompositions of cells $K_{\ell}$. To this end let $B_{\ell,\eta}(T)$ be a type A decomposition of
the bond volume \( B_{\ell, \eta} \) into six tetrahedra, that is, the decomposition where the diagonals \((x_{\ell}, x_{\ell} + e_1 \eta_1 + e_3 \eta_3)\) and \((x_{\ell} + e_2 \eta_2, x_{\ell} + \eta)\) are edges of the resulting tetrahedra; see Figure 3.

The following lemma plays a central role in our work.

**Lemma 3.1.** Let \( v \) be a piecewise linear and continuous function on a type A decomposition of the bond volume \( B_{\ell, \eta} \) into tetrahedra. Then

\[
e^3 \bar{D}_\eta v_\ell = \frac{1}{|\eta_1 \eta_2 \eta_3|} \int_{B_{\ell, \eta}} \nabla v(x) \eta \, dx. \tag{3.1}
\]

**Proof.** We present the proof for \( \eta_i > 0, i = 1, 2, 3 \). The other cases are similar. We have

\[
\frac{1}{\eta_1 \eta_2 \eta_3} \int_{B_{\ell, \eta}} \nabla v(x) \eta \, dx = \frac{1}{\eta_1 \eta_2 \eta_3} \int_{\partial B_{\ell, \eta}} v v \cdot \eta \, ds
\]

\[
= \frac{1}{\eta_1 \eta_2 \eta_3} \sum_{i=1}^{3} \left\{ \int_{\partial B_{\ell, \eta}(-e_i)} (-\eta_i) v \, ds + \int_{\partial B_{\ell, \eta}(e_i)} \eta_i v \, ds \right\}, \tag{3.2}
\]

where \( \partial B_{\ell, \eta}(e_i) \) is the face of \( B_{\ell, \eta} \) with outward unit normal \( e_i \). Since \( v \) is linear in each tetrahedron of the decomposition of \( B_{\ell, \eta} \), it will be linear in each of the two triangles comprising the face \( \partial B_{\ell, \eta}(\eta_i) \). Therefore, if \( \tau \) is such a triangle, the integral of \( v \) over \( \tau \) can be found explicitly:

\[
\int_{\tau} \eta_i v \, ds = \frac{|\tau|}{3} \sum_{j=1}^{3} \eta_i v(z_j), \tag{3.3}
\]

where \( z_j \) are the vertices of \( \tau \). Since \( \tau \) is one of the two triangles of \( \partial B_{\ell, \eta}(\eta_i) \), \( |\tau| \eta_i = \frac{\varepsilon^2}{2} \eta_1 \eta_2 \eta_3 \). Hence,

\[
\frac{1}{\eta_1 \eta_2 \eta_3} \int_{\partial B_{\ell, \eta}(e_i)} \eta_i v \, ds = \frac{\varepsilon^2}{6} \sum_{j=1}^{2} \{v(z_j) + 2v(\tilde{z}_j)\}, \tag{3.4}
\]
where \( z_j \) are the vertices shared by two triangles of \( \partial B_{\ell,\eta}(e_i) \) and \( z_j \) the vertices belonging to only one triangle of \( \partial B_{\ell,\eta}(e_i) \).

We substitute the above formula into (3.2) and group together all terms involving each vertex. For each of the vertices other than \( x_{\ell} \) or \( x_{\ell+\eta} \), there are two possibilities:

(i) It is a shared vertex in one face with outward normal \( e_i \) and it is a single vertex in two faces with normal \(-e_i\).

(ii) It is a shared vertex in one face with normal \(-e_i\) and a single vertex in two faces with normal \( e_i \).

Also, terms involving a vertex of \( \partial B_{\ell,\eta}(e_i) \) appear with coefficient 1, while terms involving a vertex of \( \partial B_{\ell,\eta}(-e_i) \) appear with coefficient \(-1\) in (3.2). Therefore, the contribution of these vertices to the sum in (3.2) is zero.

Finally, we note that \( x_{\ell+\eta} \) is a shared vertex at each \( \partial B_{\ell,\eta}(e_i) \), while \( x_{\ell} \) is a shared vertex at each \( \partial B_{\ell,-\eta}(-e_i) \) for all \( i = 1, 2, 3 \). It follows that

\[
\frac{1}{\eta_1 \eta_2 \eta_3} \int_{B_{\ell,\eta}} \nabla v(x) \cdot \eta \, dx = \epsilon^2 (v_{\ell+\eta} - v_{\ell}),
\]

and the proof is complete.

Representations of the long range difference \( \bar{D}_\eta v_\ell \) through integrals of certain functions were used previously in different forms. A representation based on line integrals over bonds was used in the two-dimensional construction of ghost-force consistent methods of methods of [20]; see also [18] and its references, where a representation based on integration over \( \mathbb{R}^n \) of expressions defined through interpolation and convolution with appropriate functions was used as a tool to derive error estimates.

4 A Coupling Method Based on Bond Volumes

4.1 Construction

In this section, we construct methods based on bond volumes. Let the atomistic region \( \Omega_a \) and the A-CB region \( \Omega_s \) each be the interior of the closure of a union of lattice tetrahedra \( T \in T_T \) and connected, and suppose

\[
\Omega = \tilde{\Omega}_a \cup \tilde{\Omega}_s, \quad \Gamma = \tilde{\Omega}_a \cap \tilde{\Omega}_s, \quad \Omega_a \cap \Omega_s = \emptyset.
\]

Here \( \Gamma \) is the interface. To avoid technicalities that may arise due to the fact that we work with periodic functions over \( \Omega \), we assume throughout that \( \tilde{\Omega}_a \) is subset of
the interior of $\Omega$ with sufficient distance from $\partial \Omega$. Let $y_\ell$ be the deformed position of $x_\ell \in \Omega_{\text{discr}}$.

Fix $\eta \in \mathbb{R}$, with $\eta_1 \eta_2 \eta_3 \neq 0$. The cases of degenerate $\eta$ can be treated with two- and one-dimensional techniques; see Remark 4.1. We shall construct an energy-based coupling method whose design relies on an appropriate handling of bond volumes $B_{\ell, \eta}$.

We consider three cases depending on the location of each bond volume $B_{\ell, \eta}$:

(a) The closure of the bond volume is contained in the atomistic region: $\bar{B}_{\ell, \eta} \subset \Omega_a$.

(b) The bond volume is contained in the region $\Omega_s$: $B_{\ell, \eta} \subset \Omega_s$.

(c) We denote by $B_{\Gamma}$ the set of bond volumes that do not satisfy (a) or (b). In fact, $B_{\ell, \eta} \in B_{\Gamma}$ if the bond volume intersects the interface: $B_{\ell, \eta} \cap \Gamma \neq \emptyset$ or if $B_{\ell, \eta} \subset \Omega_a$ and $\bar{B}_{\ell, \eta} \cap \Gamma \neq \emptyset$.

If a bond volume intersects $\partial \Omega$, then it is supposed to belong to $\Omega_s$ by periodic extension. For a fixed $\eta$, the contribution to the energy corresponding to the atomistic region (case (a)) is

$$E_{\Omega_a, \eta}^a[y] = \varepsilon^3 \sum_{\ell \in \mathcal{L}} \phi_\eta(\bar{D}_\eta y_\ell). \tag{4.1}$$

The contribution to the energy from the A-CB region (case (b)) is (cf. (2.4))

$$E_{\Omega_a, \eta}^{a, \text{CB}}[y] = \frac{\varepsilon^3}{6} \sum_{\ell \in \mathcal{L}, T \in \mathcal{K}(T), T \subset \Omega_s} \phi_\eta(\tilde{\nabla} y_\eta) = \int_{\Omega_s} \phi_\eta(\nabla \tilde{y}(x) \eta) \, dx, \tag{4.2}$$

$\tilde{y}$ being the interpolant of $\{y_\ell\}$ in $V_{\varepsilon, \eta}(\Omega_s)$; see the sentence following (2.2).

For each bond volume intersecting $\Gamma$ we denote by $y^{\ell, \eta}$ a piecewise polynomial function on $B_{\ell, \eta}$ satisfying the following conditions:

(i) We have $y^{\ell, \eta} \in C(\bar{B}_{\ell, \eta})$.

(ii) Let $T(B_{\ell, \eta})$ be a decomposition of $B_{\ell, \eta}$ with the following properties: (a) If $T \in T(B_{\ell, \eta})$ and $T \subset \Omega_s$, then $T$ is a tetrahedron resulting from a type A decomposition of an atomistic cell $K \subset \Omega_s$; (b) If $T \in T(B_{\ell, \eta})$ and $T \subset \Omega_a$, then $T$ is a lattice tetrahedron.

(iii) In case ii.(b) above, if $T$ has a face on $\partial(B_{\ell, \eta} \cap \Omega_a) \setminus \Gamma$, then it is part of a conforming decomposition that is compatible with decompositions of other bond volumes sharing a face with $B_{\ell, \eta}$. If such an attached bond volume is included in $\Omega_a$, then it is assumed to be type-A decomposed into tetrahedra.

(iv) For $T \in T(B_{\ell, \eta})$, $y^{\ell, \eta} \in \mathbb{P}_1(T)$ and it interpolates $\{y_\ell\}$ at the vertices of $T$. 

Then the energy due to bond volumes intersecting the interface is defined as

$$E_{Γ,η}(y) = \sum_{\ell ∈ Ω, B_1, ν ∈ B_2} \frac{1}{|η_1 η_2 η_3|} \int_{B_1, ν} \chi_N φ_η(∇y^{I,ν} η) \, dx.$$  \hfill (4.3)

**Remark 4.1.** In the case of degenerate $η$ with $η_1 η_2 η_3 = 0$, we proceed as follows. Let us assume that $η_3 = 0$ and $η_1 η_2 ≠ 0$. Then

$$\varepsilon^2 \sum_{ℓ ∈ Ξ} φ_η(\bar{D}_η Y_ℓ) = \varepsilon \sum_{ℓ_1 ∈ Ξ_3} \sum_{ℓ_2 ∈ Ξ'} \phi_η(\bar{D}_η Y_ℓ), \quad ℓ = (ℓ′, ℓ_3),$$  \hfill (4.4)

where $Ξ := \mathbb{Z}^2 \cap \{ (0, M_1]) \times (0, M_2) \}$, $Ξ_3 := \mathbb{Z} \cap \{ (0, M_3) \}$, and $Ξ = Ξ' × Ξ_3$. Now, for each fixed $ℓ_3 ∈ Ξ_3$, all interactions $φ_η(\bar{D}_η Y_ℓ)$ remain in the two-dimensional “sublattice” $Ξ' × \{ ℓ_3 \}$ given that $η_3 = 0$. Thus, a ghost-force consistent two-dimensional construction at each energy $\sum_{ℓ′ ∈ Ξ′} φ_η(\bar{D}_η Y_ℓ)$ will result in a ghost-force free method. To achieve this, one has to consider for each “sublattice” $Ξ' × \{ ℓ_3 \}$ a reduced two-dimensional A-CB model of the form

$$\sum_{ℓ ∈ Ξ'} \sum_{τ ∈ S_ℓ′, ℓ_3} \int_τ φ_η(∇\tilde{y}η) \, dx_1 dx_2,$$  \hfill (4.5)

where $τ ∈ S_ℓ′, ℓ_3$ are the two triangles of the face of $K_ℓ$ lying on $(0, M_1]) \times (0, M_2] \times \{ x_ℓ \}$ and $\tilde{y}$ is the natural restriction of the interpolant of $y$, $\tilde{y} ∈ V_{τ, Ω}$ on $τ$. Since $η_3 = 0$, it is a simple matter to check that (4.5) reduces to the two-dimensional A-CB model on the cell consisting of the two triangles of $S_ℓ′, ℓ_3$ of [16]. Then, for each fixed $ℓ_3$ for which the intersection of $(0, M_1]) \times (0, M_2] \times \{ x_ℓ \}$ with the interface $Γ$ is nonempty, one can construct a two-dimensional coupled model which is ghost force free consistent; see Section 4.2 and [14, 20]. It then follows that this property is preserved under summation with respect to $ℓ_3$. It is clear that the model at $Ω_∗$ is an approximation of the continuous Cauchy–Born model since

$$\varepsilon \sum_{τ ∈ S_ℓ′, ℓ_3} \int_τ φ_η(∇\tilde{y}η) \, dx_1 dx_2 \approx \int_{K_ℓ} φ_η(∇yη) \, dx.$$  \hfill (4.6)

Further, it is important to observe that, for given piecewise polynomial and continuous functions $ν_ℓ$ defined on each $(0, M_1]) \times (0, M_2] \times \{ x_ℓ \}$, and periodic with respect to $Ξ_3$, one can construct a globally defined function $\hat{v}$ with the property

$$\varepsilon \sum_{ℓ_3 ∈ Ξ_3} \int_{(0, M_1]) \times (0, M_2]} ∇_2 ν_ℓ \bar{y} \, dx_1 dx_2 = \int_Ω ∇\hat{v}η \, dx,$$  \hfill (4.7)
where $\nabla_2$ is the two-dimensional gradient and $\tilde{\eta} = (\eta_1, \eta_2)$. In fact, if $\hat{v}(x_1, x_2, \cdot)$ is the piecewise linear interpolant with respect to $x_3$ of $v_\ell(x_1, x_2)$, then (4.7) follows by a simple calculation and the exactness properties of the trapezoidal integration rule. Relation (4.7) is important since it allows one to apply the coarsening method of Section 6 to the degenerate cases as well. Similarly, if two components of $\eta$ are zero, we employ one-dimensional constructions; see Section 4.2 and [9, 14, 20].

**Remark 4.2.** Note that the energy that corresponds to the bond volume $B_{\ell, \eta} \in B_\Gamma$ would be

$$\frac{1}{|\eta_1 \eta_2 \eta_3|} \int_{B_{\ell, \eta}} \phi_\eta(\nabla y^{\ell, \eta} \cdot \eta) \, dx. \tag{4.8}$$

The part of this energy corresponding to $B_{\ell, \eta} \cap \Omega_*$ has been already taken into account in $E_{\Omega, \eta}^{a, CB}(y)$ and hence it is not included in the definition of $E_{\Gamma, \eta}(y)$. □

**Remark 4.3.** Decompositions $T(B_{\ell, \eta})$ satisfying the above properties can be explicitly constructed, after taking into account the structure of the interface $\Gamma$. In this process, one should mention that the choice of the decomposition $T(B_{\ell, \eta})$ (and of the associated piecewise polynomial function $y^{\ell, \eta}$) is somewhat flexible; it might even allow vertices that are not lattice points. See [15] for a more detailed discussion. The only essential requirement is that each function $v^{[m]}$ defined through $T(B_{\ell, \eta})$ in the proof of Proposition 4.1, should satisfy $v^{[m]} \in H^1(\Omega)$. Depending on the complexity of the interface $\Gamma$, one can construct such decompositions more or less efficiently. In many cases this can simplify the computation of the associated energy $E_{\Gamma, \eta}(y)$. See, for example, Figure 4 for such a choice of decomposition.

![Fig. 4. A possible decomposition $T(B_{\ell, \eta})$ of $B_{\ell, \eta}$.](image-url)
We then define the total energy as follows:

$$E_{b^v}(y) = \sum_{\eta \in R} E_{\eta}(y),$$  \hspace{1cm} (4.9)$$

where

$$E_{\eta}(y) = E_{\Omega_a,\eta}^a(y) + E_{\Omega_a,\eta}^{a,\text{CB}}(y) + E_{\Gamma,\eta}(y).$$  \hspace{1cm} (4.10)$$

### 4.2 Discussion in one and two dimensions

In order to better understand the proposed method, we shall briefly discuss its adaptation in one dimension. To this end, we first write the one-dimensional atomistic energy:

$$\Phi^a(y) := \varepsilon \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \phi_\eta(\tilde{D}_\eta y_\ell),$$  \hspace{1cm} (4.11)$$

where $R \subset \mathbb{Z}$ and $\mathcal{L} = \mathbb{Z} \cap \frac{1}{\varepsilon} (0, M]$. The one-dimensional Cauchy–Born energy is

$$\Phi^{\text{CB}}(y) := \int_0^M W_{\text{CB}}(y'(x)) \, dx.$$ 

Following the plan of Section 4.1, we define bond volumes $B_{\ell,\eta}$ in one dimension. These are simply the open intervals connecting $x_\ell$ and $x_{\ell+\eta}$. Note that in one dimension bond volumes are the same as bonds, which is not true in higher dimensions. Further, we use the same notation as before for one-dimensional counterparts of the atomistic region $\Omega_a$ and the A-CB region $\Omega_a^*$; let each be the interior of the closure of a union of lattice intervals $I_\ell = (x_\ell, x_{\ell+1})$. Fix $\eta \in R$, with $\eta > 0$. As before, we consider three cases depending on the location of each bond volume $B_{\ell,\eta}$. First, the contribution to the energy of the atomistic region is

$$E_{\Omega_a,\eta}^a(y) = \varepsilon \sum_{\ell \in \mathcal{L}} \sum_{B_{\ell,\eta} \subset \mathcal{B}_a} \phi_\eta(\tilde{D}_\eta y_\ell).$$  \hspace{1cm} (4.12)$$

The contribution to the energy of the A-CB region is

$$E_{\Omega_a,\eta}^{a,\text{CB}}(y) = \varepsilon \sum_{\ell \in \mathcal{L}, I_\ell \subset \Omega_a} \phi_\eta(\tilde{D}_1 y_\ell \eta) = \int_{\Omega_a^*} \phi_\eta(\tilde{y}'(x) \eta) \, dx,$$  \hspace{1cm} (4.13)$$

$\tilde{y}$ being the piecewise linear interpolant of $\{y_\ell\}_{\ell \in \mathcal{L}}$.

It remains to consider bond volumes $B_{\ell,\eta}$ intersecting $\Gamma$. To fix ideas, let $\tilde{B}_{\ell,\eta} = [x_\ell, x_{\ell+\eta}] \cup [x_{\ell+\eta}, x_{\ell+\eta}]$ where $x_{\ell+\eta}$ is a point on the interface $\Gamma$. We denote by $y_{\ell,\eta}^{\prime}$ the continuous, piecewise linear function on $B_{\ell,\eta}$, such that $y_{\ell,\eta}^{\prime}$ is linear on $(x_\ell, x_{\ell+\eta})$ and linear at each $I_j \subset (x_{\ell+\eta}, x_{\ell+\eta})$. Then the energy due to bond volumes intersecting the
interface is defined as

\[ E_{\Gamma, \eta}(y) = \sum_{\ell \in \Omega} \frac{1}{\eta} \int_{B_{\ell, \eta}} \chi_{\Omega_{\ell}} \phi_{\eta} ( (y^{\ell, \eta})' \eta ) \, dx = \sum_{\ell \in \Omega} \frac{1}{\eta} \varepsilon \eta_{\Gamma} \phi_{\eta} \left( \frac{y_{\ell} + \eta_{\Gamma} - y_{\ell} - \eta_{\Gamma}}{\varepsilon \eta_{\Gamma}} \right) \]

(4.14)

The resulting method which follows by summing the corresponding energies over \( \eta \in \mathbb{R} \) is essentially the same as the method of [9, 20]. One can show directly using a covering argument based on bond volume decompositions, presented in the next section, that this method is free of ghost forces.

As noted in the introduction, the method of [20] in two dimensions expresses finite differences related to long range interactions of atoms as appropriate line integrals over bonds. In two space dimensions it is possible to transform the assembly of line integrals over all possible interactions into an area integral, through the bond density lemma, a key result employed in the proof of ghost-force consistency, [20]. Our method of construction of the energy differs from that of Shapeev [20] in the following way: Shapeev's method is based on line integrals over bonds, while ours is based directly on volume integrals over bond volumes. In two space dimensions our approach gives rise to a family of ghost-force free methods which are described in detail in [14], along with approaches leading to efficient implementation.

The bond density lemma fails to hold in three space dimensions, thus this approach for construction of energy-based consistent couplings does not seem to be extendable to this case. In [21], a ghost-force consistent method for three dimensions is presented based on line integrals; however, the approximation of the continuum region in this method is not based on a discretization of the continuum Cauchy–Born energy.

4.3 Ghost-force consistency

The energy (4.9) based on bond volumes is ghost-force free, as we prove in the following proposition.

**Proposition 4.1.** The energy (4.9) is free of ghost forces, in the sense that

\[ \langle D \mathcal{E}_{b\nu}(y_F), v \rangle = 0, \quad y_F(x) = Fx, \]

(4.15)

for all \( v \in \mathcal{V} \). \( \square \)
To show this proposition, we shall need some more notation. First, we fix $\eta$ and consider decompositions into bond volumes which cover $\mathbb{R}^3$:

$$S^m_B := \{ B_{\ell, \eta} : (i) B_{\ell, \eta} \cap B_{j, \eta} = \emptyset, \text{if } \ell \neq j, \text{ (ii) } \mathbb{R}^3 = \bigcup B_{\ell, \eta} \}, \quad m = 1, \ldots, |\eta_{123}|. \quad (4.16)$$

$S^m_B$ will be used for counting purposes in the proof; the associated functions introduced below will be defined on $\Omega$. The number of different such coverings is $|\eta_{123}|$, hence the numbering $m = 1, \ldots, |\eta_{123}|$. Note that bond volumes corresponding to different $m$ may overlap, but the elements of a single $S^m_B$ are nonoverlapping bond volumes; see Figure 5 for a two-dimensional visualization.

For a lattice function $\{ v_\ell \}$ construct the functions $\nabla \tilde{v}$ and $v^{\ell, \eta}$ in analogy with $\nabla \tilde{y}$ and $y^{\ell, \eta}$ in the construction below (4.13). Then, for a fixed $\eta$, we have

$$\langle D\mathcal{E}_\eta(y_F), v \rangle = \phi'_\eta(F\eta) \cdot \left\{ \varepsilon^3 \sum_{\ell \in \Sigma} \tilde{D}_\eta v_\ell + \int_{B_{\eta}} \tilde{\nabla} v(x) \eta \ dx + \sum_{\ell \in \Sigma} \frac{1}{|\eta_{123}|} \int_{B_{\ell, \eta}} \chi_{B_\eta} \nabla v^{\ell, \eta} \eta \ dx \right\}. \quad (4.17)$$

The main idea in the proof of Proposition 4.1 is to rewrite the expression within brackets above in the following way:

$$\varepsilon^3 \sum_{\ell \in \Sigma} \tilde{D}_\eta v_\ell + \int_{\Omega} \tilde{\nabla} v(x) \eta \ dx + \sum_{\ell \in \Sigma} \frac{1}{|\eta_{123}|} \int_{B_{\ell, \eta}} \chi_{B_\eta} \nabla v^{\ell, \eta} \eta \ dx$$

$$= \frac{1}{|\eta_{123}|} \sum_{m=1}^{\eta_{123}} \int_{\Omega} \nabla v^{[m]}(x) \eta \ dx, \quad (4.18)$$
where $v^{[m]}$, $m = 1, \ldots, |\eta_1| \eta_2 \eta_3|$ are appropriate conforming functions in $H^1(\Omega)$, each associated with a different covering $S^m_{B_0}$ consisting of bond volumes. The details are provided below.

**Proof of Proposition 4.1.** We start by defining $v^{[m]}$. For a given lattice function $\{v_\ell\}$, a fixed $m$, and a covering $S^m_{B_0}$, $v^{[m]}$ is equal to

1. the piecewise linear interpolant of $\{v_\ell\}$ on a type A decomposition of the bond volume $B_{l,\eta}$ into tetrahedra if $\bar{B}_{l,\eta} \subset \Omega$;
2. $v_\ell^{l,\eta}$, for $B_{l,\eta} \cap \Gamma \neq \emptyset$, where the piecewise polynomial $v_\ell^{l,\eta}$ on $B_{l,\eta}$ is defined through (i–iv) below (4.13);
3. the piecewise linear function interpolating $\{v_\ell\}$ at lattice tetrahedra $T \subset B_{l,\eta} \subset \Omega$.

It is clear by construction that each $v^{[m]} \in H^1(\Omega)$. The superscript $m$ indicates the covering $S^m_{B_0}$ to which $B_{l,\eta}$ belongs.

Since $v^{[m]}$ is a piecewise linear continuous function on a type A decomposition of the bond volume $B_{l,\eta}$, we use Lemma 3.1 to write

$$
\varepsilon^3 \sum_{l \in \Sigma} \bar{D}_{l,\eta} v_\ell = \frac{1}{|\eta_1| \eta_2 \eta_3|} \sum_{l \in \Sigma} \int_{B_{l,\eta} \subset \Omega} \nabla v^{[m]}(x) \eta \, dx. \tag{4.19}
$$

Further, each tetrahedron corresponds to exactly one atomistic cell $K \subset \Omega_*$ belonging to $|\eta_1| \eta_2 \eta_3|$ different bond volumes $B_{l,\eta}$, each one belonging to a different covering $S^m_{B_0}$. Thus, for $T \subset \Omega_*$, we have

$$
\int_T \nabla \bar{v}(x) \eta \, dx = \frac{1}{|\eta_1| \eta_2 \eta_3|} \sum_{m=1}^{[\eta_1| \eta_2| \eta_3]} \int_{T \cap B_{l,\eta} \in S^m_{B_0}} \nabla v^{[m]}(x) \eta \, dx. \tag{4.20}
$$

Therefore,

$$
\int_{\Omega_*} \nabla \bar{v}(x) \eta \, dx = \frac{1}{|\eta_1| \eta_2 \eta_3|} \sum_{m=1}^{[\eta_1| \eta_2| \eta_3]} \int_{\Omega_*} \nabla v^{[m]}(x) \eta \, dx. \tag{4.21}
$$

By construction of $v^{l,\eta}$ and $v^{[m]}$ we have

$$
\sum_{l \in \Sigma} \frac{1}{|\eta_1| \eta_2 \eta_3|} \int_{B_{l,\eta}} \chi_{\Omega_a} \nabla v^{l,\eta} \eta \, dx = \frac{1}{|\eta_1| \eta_2 \eta_3|} \sum_{m=1}^{[\eta_1| \eta_2| \eta_3]} \sum_{B_{l,\eta} \in S^m_{B_0}} \int_{B_{l,\eta}} \chi_{\Omega_a} \nabla v^{[m]}(x) \eta \, dx. \tag{4.22}
$$
Thus rewriting (4.19) as

\[ \varepsilon^3 \sum_{\ell \in \Sigma \atop \bar{B}_{\ell,\alpha} \subset \Omega_a} \mathcal{D}_m \eta \ell = \frac{1}{|\eta_1 \eta_2 \eta_3|} \sum_{m=1} |\eta_1 \eta_2 \eta_3| \sum_{B_{\ell,\alpha} \in \mathcal{S}_m} \int_{B_{\ell,\alpha}} \nabla v_{m}^{[m]}(x) \eta \, dx, \]  

we finally obtain

\[ \varepsilon^3 \sum_{\ell \in \Sigma \atop \bar{B}_{\ell,\alpha} \subset \Omega_a} \mathcal{D}_m \eta \ell + \sum_{\ell \in \Sigma \atop B_{\ell,\alpha} \subset B_F} \frac{1}{|\eta_1 \eta_2 \eta_3|} \int_{B_{\ell,\alpha}} \chi_{\Omega_a} \nabla v_{m}^{[m]}(x) \eta \, dx \]

\[ = \frac{1}{|\eta_1 \eta_2 \eta_3|} \sum_{m=1} |\eta_1 \eta_2 \eta_3| \sum_{B_{\ell,\alpha} \in \mathcal{S}_m} \int_{B_{\ell,\alpha}} \chi_{\Omega_a} \nabla v_{m}^{[m]}(x) \eta \, dx \]

\[ = \frac{1}{|\eta_1 \eta_2 \eta_3|} \sum_{m=1} \int_{\Omega_a} \nabla v_{m}^{[m]}(x) \eta \, dx. \]  

Hence (4.18) follows in view of (4.20). Therefore, the proof of proposition is complete in view of the Gauss–Green theorem.

5 A Discontinuous Bond Volume-Based Coupling Method

In this section, we show that it is possible to modify energies to allow underlying functions which might be discontinuous at the interface. This allows greater flexibility on the construction of the underlying meshes and thus the computation of the energy at the interface might become simpler. To retain consistency, the interfacial energies should include terms accounting for the possible discontinuity of the underlying functions. There are many alternatives, such as the possibility of adding extra stabilization terms; cf. [1]. The purpose of this paper is however to present the general framework and we will not insist on the various modifications and extensions of the methods developed herein.

Let \( \Omega, \Omega_a, \Omega_s, \) and \( \Gamma \) be as in the previous section. Further, we distinguish the same cases (a), (b), and (c) regarding the location of each bond volume \( B_{\ell,\eta} \). The corresponding energies are still defined by

\[ E_{\Omega_a,\eta} \{ y \} = \varepsilon^3 \sum_{\ell \in \Sigma \atop \bar{B}_{\ell,\alpha} \subset \Omega_a} \phi_\eta(\mathcal{D}_m \eta \ell) \]

and

\[ E_{\Omega_s,\eta} \{ y \} = \frac{\varepsilon^3}{6} \sum_{\ell \in \Sigma \atop T \in \mathcal{K}(T), T \subset \Omega_s} \phi_\eta(\nabla \cdot y \eta) = \int_{\Omega_s} \phi_\eta(\nabla \cdot y \eta) \, dx, \]
\( \bar{y} \) being the piecewise linear function at the lattice tetrahedra interpolating \( \{ y_\ell \} \). The main difference from the previous construction in Section 3 is the choice of \( y^{\ell, \eta} \) and the corresponding energies for each bond volume intersecting the interface. Specifically:

(i) Let \( y^{\ell, \eta} \in C(\overline{B_{\ell, \eta}} \setminus \Gamma) \).

(ii) Further, let \( T(\overline{B_{\ell, \eta}}) \) be a decomposition of \( B_{\ell, \eta} \) with the following properties:

(a) If \( T \in T(\overline{B_{\ell, \eta}}) \) and \( T \subset \Omega_\ast \), then \( T \) is an atomistic tetrahedron resulting from a type A decomposition of an atomistic cell. (b) If \( T \in T(\overline{B_{\ell, \eta}}) \) and \( T \subset \Omega_a \), then \( T \) is a lattice tetrahedron.

(iii) In the case ii.(b) above if \( T \) has a face on \( \partial(\overline{B_{\ell, \eta}} \cap \Omega_a) \setminus \Gamma \), then it will allow for a compatible conforming decomposition with respect to attached bond volumes. In that case if the attached bond volume is included in \( \Omega_a \), it is assumed to be type-A decomposed into tetrahedra.

(iv) For \( T \in T(\overline{B_{\ell, \eta}}) \), \( y^{\ell, \eta} \in P_1(T) \), interpolating \( \{ y_\ell \} \) at the vertices of \( T \).

We then define the energy due to bond volumes intersecting the interface as

\[
E_{D, \eta}^{\Gamma, \eta} \{ y \} = \sum_{\ell \in \Sigma} \frac{1}{|\eta_1 \eta_2 \eta_3|} \left[ \int_{B_{\ell, \eta}} \chi_{\Omega_a} \phi_{\eta}(\nabla y^{\ell, \eta} \eta) \, dx - \int_{B_{\ell, \eta} \cap \Gamma} \phi_{\eta}'(\{ \nabla y^{\ell, \eta} \eta \}) \cdot [y^{\ell, \eta}] \, dS \right].
\] (5.3)

Here, \( [w, \eta] \), \( \{w\} \) denote the jump and the average of a possibly discontinuous function on the interface

\[
[w, \eta] := (v_{\Omega_a} \cdot \eta) w^- + (v_{\Omega_\ast} \cdot \eta) w^+, \quad \{w\} := \frac{1}{2} (w^- + w^+),
\] (5.4)

\( w^- \) and \( w^+ \) being the limits taken from \( \Omega_a \) and \( \Omega_\ast \), respectively, and \( v_{\Omega_a}, v_{\Omega_\ast} \) the corresponding exterior normal unit vectors, with \( v_{\Omega_a} = -v_{\Omega_\ast} \) on \( \Gamma \).

A key observation here is that \( E_{D, \eta}^{\Gamma, \eta} \{ y \} \) does not induce inconsistencies on the energy level. In fact, it is obvious that if \( y^{\ell, \eta} \in C(\overline{B_{\ell, \eta}}) \) as in the previous section, then

\[
E_{D, \eta}^{\Gamma, \eta} \{ y \} = E_{\Gamma, \eta} \{ y \},
\] (5.5)

since the extra term on the interface vanishes. Then, as in the previous section, we define the total energy as follows:

\[
E_{D, \eta}^D \{ y \} = \sum_{\eta \in R} E_{\eta}^D \{ y \},
\] (5.6)
where
\[ E_D^{\eta}(y) = E^{a}_{\omega_{a},\eta}(y) + E^{a,GB}_{\omega_{a},\eta}(y) + E^{D}_{\Gamma,\eta}(y). \] (5.7)

Despite the fact that we allow discontinuities, the energy \( E_D^{D_{\eta}} \) is still ghost-force free:

**Proposition 5.1.** The energy (5.6) is free of ghost forces, in the sense that
\[ \langle D\mathcal{E}_{\eta}^{D}(y_{F}), v \rangle = 0, \quad y_{F}(x) = Fx, \] (5.8)
for all \( v \in \mathcal{V} \).

**Proof.** The structure of the proof is the same as that of Proposition 4.1, hence we present in detail only the main differences. We still need the coverings \( S_{B_{\eta}} \) and recall that their elements define a decomposition of nonoverlapping bond volumes. As in the proof of Proposition 4.1, for a given lattice function \( \{v_{\ell}\} \) we define the functions \( \nabla \bar{v} \) and \( v_{\ell,\eta} \) in analogy with \( \nabla y \) and \( y_{\ell,\eta} \); cf. (4.13). Then, we have
\[ \langle D\mathcal{E}_{\eta}^{D}(y_{F}), v \rangle = \phi'_{\eta}(F_{\eta}) \cdot \sum_{\ell \in \Omega, B_{\ell,\eta} \subseteq \Omega_{a}} \bar{D}_{\eta}v_{\ell} + \int_{\Omega,} \nabla \bar{v}(x)\eta \, dx \]
\[ + \frac{1}{|\eta_{1}\eta_{2}\eta_{3}|} \sum_{\ell \in \Omega, B_{\ell,\eta} \subseteq B_{\Gamma}} \int_{B_{\ell,\eta}} \chi_{\Omega_{a}} \nabla v_{\ell,\eta} \, dx - \int_{B_{\eta,\Gamma} \cap \Gamma} \|v_{\ell,\eta}\| \, dS. \] (5.9)

Indeed, to show this, it suffices to observe that
\[ \langle D\phi'_{\eta}(\{\nabla w_{\eta}\}) \cdot \{w_{\eta}\}, v \rangle = (\phi''_{\eta}(\{\nabla w_{\eta}\}) \cdot \{w_{\eta}\}) \cdot \{\nabla v_{\eta}\} + \phi'_{\eta}(\{\nabla w_{\eta}\}) \cdot \{v_{\eta}\}, \] (5.10)
which is equal to \( \phi'_{\eta}(F_{\eta}) \cdot \|v_{\eta}\| \) for \( w = y_{F} \) (details are omitted).

In parallel to the proof of Proposition 4.1, we will prove
\[ \sum_{\ell \in \Omega, B_{\ell,\eta} \subseteq \Omega_{a}} \bar{D}_{\eta}v_{\ell} + \int_{\Omega_{a}} \nabla \bar{v}(x)\eta \, dx \]
\[ + \frac{1}{|\eta_{1}\eta_{2}\eta_{3}|} \sum_{\ell \in \Omega, B_{\ell,\eta} \subseteq B_{\Gamma}} \int_{B_{\ell,\eta}} \chi_{\Omega_{a}} \nabla v_{\ell,\eta} \, dx - \int_{B_{\eta,\Gamma} \cap \Gamma} \|v_{\ell,\eta}\| \, dS \]
\[ = \frac{1}{|\eta_{1}\eta_{2}\eta_{3}|} \sum_{m=1}^{\mid\eta_{1}\eta_{2}\eta_{3}\mid} \int_{\Omega_{a} \setminus \Gamma} \nabla v_{[m]}(x)\eta \, dx - \int_{\Gamma} \|v_{[m]}\| \, dS, \] (5.11)
where \( v_{[m]}, m = 1, \ldots, |\eta_{1}\eta_{2}\eta_{3}|, \) are appropriate functions in \( H^{1}(\Omega \setminus \Gamma) \cap C(\hat{\Omega} \setminus \Gamma) \), possibly discontinuous at \( \Gamma \); each \( v_{[m]} \) is associated with a different covering \( S_{B_{\eta}} \) consisting of bond volumes. Relation (5.11) then implies \( \langle D\mathcal{E}_{\eta}^{D}(y_{F}), v \rangle = 0, \) since by the Gauss–Green
theorem,
\[ \int_{\Omega \setminus \Gamma} \nabla v^{|m|}(x) \eta \, dx = \int_{\Gamma} [v^{|m|}\eta] \, dS. \]

It remains therefore to establish (5.11). To this end, we proceed exactly as in the proof of Proposition 4.1. In particular, for a given lattice function \( \{v_\ell\} \), a fixed \( m \), and a covering \( S^m_{B_{\ell,\eta}} \), define \( v^{|m|} \) as

1. the piecewise linear interpolant of \( \{v_\ell\} \) on a type A decomposition of the bond volume \( B_{\ell,\eta} \) into tetrahedra if \( \bar{B}_{\ell,\eta} \subset \Omega_{\bar{a}} \);
2. \( v_\ell \), for \( B_{\ell,\eta} \cap \Gamma \neq \emptyset \), where the piecewise polynomial on \( B_{\ell,\eta} \), \( v_\ell \), is possibly discontinuous on \( B_{\ell,\eta} \cap \Gamma \), and is defined through (i–iv) above;
3. the piecewise linear function at the lattice tetrahedra interpolating \( \{v_\ell\} \), if \( T \) is an atomistic tetrahedron such that \( T \subset B_{\ell,\eta} \subset \Omega_a \).

Now, by construction \( v^{|m|} \in H^1(\Omega \setminus \Gamma) \cap C(\bar{\Omega} \setminus \Gamma) \), and is possibly discontinuous at \( \Gamma \). The rest of the proof is identical to the one of Proposition 4.1 with the exception that (4.22) should be replaced by

\[
\sum_{\ell \in \Omega} \frac{1}{|\eta_1,\eta_2,\eta_3|} \int_{B_{\ell,\eta}} \chi_{\Omega_a} \nabla v_\ell \eta \, dx - \int_{B_{\ell,\eta} \cap \Gamma} [v_\ell \eta] \, dS
= \frac{1}{|\eta_1,\eta_2,\eta_3|} \sum_{m=1}^{\text{atoms}} \sum_{\ell \in \Omega} \chi_{\Omega_a} \nabla v^{|m|}(x) \eta \, dx - \int_{B_{\ell,\eta} \cap \Gamma} [v^{|m|}\eta] \, dS, \quad (5.12)
\]

with (4.24) modified accordingly.

6 Coarse Mesh and High-Order Finite Element Coupling

In this section, we shall see how the previous analysis can lead to energy-based methods that employ coarse mesh and high-order (even \( hp \)-) finite element approximations of the Cauchy–Born energy on the continuum region, while remaining ghost-force free. First, we relax the assumption that the continuum region \( \Omega_a \) is decomposed into atomistic size elements. This can be done gradually, since close to the interface, the elements should be of atomistic size. To this end, let \( T_{ac} \) be a decomposition of \( \Omega \) into elements with the following properties: Let \( \Omega, \Omega_a, \Omega_s, \) and \( \Gamma \) be as before. The approximations will be based on decompositions of the continuum region \( \Omega_s \) that are compatible on \( \Gamma \).
to $V_{c,T}(\Omega_s)$. To do that, let

$$T_c(\Omega_s)$$

be a conforming decomposition of $\Omega_s$ into lattice tetrahedra,

such that, if $T \in T_c(\Omega_s), \bar{T} \cap \Gamma \neq \emptyset$, then $T \in T_T(\Omega_s)$. \hfill (6.1)

We consider the discrete space

$$V_{h,ac}(\Omega_s) = \{v \in C(\bar{\Omega}_s) : v|_T \in \mathbb{P}_1(T) \text{ for } \bar{T} \cap \Gamma \neq \emptyset \text{ and } v|_T \in \mathbb{P}_k(T) \text{ for all other } T \in T_c(\Omega_s), \} \hfill (6.2)$$

where $\mathbb{P}_k(T)$ is the space of polynomials of degree $k$ on $T$. The space $V_{h,ac}(\Omega_s)$ can be extended to include the atomistic region as well by

$$V_{h,ac} = \{v \in C(\bar{\Omega}) : v|_T \in \mathbb{P}_1(T) \text{ for } T \in T_T(\Omega_a) \text{ and } v|_T \in V_{h,ac}(\Omega_s) \text{ for all } T \in T_c(\Omega_s), v \text{ periodic on } \Omega \}. \hfill (6.3)$$

For $v \in V_{h,ac}$ one can define the corresponding lattice function $\{v_\ell\}$, simply by evaluating $v$ at vertices. Conversely, one can find $v \in V_{h,ac}$ that coincides with corresponding values of a given $\{v_\ell\}$ at the vertices. However, at regions where high-order finite elements are employed, the remaining degrees of freedom which might not correspond directly to lattice points should be defined using appropriate averaging. In the following, given the deformation $y$, $y(x) = Fx + v(x), v \in V_{h,ac}$, we shall define its A/C energy. To this end, let

$$\mathcal{E}_h = \sum_{\eta \in R} \mathcal{E}_{h,\eta}, \hfill (6.4)$$

where

$$\mathcal{E}_{h,\eta}[y] = E^a_{\Omega_a,\eta}[y] + \int_{\Omega_s} \phi_\eta(\nabla y(x)\eta) \, dx + E_{\Gamma,\eta}[y]. \hfill (6.5)$$

Here, for an atomistic point $x_\ell \in \Omega_a, y_\ell = y(x_\ell)$, and the local energies $E^a_{\Omega_a,\eta}[y], E_{\Gamma,\eta}[y]$ are defined as in Section 4; see (4.12), (4.14).

The above method can be designed to have accuracy of arbitrarily high order for the Cauchy–Born energy at the continuum region $\Omega_s$. This is important because, by tuning the discretization parameters (decomposition of $\Omega_s$ and polynomial degrees), we have the possibility of matching $O(\varepsilon^2)$, which is the best possible accuracy of the approximation of the atomistic model by the continuum Cauchy–Born model at this region; see Remark 6.1.

The energy $\mathcal{E}_h$ is ghost-force free as we show next.
Proposition 6.1. The energy (6.4) is free of ghost forces, in the sense that
\[
\langle D\mathcal{E}_h(y_F), v \rangle = 0, \quad y_F(x) = Fx,
\]  
(6.6)
for all \( v \in V_{h,ac} \).

**Proof.** Since \( v \in V_{h,ac} \), we have
\[
\langle D\mathcal{E}_h(y_F), v \rangle = \phi'_\eta(F\eta) \cdot \left\{ \varepsilon^3 \sum_{\ell \in \Sigma} \bar{D}_\eta v_\ell + \int_{\Omega_a} \nabla v(\eta)^x \eta \, dx + \sum_{\ell \in \Sigma} \frac{1}{|\eta_1\eta_2\eta_3|} \int_{B_{\ell,\eta} \subset B_{\ell,\eta}} \chi_{\Omega_a} \nabla v^{m,\eta} \eta \, dx \right\}.
\]  
(6.7)
Exactly as in the proof of Proposition 4.1, we may write the first and the third term of above sum as
\[
\varepsilon^3 \sum_{\ell \in \Sigma} \bar{D}_\eta v_\ell + \sum_{\ell \in \Sigma} \frac{1}{|\eta_1\eta_2\eta_3|} \int_{B_{\ell,\eta} \subset B_{\ell,\eta}} \chi_{\Omega_a} \nabla v^{m,\eta} \eta \, dx = \frac{1}{|\eta_1\eta_2\eta_3|} \sum_{m=1}^{\eta_1\eta_2\eta_3} \int_{\Omega_a} \nabla v^{[m]}(x) \eta \, dx,
\]  
(6.8)
where \( v^{[m]}, \, m = 1, \ldots, |\eta_1\eta_2\eta_3| \), are the functions defined in the proof of Proposition 4.1. Define now
\[
\tilde{v}(x) = \begin{cases} 
\frac{1}{|\eta_1\eta_2\eta_3|} \sum_{m=1}^{\eta_1\eta_2\eta_3} v^{[m]}(x) & \text{for } x \in \Omega_a, \\
v(x) & \text{for } x \in \Omega_*. 
\end{cases}
\]  
(6.9)
Then tracing back the definition of \( V_{h,ac} \) at the elements next to the interface \( \Gamma \) and the proof of Proposition 4.1, we can show that \( \tilde{v} \) is continuous at the interface \( \Gamma \). Thus \( \tilde{v} \in H^1(\Omega) \), and is periodic. Further, by the Gauss–Green theorem,
\[
\langle D\mathcal{E}_h(y_F), v \rangle = \phi'_\eta(F\eta) \cdot \left\{ \int_{\Omega_a} \nabla \tilde{v} \eta + \int_{\Omega_*} \nabla v \eta \right\} = \phi'_\eta(F\eta) \cdot \int_{\Omega} \nabla \tilde{v} \eta = 0,
\]  
(6.10)
and the proof is complete.

Remark 6.1 (Consistency and finite element discretization). In the classical numerical analysis terminology, consistency refers to a quantity which measures to what extent an exact smooth solution fails to satisfy the numerical scheme. In analogy, we are interested in the consistency error of coupled models that approximate the exact atomistic model. As in [16], we distinguish between energy and variational consistency errors. Let \( \Phi^{AC} \) be the energy of a coupled A/C model approximating the atomistic model (1.4). The
energy consistency error refers to the quantity

$$C_E(y) := |\Phi^a(y) - \Phi^{AC}(y)|$$

for any smooth enough $y$. The corresponding error for first variations can be quantified as

$$C_V(y) := \sup\{\|\langle D\Phi^a(y), v \rangle \epsilon - \langle D\Phi^{AC}(y), v \rangle \| : v \in \mathcal{V} \text{ with } \|v\|_{W^{1,p}(\Omega)} = 1\}. $$

Here, by $\|v\|_{W^{1,p}(\Omega)}$ we denote the standard $W^{1,p}$ Sobolev norm of an appropriate interpolant of $v \in \mathcal{V}$. We shall refer to $C_V(y)$ as the variational consistency error. Note that if $\Phi^{AC}$ corresponds to a ghost-force free coupling, then $C_V(y_F) = 0$. As first proved in [3] for $C_E(y)$ and in [16] for $C_V(y)$, both consistency errors for the Cauchy–Born model are of second order in $\epsilon$; see also [7, 18].

Note that when $\Phi^{AC}$ is ghost-force free, both errors can be localized by appropriately selecting $u$ in $y(x) = Fx + u(x)$. Therefore, the best possible error of a coupled model that is based on the Cauchy–Born rule in the continuum region is $O(\epsilon^2)$. However, if we use piecewise linear finite elements on coarse decompositions, the error between the continuum model and its finite element approximation on elements over decompositions without symmetric structure, will be typically of order $O(h_K)$ locally ($h_K$ being the diameter of the element $K$). Since we aim at local mesh sizes $h_K$ significantly larger than $\epsilon$, it might be profitable to use higher-order elements where the local error can be $O(h_K^r)$, $r$ being the polynomial degree.

Note that the overall consistency error of a coupled method is influenced, as expected, by errors due to the treatment of the interface. In [17], it is shown that ghost-force consistency implies a first-order error estimate under certain assumptions on the coupling method. See the review [13] and its references for results related to error estimates of various coupled methods.

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