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ANALYSIS OF AN OPTIMIZATION-BASED ATOMOSTIC-TO-CONTINUUM COUPLING METHOD FOR POINT DEFECTS*

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Abstract. We formulate and analyze an optimization-based Atomistic-to-Continuum (AtC) coupling method for problems with point defects. Near the defect core the method employs a potential-based atmostic model, which enables accurate simulation of the defect. Away from the core, where site energies become nearly independent of the lattice position, the method switches to a more efficient continuum model. The two models are merged by minimizing the mismatch of their states on an overlap region, subject to the atomistic and continuum force balance equations acting independently in their domains. We prove that the optimization problem is well-posed and establish error estimates.

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Introduction

Atomistic-to-continuum (AtC) coupling methods combine the accuracy of potential-based atomistic models of solids with the efficiency of coarse-grained continuum elasticity models by using the former only in small regions where the deformation of the material is highly variable such as near a crack tip or dislocation. The past two decades have seen an abundance of interest in AtC methods both in the engineering community to enable predictive simulations of crystalline materials and in the mathematical community to understand the errors introduced by AtC approximations. Of prime importance is the use of AtC methods to model material

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defects such dislocations and interacting point defects, which play roles in determining the elastic and plastic response of a material [34].

A prototypical AtC method consists of dividing a computational domain into atomistic and continuum regions. A discrete system involving non-local interactions between atoms models the atomistic region whereas a conventional continuum model such as a hyperelastic continuum mechanics, represents the material in the continuum region. AtC methods differ chiefly in how they couple the distinct models with each roughly being able to be categorized as either force or energy-based [21]. Energy based couplings define a hybrid energy functional as a combination of atomistic and continuum energy functionals, and this hybrid energy functional is then minimized over a class of admissible deformations. Force based couplings instead derive atomistic and continuum forces from the separate energies and then equilibrate them. We refer to [19, 21] for a review of many existing AtC methods.

The primary challenge in developing energy-based methods has been the existence of "ghost forces" [19, 24] near the interface between the atomistic and continuum regions. These ghost forces may lead to uncontrollable errors in predicted strains, and to date, no method has been implemented that completely eliminates these errors for general many-body potentials and general interface geometry in two and three dimensions. Many force-based methods do not suffer from the perils of ghost forces; however, for two and three dimensions establishing the stability of these methods in the absence of an energy functional remains a difficult task.

Owing to the practical potential of AtC methods, their error analysis has recently attracted a significant attention from mathematicians and engineers. In one dimension, this analysis is well-developed, see e.g., [19] for a thorough review. In two and three dimensions, analytic results have been obtained for quasinonlocal (QNL) type methods [8, 26, 27, 29, 32, 38], and blended methods [12–14, 18, 43]. Sharp error estimates for the energy-based method of [37] have only been established in two dimensions assuming pair interactions with an additional *a priori* assumption on the magnitude of the true atomistic solution in [32]. The analyses of the QNL method of [38] and its subsequent extensions [8, 32] are valid for arbitrary interactions but are limited to two dimensions and by allowing only planar interfaces [8] or corners [32] between the atomistic and continuum domains. The work [18] has presented a force-based AtC method and established sharp error estimates in three dimension, but it is not applicable to defects. Most recently, [14] has presented a complete analysis valid in two and three dimensions of the blended quasicontinuum energy (BQCE) [12, 20] and blended quasicontinuum force (BQCF) [13, 15] methods valid for finite-range interactions with no geometrical restrictions on the interface between atomistic and continuum regions. A recent modification of a BQCE method was also proposed and analyzed in [33].

The purpose of the present paper is to analyze an optimization-based AtC, introduced in [22, 23], which couches the coupling of the two models into a constrained minimization problem. Specifically, a suitable measure of the mismatch between the atomistic and continuum states, the "mismatch energy," is minimized over a common *overlap* region, subject to the atomistic and continuum force balance equations holding in atomistic and continuum subdomains. This differs substantially from energy AtC based methods such as [1, 12, 24, 36, 38] which minimize a hybrid combination of atomistic and continuum energies, approximating the original atomistic energy. Also, unlike the force-based, non-energy methods [7, 13, 18], we do not directly equilibrate forces but instead employ the force balance equations as constraints in a minimization problem.

Our approach is related to non-standard optimization-based domain decomposition methods for Partial Differential Equationa (PDEs); see e.g., [6, 10, 16, 17] and the references therein. In [23], we analyzed an optimization-based AtC formulation for a linear system with next-nearest neighbor interactions using the L^2 norm of the difference between the states as a cost functional, and in [22] we formulated the approach for many dimensions with nonlinear interactions and studied it numerically for a 1D chain of atoms interacting through a Lennard-Jones potential.

A useful setting for studying the errors of various AtC methods, and the setting we utilize in the present work, is a single defect embedded in an infinite lattice. A comprehensive analysis of several AtC methods has been carried out in one dimension in [19]. In addition to the continuum error and coupling error, this setting introduces a third error resulting from truncating the infinite domain to a finite domain in order to obtain a computable quantity. We provide a comprehensive analysis of the optimization-based AtC method in $\mathbb{R}^d$ for $d \geq 2$ in the context of a point[1] defect located at the origin of an infinite lattice and establish bounds on the error of the method in terms of two parameters: the "diameter" of the defect core, R_{core}, and the size of the continuum region, R_{c}.

Our results are comparable to the results for BQCF method in [14] in that the coupling error of our method is dominated by the continuum error and truncation error. In contrast, the leading order error term established in [14] for the BQCE method is precisely the coupling error, which can be minimized but never altogether removed [12,14]. Our analytical results have been numerically confirmed in [22] in one dimension; however, the analysis presented here is not directly applicable in that scenario because the continuum region is a disconnected set in one dimension after a neighborhood of the defect core at the origin is removed.

This paper is organized as follows. We begin by describing the atomistic defect problem in an infinite domain and formulate the associated AtC method in Section 1. In Section 2, we prove that the AtC problem has a solution and subsequently estimate a broken norm error. These results rely on an essential norm equivalence property established in Section 3. The norm equivalence result generalizes a 1D linear result established in [23] and draws upon ideas from heterogeneous domain decomposition methods developed in [10].

0.1. **Notation**

For the convenience of the readers below we summarize the key notation used throughout the paper.

- ξ - an element of $\mathbb{Z}^d$ or $\epsilon\mathbb{Z}^d$ for $\epsilon > 0$.
- $|\cdot|$ - meaning depends on context: $|\cdot|$ is ℓ^2 norm of a vector, matrix, or higher order tensor, $|T|$ is area or volume of element T in a finite element partition, $|\alpha|$ is order of a multiindex.
- $\|\cdot\|_{\ell^2(A)}$ - ℓ^2 norm over a set A. If $f : A \to \mathbb{R}^d$ is a vector valued function, $\|f\|_{\ell^2(A)} = (\sum_{\alpha\in A} |f(\alpha)|^2)^{1/2}$.
- $B_r(\boldsymbol{y}) = \{\boldsymbol{x} \in \mathbb{R}^d \,|\, |\boldsymbol{y} - \boldsymbol{x}| \leq r\}$ - Ball of radius r in $\mathbb{R}^d$
- $\bar{U}$ - closure of a domain U.
- U° - interior of a domain U.
- $\text{conv}(x, y)$ - convex hull of x and y.
- $(\mathbb{R}^d)^{\mathcal{R}}$ - direct product with $|\mathcal{R}|$ terms.
- G - a $d \times d$ matrix.
- $\top$ - transpose of a matrix.
- $\otimes$ - tensor product.
- ∇^j - jth Frechet derivative of a function defined on $\mathbb{R}^d$.
- ∂^α - multiindex notation for derivatives.
- $L^p(U) = \left\{f : U \to \mathbb{R}^d | \int_U |f(x)|^p \, dx < \infty\right\}$
- $W^{k,p}(U) = \left\{f : U \to \mathbb{R}^d | \int_U |\partial^\alpha f(x)|^p \, dx < \infty \, \forall |\alpha| \leq k\right\}$
- $W^{k,p}_{\text{loc}}(U) = \left\{f : U \to \mathbb{R}^d | f \in W^{k,p}(V) \, \forall \, V \subset\subset U\right\}$.
- $H^k(U) = W^{k,2}(U)$, $H^1_0(U) = \left\{f \in H^k(U) | \text{Trace}(f) = 0 \, \text{on} \, \partial U\right\}$.
- $\text{C}^{k,\gamma}(\bar{U}) = \left\{f : U \to \mathbb{R}^d | \sum_{|\alpha|\leq K} \sup_{x\in U} |f(x)| + \sum_{|\alpha|=k} \sup_{\substack{x,y\in U \\ x\neq y}} \frac{|f(x)-f(y)|}{|x-y|^k}\right\}$
- $*$ - used to denote convolution
- $⨍_U f \, dx$ - average value of f over U.
- $\mathcal{T}$ - a finite element discretization of triangles in $2D$ or tetrahedra in $3D$.
- $\mathcal{P}^1(T)$ - set of affine functions over a triangle or tetrahedron, T.
- $\mathcal{P}^1(\mathcal{T})$ - set of piecewise affine functions with respect to the discretization $\mathcal{T}$.
- $Q_5(\xi + (0, 1)^d)$ - set of biquintic functions over the square $\xi + (0, 1)^d$ for $d = 2$ or triquintic functions over the cube $\xi + (0, 1)^d$ for $d = 3$.

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[1] Aside from additional technicalities needed to account for differences in a suitable reference configuration and the decay of the elastic deformation fields of a dislocation, our analysis can also include dislocations.

1. Problem Formulation

We consider a point defect such as a vacancy, interstitial, or impurity located at the origin on the infinite lattice, $\mathbb{Z}^d$. To formulate the AtC method, we will introduce a finite atomistic domain $\Omega_{\rm a}$ surrounding the defect, and a finite continuum domain, $\Omega_{\rm c}$, which overlaps with $\Omega_{\rm a}$ in $\Omega_{\rm o}$. Restriction of the atomistic energy to Ω_a and application of the Cauchy-Born strain energy on Ω_c yield notions of restricted atomistic and continuum energies. Minimizing the H^1-(semi)norm of the mismatch between the atomistic and continuum states in $\Omega_{\rm o}$, subject to the Euler-Lagrange equations of these energies in $\Omega_{\rm a}$ and $\Omega_{\rm c}$, respectively, completes the formulation of the AtC method.

1.1. **Atomistic Model**

In this paper, we will model atoms located on the integer lattice $\mathbb{Z}^d$. We assume the atoms interact via a classical interatomic potential, and the displacement of atoms from their reference configuration will be denoted by $u : \mathbb{Z}^d \to \mathbb{R}^d$. We require that atomistic energy can be written as a sum of site energies, V_ξ, associated to each lattice site $\xi \in \mathbb{Z}^d$. This site energy is not unique, and there is great freedom in defining it, see e.g [40]. From the axiom of material frame indifference, V_ξ is allowed to depend only upon interatomic distances. Furthermore, we assume a finite cut-off radius in the reference configuration, $r_{\rm cut}$, so that V_ξ depends only on a subset of the position of atoms in $B_{r_{\rm cut}}(\xi)$. The set of atoms interacting with an arbitrary $\xi \in \mathbb{Z}^d$ is given by $\xi + \mathcal{R}$ where

$$\mathcal{R} \subset \left\{\rho \in \mathbb{Z}^d : 0 < |\rho| \leq r_{\rm cut}\right\}$$

Note that we measure distance in the reference configuration rather than the deformed configuration. An example interaction range is displayed in Figure 1.

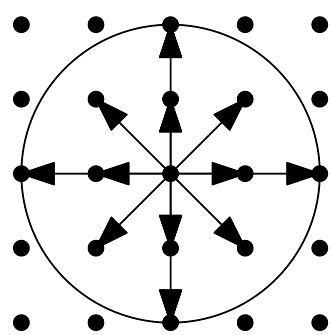

Figure 1. A possible interaction range with $r_{\rm cut} = 2$ in $\mathbb{R}^2$.

It is convenient to write differences between atoms' displacements using finite difference operators, $D_\rho u$ for $\rho \in \mathcal{R}$, defined by

$$D_\rho u(\xi) := u(\xi + \rho) - u(\xi).$$

The collection of finite differences for $\rho \in \mathcal{R}$ yields a stencil in $(\mathbb{R}^d)^{\mathcal{R}}$, which we denote by

$$Du(\xi) := \big(D_\rho u(\xi)\big)_{\rho \in \mathcal{R}}.$$

Thus, formally, the site energy at ξ is a mapping $(\mathbb{R}^d)^{\mathcal{R}} \mapsto \mathbb{R}$, which we denote by $V_\xi(Du)$. The atomistic energy is then given by

$$\mathcal{E}^{\rm a}(u) := \sum_{\xi \in \mathbb{Z}^d} V_\xi(Du). \tag{1.1}$$

We refer to [9] for a discussion of how to define V_ξ for various point defects such as vacancies or impurities and the case of dislocations.

Remark 1.1. *By allowing V to depend upon the lattice site, ξ, we can include both point and line defects in the analysis. For simplicity, we state our results for the case of point defects.*

Admissible states of the atomic configuration correspond to *local minima* of (1.1). To define the relevant displacement spaces of lattice functions, we introduce a continuous representation of a discrete displacement via interpolation. To that end, let $\mathcal{T}_{\rm a}$ be a partition of $\mathbb{Z}^d$ into simplices such that (i) ξ is a node of $\mathcal{T}_{\rm a}$ if and only if $\xi \in \mathbb{Z}^d$ and (ii) for each $\rho \in \mathbb{Z}^d$ and each $\tau \in \mathcal{T}_{\rm a}$, $\rho + \tau \in \mathcal{T}_{\rm a}$; see Figure 2.

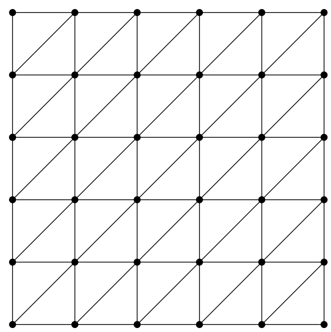

Figure 2. An atomistic triangulation of $\mathbb{Z}^2$.

Let $\mathcal{P}^1(\mathcal{T}_{\rm a})$ be the standard finite element space of C^0 piecewise linear functions with respect to $\mathcal{T}_{\rm a}$. The nodal interpolant, $Iu \in \mathcal{P}^1(\mathcal{T}_{\rm a})$, of a lattice function u is defined by setting

$$Iu(\xi) = u(\xi) \quad \forall\, \xi \in \mathbb{Z}^d.$$

Using this interpolant, we define the admissible space of displacements as

$$\mathcal{U} := \left\{ u : \mathbb{Z}^d \to \mathbb{R}^d : \nabla I u \in L^2(\mathbb{R}^d) \right\}, \tag{1.2}$$

and endow it with a semi-norm, $\|\nabla I u\|_{L^2(\mathbb{R}^d)}$.

The kernel of the semi-norm is the space of constant functions, $\mathbb{R}^d$, and elements of the associated quotient space, $\boldsymbol{\mathcal{U}} := \mathcal{U}/\mathbb{R}^d$ are equivalence classes

$$\boldsymbol{u} = \left\{ v \in \mathcal{U} : \exists\, c \in \mathbb{R}^d, v - u = c \right\}.$$

In order to define the interpolation operator on equivalence classes, we define the space

$$\dot{W}^{1,2}(\mathbb{R}^d) := \left\{ f \in W^{1,2}_{\rm loc}(\mathbb{R}^d) : \nabla f \in L^p(\mathbb{R}^d) \right\}$$

and its quotient space modulo constant functions,

$$\boldsymbol{W}^{1,2}(\mathbb{R}^d) := \dot{W}^{1,2}(\mathbb{R}^d)/\mathbb{R}^d.$$

Since the interpolation operator preserves constants $I\boldsymbol{u} := \{Iu : u \in \boldsymbol{u}\}$ is a well-defined equivalence class. Consequently, the mapping $I : \boldsymbol{\mathcal{U}} \to \boldsymbol{W}^{1,2}(\mathbb{R}^d)$ is well-defined and $|\nabla I u|_{L^2(\mathbb{R}^d)}$ induces a norm on $\boldsymbol{\mathcal{U}}$. Because $\mathcal{E}^{\rm a}(u)$ is invariant under shifts by constants, it is also well-defined on $\boldsymbol{\mathcal{U}}$. As a result, we can state the atomistic problem as

$$\boldsymbol{u}^\infty = \arg\min_{\boldsymbol{u} \in \boldsymbol{\mathcal{U}}} \mathcal{E}^{\rm a}(\boldsymbol{u}), \tag{1.3}$$

where arg min represents the set of local minimizers and the superscript "∞" is used throughout to indicate the *exact* solution displacement field defined on $\mathbb{Z}^d$. Note that minimization over equivalence classes effectively enforces a boundary condition[2] $u(\xi) \sim const$ for $\xi \to \infty$.

We formulate and study our AtC method for approximating (1.3) under several hypotheses on the site energy V_ξ. First, we assume that the defect core is concentrated at the origin, i.e., outside of this core V_ξ is independent of ξ. Succinctly,

Assumption A. *There exists $M > 0$ and $V : (\mathbb{R}^d)^{\mathcal{R}} \to \mathbb{R}$ such that for all $|\xi| > M$, $V_\xi(Du) \equiv V(Du)$.*

Second, since $\mathcal{E}^{\rm a}(u)$ may be infinite at the reference configuration, $u \equiv 0$, we should instead consider energy differences from the homogeneous lattice, $\mathbb{Z}^d$. In lieu of this, without loss of generality, we ask that

Assumption B. *The site energy vanishes at the reference configuration, i.e., $V(0) = 0$.*

Finally, we will make the following assumption concerning the regularity of V_ξ.

Assumption C. *The site potential V_ξ is C^4 on all of $(\mathbb{R}^d)^{\mathcal{R}}$. Furthermore, for $k \in \{1, 2, 3, 4\}$, there exists M_k such that*

$$|\partial^\alpha V_\xi(\boldsymbol{\rho})| \leq M_k \quad \forall \xi \in \mathbb{Z}^d, \, \boldsymbol{\rho} \in (\mathbb{R}^d)^{\mathcal{R}}, \, |\alpha| \leq k. \tag{1.4}$$

Assumption C allows us to avoid technicalities associated with handling potentials that are singular at the origin, such as the Lennard-Jones potential[3]. This assumption also implies that $\mathcal{E}^{\rm a}$ is four times Frechet differentiable on the space of displacements

$$\boldsymbol{\mathcal{U}}_0 := \{ \boldsymbol{u} \in \boldsymbol{\mathcal{U}} : \mathrm{supp}(\nabla I \boldsymbol{u}) \, \text{is compact} \} \,, \tag{1.5}$$

from which it is easy to deduce the regularity of the atomistic energy.

Theorem 1.2. *The atomistic energy $\mathcal{E}^{\rm a}$ can be extended by continuity to $\boldsymbol{\mathcal{U}}$ and is four times Frechet differentiable on $\boldsymbol{\mathcal{U}}$.*

We omit the proof, which is a minor modification of the proof of Theorem 2.3 of [9].

The Euler-Lagrange equation corresponding to the local minimization problem (1.3) is

$$\langle \delta \mathcal{E}^{\rm a}(\boldsymbol{u}^\infty), \boldsymbol{v} \rangle = \; 0 \quad \forall \boldsymbol{v} \, \in \boldsymbol{\mathcal{U}}_0. \tag{1.6}$$

We make the following assumption regarding the local minima of (1.6).

Assumption D. *There exists a local minimum, $\boldsymbol{u}^\infty \in \boldsymbol{\mathcal{U}}$, of $\mathcal{E}^{\rm a}(\boldsymbol{u})$ and a real number $\gamma_{\rm a} > 0$ such that*

$$\gamma_{\rm a} \| \nabla I \boldsymbol{v} \|^2_{L^2(\mathbb{R}^d)} \leq \langle \delta^2 \mathcal{E}^{\rm a}(\boldsymbol{u}^\infty) \boldsymbol{v}, \boldsymbol{v} \rangle \quad \forall \boldsymbol{v} \in \boldsymbol{\mathcal{U}}_0. \tag{1.7}$$

For point and line defects, solutions of (1.6) decay algebraically in their elastic far fields [9]. We quantify the rates of decay using a smooth nodal interpolant of a lattice function, v, which we denote by $\tilde{I} v \in W^{3,\infty}_{\rm loc}(\mathbb{R}^d)$. Its existence follows from [14, Lemma 2.1], which we state below. We refer to [14] for the proof.

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[2]This technique is also useful in establishing well-posedness results for linear elliptic systems on all of $\mathbb{R}^d$ [30].

[3]A more realistic assumption would be to assume smoothness in region of displacements in an energy well, which unduly complicates the analysis.

Lemma 1.3. *There exists a unique operator* $\tilde{I} : \mathcal{U} \to \mathrm{C}^{2,1}(\mathbb{R}^d)$ *such that for all* $\xi \in \mathbb{Z}^d$, $\tilde{I}v \in Q_5(\xi + (0,1)^d)$, $\tilde{I}v(\xi) = v(\xi)$, *and for all multiindices* $|\alpha| \le 2$, $\partial^\alpha \tilde{I}v(\xi) = D^{nn}_\alpha v(\xi)$ *where* D^{nn}_α *is defined by*

$$
\begin{aligned}
D_i^{nn,0} v(\xi) &:= v(\xi),\\
D_i^{nn,1} v(\xi) &:= \frac{1}{2}(v(\xi + e_i) - v(\xi - e_i)),\\
D_i^{nn,2} v(\xi) &:= v(\xi + e_i) - 2v(\xi) + v(\xi - e_i),\\
D_\alpha^{nn} v(\xi) &:= D_1^{nn,|\alpha_1|} \cdots D_d^{nn,|\alpha_d|} v(\xi).
\end{aligned}
$$

Furthermore,

$$\|\nabla^j \tilde{I}u\|_{L^2(\xi+(0,1)^d)} \lesssim \|D^j u\|_{\ell^2(\xi+\{-1,0,1\}^d)} \quad \text{for} \quad j = 1, 2, 3,^{4} \tag{1.8}$$

where

$$D^j u(\xi) = \left(D_{\rho_1} D_{\rho_2} \cdots D_{\rho_j} u(\xi)\right)_{(\rho_1,\rho_2,\ldots,\rho_j)\in\mathcal{R}^j}.$$

The uniqueness assertion of Lemma 1.3 and the condition that $\partial^\alpha \tilde{I}v(\xi) = D^{nn}_\alpha v(\xi)$ for all $\xi \in \mathbb{Z}^d$ imply that for any constant vector field, $u(\xi) \equiv c \in \mathbb{R}^d$, $\tilde{I}u = c$. Thus $\tilde{I}$ is well defined as an operator from $\boldsymbol{\mathcal{U}}$ to $\boldsymbol{\mathcal{U}}$ with $\tilde{I}\boldsymbol{u} = \left\{\tilde{I}u : u \in \boldsymbol{u}\right\}$. From (1.8) and a straightforward calculation it follows that

$$\|\nabla \tilde{I}\boldsymbol{u}\|_{L^2(\mathbb{R}^d)} \lesssim \|\nabla I\boldsymbol{u}\|_{L^2(\mathbb{R}^d)}. \tag{1.9}$$

The following theorem provides a sharp estimate on the algebraic decay of the minimizers for point defects only.

Theorem 1.4 (Regularity of a point defect)**.** *The local minimum,* $\boldsymbol{u}^\infty$, *of (1.3) satisfies*

$$\left|\nabla^j \tilde{I}\boldsymbol{u}^\infty(\xi)\right| \lesssim |\xi|^{1-j-d} \quad \text{for } j = 1, 2, 3. \tag{1.10}$$

Proof. Theorem 3.1 and Lemma 3.5 of [9] imply

$$\left|D^j \boldsymbol{u}^\infty(\xi)\right| \lesssim |\xi|^{1-j-d} \quad \text{for } j = 1, 2, 3.$$

□

The first step towards an AtC formulation for (1.3) is to approximate this problem by truncating the support of the admissible functions to a regular polygon or polyhedron Ω of diameter N. The resulting displacement space

$$\boldsymbol{\mathcal{U}}_\Omega := \left\{\boldsymbol{u} \in \boldsymbol{\mathcal{U}} : \mathrm{supp}(\nabla I u) \subset \overline{\Omega}\right\} \tag{1.11}$$

is finite-dimensional and comprises all functions that are constant outside of Ω. Restriction of the optimization problem (1.3) to (1.11) yields a finite dimensional atomistic problem

$$\boldsymbol{u}_\Omega = \arg\min_{\boldsymbol{\mathcal{U}}_\Omega} \mathcal{E}^{\mathrm{a}}(\boldsymbol{u}). \tag{1.12}$$

The corresponding Euler-Lagrange equation: seek $\boldsymbol{u}_\Omega \in \boldsymbol{\mathcal{U}}_\Omega$ such that

$$\langle \delta\mathcal{E}^{\mathrm{a}}(\boldsymbol{u}_\Omega), \boldsymbol{v}\rangle = 0 \qquad \forall \boldsymbol{v} \in \boldsymbol{\mathcal{U}}_\Omega, \tag{1.13}$$

[4]In this context, the modified Vinogradov notation $A \lesssim B$ means there is a constant C such that $A \le CB$ where C may depend on the dimension d. After introducing the relevant approximation parameters for the AtC method, we will explicitly state what the constant C is allowed to depend upon.

is a finite-dimensional approximation of (1.6). The truncated problem (1.13) provides an accurate and computationally feasible approximation for a single point defect [9]. However, its numerical solution quickly becomes intractable as the number of defects increases.

Thus, the next step in the AtC formulation is to replace (1.13) with a local hyperelastic model in parts of the domain that are sufficiently far away from the defect core; at a minimum, we require $V_\xi \equiv V$ in these regions. In such regions, the hyperelastic model is derived from the Cauchy-Born rule [3], which defines a strain energy per unit volume according to

$$W(\mathsf{G}) := V\big((\mathsf{G}\rho)_{\rho\in\mathcal{R}}\big) \quad \text{for } \mathsf{G} \in \mathbb{R}^{d\times d}. \tag{1.14}$$

Integration of the strain energy yields a continuum energy

$$\mathcal{E}^{\rm c}(u) := \int_{\mathbb{R}^d} W(\nabla u(x))\, dx, \tag{1.15}$$

which is defined for a suitable class of functions such as $W^{1,2}(\mathbb{R}^d)$. We use the Cauchy-Born rule far from the defect core because in the absence of defects it provides a second-order accurate approximation for smoothly decaying elastic fields [2, 42]. The advantage of (1.15) over (1.1) is that local minima of the former energy can efficiently be approximated by the finite element method.

1.2. **AtC Approximation**

AtC methods use the more accurate but expensive atomistic model only in a small region surrounding the defect core and switch to a more computationally efficient continuum model in the bulk of the domain where the lattice and site energy are homogeneous. The challenge is to couple the models in a stable and accurate manner without creating spurious numerical artifacts.

To describe our AtC approach we consider a configuration comprising a finite domain Ω, a defect core $\Omega_{\rm core} \subset \Omega$, and atomistic and continuum subdomains $\Omega_{\rm a}, \Omega_{\rm c} \subset \Omega$. Let

$$R_{\rm t} := \frac{1}{2}{\rm Diam}(\Omega_{\rm t}) \tag{1.16}$$

denote the outer radius of $\Omega_{\rm t}$ (${\rm t} = {\rm a}, {\rm c}, {\rm core}$), and let $r_{\rm core}, r_{\rm a}$, and $r_{\rm c}$ be the radii of the largest circle inscribed in $\Omega_{\rm core}, \Omega_{\rm a}$, and Ω respectively.[5]

We first select Ω_0 so that (i) it contains all ξ for which $V_\xi \not\equiv V$; (ii) its boundary, $\partial\Omega_0$, is Lipschitz, and (iii) $\partial\Omega_0$ is a union of edges from $\mathcal{T}_{\rm a}$. Then we choose integers $R_{\rm core} \geq 1$ and $\psi_{\rm a} > 1$ and set $\Omega_{\rm core} = R_{\rm core}\Omega_0$ and $\Omega_{\rm a} = \psi_{\rm a}\Omega_{\rm core}$ with the requirement that $(\psi_{\rm a}-1)r_{\rm core} \geq 4r_{\rm cut}$. Finally, we choose Ω so that $R_{\rm c}/R_{\rm core} = R_{\rm core}^{\kappa}$ for some integer $\kappa \geq 1$. The continuum domain is then defined by $\Omega_{\rm c} := \Omega\backslash\Omega_{\rm core}$, and we also define the "annular" overlap region $\Omega_{\rm o} := \Omega_{\rm a}\backslash\Omega_{\rm core}$. The requirement that $(\psi_{\rm a}-1)r_{\rm core} \geq 4r_{\rm cut}$ can now be interpreted as requiring the overlap "width" to be twice the size of the interaction range of the site potential. See Figure 3 for an illustration in two dimensions.

The atomic lattices associated with the new domains are

$$\mathcal{L}_{\rm t} := \mathbb{Z}^d \cap \Omega_{\rm t} \quad \text{where} \quad {\rm t} = {\rm a}, {\rm c}, {\rm o}, {\rm core}, \tag{1.17}$$

and their atomistic interiors are

$$\mathcal{L}_{\rm t}^{\circ} := \{\xi \in \mathcal{L}_{\rm t} : \xi - \rho \in \mathcal{L}_{\rm t} \quad \forall \rho \in \mathcal{R}\}\,. \tag{1.18}$$

The atomistic interiors of the interiors are $\mathcal{L}_{\rm t}^{\circ\circ} = (\mathcal{L}_{\rm t}^{\circ})^{\circ}$ while the atomistic boundary of $\mathcal{L}_{\rm t}$ is

$$\partial_{\rm a}\mathcal{L}_{\rm t} := \mathcal{L}_{\rm t}\backslash\mathcal{L}_{\rm t}^{\circ\circ}. \tag{1.19}$$

[5] We define $r_{\rm c}$ as the inner radii of Ω since $\Omega_{\rm c}$ itself will later be constructed to have a hole at the defect core and hence not have an inscribed circle.

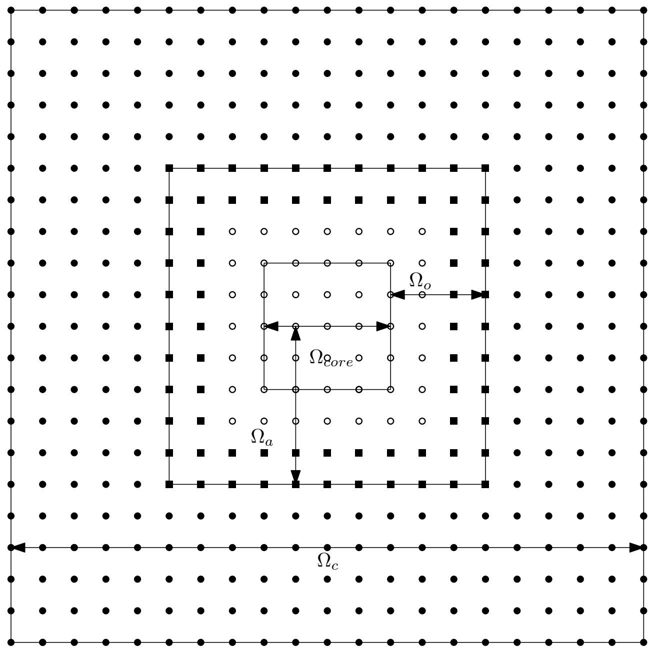

FIGURE 3. An example AtC configuration in two dimensions. The set $\Omega_{\mathrm{a}}^{\circ\circ}$ is shown as open circles. The boxes show $\partial_{\mathrm{a}}\mathcal{L}_{\mathrm{a}}$ for the case $\mathcal{R} = \{\pm \boldsymbol{e}_1, \pm \boldsymbol{e}_2\}$.

See Figure 3 for an illustration of $\Omega_{\mathrm{a}}^{\circ\circ}$ (open circles) and $\partial_{\mathrm{a}}\mathcal{L}_{\mathrm{a}}$ (closed boxes) for the case $\mathcal{R} = \{\pm \boldsymbol{e}_1, \pm \boldsymbol{e}_2\}$.

Remark 1.5. *Throughout the paper we state results involving a parameter R_{core}^* such that if $R_{\mathrm{core}} \geq R_{\mathrm{core}}^*$, then a solution to a specific problem defined on the domains constructed above will be guaranteed to exist. Because $R_{\mathrm{c}} \gg R_{\mathrm{core}}$, this will automatically ensure that $R_{\mathrm{c}} \gg R_{\mathrm{core}}^*$ as well. These results always assume AtC domain configurations constructed according to the above guidelines. Furthermore, when stating inequalities, we will use modified Vinogradov notation, $A \lesssim B$ in lieu of $A \leq C \cdot B$, where $C > 0$ is a constant. This constant may only depend upon $\Omega_0, d, R_{\mathrm{core}}^*, r_{\mathrm{cut}}$, ψ_{a}, and an additional constant, β, introduced in Section 1.2.2 as the minimum angle of a finite element mesh.*

1.2.1. *Restricted Atomistic Problem*

The basis for defining an atomistic problem restricted to Ω_{a} are the Euler-Lagrange equations (1.13). By requiring $\boldsymbol{u}_\Omega \in \boldsymbol{\mathcal{U}}_\Omega$, we are effectively imposing Dirichlet boundary conditions (in the sense of equivalence classes) for the variational problem by requiring the function to be constant outside Ω. Accordingly, we will define a restricted atomistic problem by also specifying Dirichlet boundary conditions on $\partial_{\mathrm{a}}\mathcal{L}_{\mathrm{a}}$.

The admissible displacement space for this problem is $\boldsymbol{\mathcal{U}}^{\mathrm{a}} := \mathcal{U}^{\mathrm{a}}/\mathbb{R}^d$ where

$$\mathcal{U}^{\mathrm{a}} := \left\{ u^{\mathrm{a}} : \mathcal{L}_{\mathrm{a}} \to \mathbb{R}^d \right\}. \tag{1.20}$$

The elements of $\boldsymbol{\mathcal{U}}^{\mathbf{a}}$ are equivalence classes, $\boldsymbol{u}^{\mathrm{a}}$, of lattice functions on $\mathcal{L}_{\mathrm{a}}$ differing by a constant $c \in \mathbb{R}^d$. We again use I to denote the piecewise linear interpolant of a lattice function on $\mathcal{L}_{\mathrm{a}}$ and endow $\boldsymbol{\mathcal{U}}^{\mathrm{a}}$ with the norm $\|\nabla I \boldsymbol{u}^{\mathrm{a}}\|_{L^2(\Omega_a)}$. We then define a restricted atomistic energy functional on $\boldsymbol{\mathcal{U}}^{\mathrm{a}}$ via

$$\tilde{\mathcal{E}}^{\mathrm{a}}(\boldsymbol{u}^{\mathrm{a}}) := \sum_{\xi \in \mathcal{L}_{\mathrm{a}}^{\circ\circ}} V_\xi(D\boldsymbol{u}^{\mathrm{a}}(\xi)). \tag{1.21}$$

We seek to minimize $\tilde{\mathcal{E}}^{\rm a}(\boldsymbol{u}^{\rm a})$ over $\boldsymbol{\mathcal{U}}^{\rm a}$ subject to Dirichlet boundary conditions on $\partial_{\rm a}\mathcal{L}_{\rm a}$. The set of all possible boundary values is the quotient space $\boldsymbol{\Lambda}^{\rm a} := \Lambda^{\rm a}/\mathbb{R}^d$, where

$$\Lambda^{\rm a} := \left\{\lambda_{\rm a} : \partial_{\rm a}\mathcal{L}_{\rm a} \to \mathbb{R}^d\right\}. \tag{1.22}$$

Elements of $\boldsymbol{\Lambda}^{\rm a}$ are denoted again by $\lambda_{\rm a}$ (without boldface). Thus, the restricted atomistic problem reads

$$\boldsymbol{u}^{\rm a} = \arg\min_{\boldsymbol{\mathcal{U}}^{\rm a}} \tilde{\mathcal{E}}^{\rm a}(\boldsymbol{w}^{\rm a}) \quad \text{subject to} \quad \boldsymbol{u}^{\rm a} = \lambda_{\rm a} \quad \text{on} \quad \partial_{\rm a}\mathcal{L}_{\rm a}. \tag{1.23}$$

We refer to $\lambda_{\rm a}$ as a *virtual atomistic controls.* They are virtual because $\partial_{\rm a}\mathcal{L}_{\rm a}$ is an artificial rather than a physical boundary. They are controls because by varying $\lambda_{\rm a}$ we can vary, i.e. "control," the solutions of (1.23).

The Euler-Lagrange equation for (1.23) is: seek $\boldsymbol{u}^{\rm a} \in \boldsymbol{\mathcal{U}}^{\rm a}$ such that

$$\begin{aligned} \langle \delta\tilde{\mathcal{E}}^{\rm a}(\boldsymbol{u}^{\rm a}), \boldsymbol{v}^{\rm a}\rangle = 0 \quad \forall \boldsymbol{v}^{\rm a} \in \boldsymbol{\mathcal{U}}^{\rm a}_0, \\ \boldsymbol{u}^{\rm a} = \lambda_{\rm a} \quad \text{on} \quad \partial_{\rm a}\mathcal{L}_{\rm a}, \end{aligned} \tag{1.24}$$

where the space of atomistic test functions, $\boldsymbol{\mathcal{U}}^{\rm a}_0 := \mathcal{U}^{\rm a}_0/\mathbb{R}^d$, is the quotient space of

$$\mathcal{U}^{\rm a}_0 := \left\{u^{\rm a} \in \mathcal{U}^{\rm a} : \exists\, c \in \mathbb{R}^d,\, u^{\rm a}|_{\partial_{\rm a}\mathcal{L}_{\rm a}} = c\right\}. \tag{1.25}$$

After extending $\boldsymbol{v}^{\rm a} \in \boldsymbol{\mathcal{U}}^{\rm a}_0$ by a constant to a function defined on all of $\mathbb{R}^d$, [9, (2.5) in Lemma 2.1] implies

$$\sum_{\xi \in \mathcal{L}^{\circ\circ}_{\rm a}} \sup_{\rho \in \mathcal{R}} |D_\rho \boldsymbol{v}^{\rm a}|^2 \lesssim \|\nabla I\boldsymbol{v}^{\rm a}\|^2_{L^2(\Omega_{\rm a})} \quad \forall \boldsymbol{v}^{\rm a} \in \boldsymbol{\mathcal{U}}^{\rm a}_0. \tag{1.26}$$

The following result is then a direct consequence of Assumption C and (1.26).

Theorem 1.6. *The restricted energy functional $\tilde{\mathcal{E}}^{\rm a}$ is four times Frechet differentiable on $\boldsymbol{\mathcal{U}}^{\rm a}$, and each derivative is uniformly bounded in the parameter $R_{\rm core}$. In particular, $\delta^2\tilde{\mathcal{E}}^{\rm a}$ is Lipschitz continuous on $\boldsymbol{\mathcal{U}}^{\rm a}$ with Lipschitz bound independent of $R_{\rm core}$.*

Given the exact solution $\boldsymbol{u}^\infty$, we will later require solving (1.24) where we take $\lambda_{\rm a} = \boldsymbol{u}^\infty|_{\partial_{\rm a}\mathcal{L}_{\rm a}}$. To do that, first set $\boldsymbol{u}^\infty_{\rm a} := \boldsymbol{u}^\infty|_{\mathcal{L}_{\rm a}}$, and next note that elements of $\boldsymbol{\mathcal{U}}^{\rm a}_0$ can be extended by a constant to functions defined on all of $\mathbb{Z}^d$, and this extension will belong to $\boldsymbol{\mathcal{U}}_0$. By identifying $\boldsymbol{v}^{\rm a} \in \boldsymbol{\mathcal{U}}^{\rm a}_0$ as an element of $\boldsymbol{\mathcal{U}}_0$, we have

$$\left\langle \delta\tilde{\mathcal{E}}^{\rm a}(\boldsymbol{u}^\infty_{\rm a}), \boldsymbol{v}^{\rm a}\right\rangle = \langle \mathcal{E}^{\rm a}(\boldsymbol{u}^\infty), \boldsymbol{v}^{\rm a}\rangle = 0. \tag{1.27}$$

The final equality holds since $\boldsymbol{u}^\infty$ solves the Euler Lagrange equations (1.6). Similarly, Assumption D implies

$$\gamma_{\rm a}\|\nabla I\boldsymbol{v}^{\rm a}\|_{L^2(\Omega_{\rm a})} = \gamma_{\rm a}\|\nabla I\boldsymbol{v}^{\rm a}\|_{L^2(\mathbb{R}^d)} \leq \left\langle \delta^2\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty_{\rm a})\boldsymbol{v}^{\rm a}, \boldsymbol{v}^{\rm a}\right\rangle = \left\langle \delta^2\tilde{\mathcal{E}}^{\rm a}(\boldsymbol{u}^\infty)\boldsymbol{v}^{\rm a}, \boldsymbol{v}^{\rm a}\right\rangle \tag{1.28}$$

Hence the solution to (1.24) for $\lambda_{\rm a} = \boldsymbol{u}^\infty|_{\partial_{\rm a}\mathcal{L}_{\rm a}}$ is precisely $\boldsymbol{u}^\infty_{\rm a} := \boldsymbol{u}^\infty|_{\mathcal{L}_{\rm a}}$. To avoid unnecessary notation, we will often drop the subscript and just write $\boldsymbol{u}^\infty$ as the solution to this problem.

1.2.2. *Restricted Continuum*

We define the continuum subproblem analogously by using the Euler-Lagrange equations corresponding to minimizing the Cauchy-Born energy (1.15). In addition to the atomistic mesh, $\mathcal{T}_a$, that covers Ω_a and Ω_c, we introduce a partition, $\mathcal{T}_h$, of Ω_c into finite elements. This is required to define the admissible continuum displacement space. Let $\mathcal{N}_h$ be the nodes of $\mathcal{T}_h$. We assume that (i) an atomistc position $\xi \in \overline{\Omega}_{\rm a}$ is a node of

$\mathcal{T}_h$ *if and only if* $\xi \in \mathcal{L}_{\rm a} \cap \Omega_{\rm c}$, (ii) nodes in $\mathcal{N}_h$ are also nodes of $\mathcal{T}_{\rm a}$, and (iii) the elements $T \in \mathcal{T}_h$ satisfy a minimum angle condition for some fixed $\beta > 0$. Further define

$$h_T := \mathrm{Diam}(T), \quad \text{and} \quad h(x) := \sup_{\{T \in \mathcal{T}_h : x \in T\}} h_T.$$

For example, if x is a vertex of a triangle, then $h(x)$ is the largest diameter of the triangles which share this vertex. Error estimates require an additional assumption on this function.

Assumption E. *The mesh size function satisfies* $h(x) \lesssim (|x|/R_{\rm core})^{\upsilon}$ *for some* $(d+2)/2 \geq \upsilon \geq 1$.

We will also need the inner and outer continuum boundaries defined as

$$\Gamma_{\rm core} = \partial\Omega_{\rm core} \quad \text{and} \quad \Gamma_{\rm c} = \partial\Omega_{\rm c} \backslash \Gamma_{\rm core},$$

respectively.

Our analysis uses two families of interpolants. The first family comprises the standard piecewise linear interpolants I_h and I defined on the finite element mesh $\mathcal{T}_h$ and the atomistic mesh $\mathcal{T}_a$ on Ω_c, i.e.,

$$\begin{aligned} I_h u \in \mathcal{P}^1(\mathcal{T}_h), \quad I_h u(\zeta) = u(\zeta) \quad \forall \zeta \in \mathcal{N}_h. \\ Iu \in \mathcal{P}^1(\mathcal{T}_a), \quad Iu(\xi) = u(\xi) \quad \forall \xi \in \mathcal{L}. \end{aligned} \tag{1.29}$$

The second family comprises Scott-Zhang (quasi-)interpolants [4,35] $S_{\rm a}$, $S_{{\rm a},n}$, and $S_{h,n}$ defined on $\Omega_{\rm c}$ with the atomistic discretization, $\mathcal{T}_{\rm a}$, a domain $\tilde{\Omega}_{\rm a}$ with a discretization $\tilde{\mathcal{T}}_{{\rm a},n} = \epsilon_n \mathcal{T}_{\rm a}$ for some $\epsilon_n > 0$; and a domain $\tilde{\Omega}_{\rm c}$ with discretization $\tilde{\mathcal{T}}_{h,n} = \epsilon_n \mathcal{T}_h$, respectively. We recall that for a given domain U, a mesh partition $\mathcal{T}$ and a function $f \in H^1(U)$, the Scott-Zhang interpolant Sf has the following four properties [4, Chapter 4]:

- **P.1:** (Projection) $Sf = f$ for all $f \in \mathcal{P}^1(\mathcal{T})$.
- **P.2:** (Preservation of Homogeneous Boundary Conditions) If f is constant on ∂U, then so is Sf.
- **P.3:** (Stability of semi-norm) $\|\nabla Sf\|_{L^2(U)} \lesssim \|\nabla f\|_{L^2(U)}$ - the implied constant depending upon the shape regularity constant, or minimum angle of the mesh $\mathcal{T}$.
- **P.4:** (Interpolation Error for S) $\|Sf - f\|_{L^2(U)} \lesssim \max_{T \in \mathcal{T}} \mathrm{Diam}(T) \|\nabla f\|_{L^2(U)}$.

The space of admissible continuum displacements is $\boldsymbol{\mathcal{U}}_h^{\rm c} := \mathcal{U}_h^{\rm c}/\mathbb{R}^d$, where

$$\mathcal{U}_h^{\rm c} := \left\{ u^{\rm c} \in C^0(\Omega_{\rm c}) : u^{\rm c}|_T \in \mathcal{P}^1(T) \; \forall T \in \mathcal{T}_h, \, \exists K \in \mathbb{R}^d, \, u^{\rm c} = K \; \text{ on } \Gamma_{\rm c} \right\}. \tag{1.30}$$

The norm on this space is $\|\nabla \boldsymbol{u}^{\rm c}\|_{L^2(\Omega_{\rm c})}$. Similar to the definition of $\boldsymbol{\mathcal{U}}_\Omega$, we require the elements of $\boldsymbol{\mathcal{U}}_h^{\rm c}$ to be constant on the *outer* continuum boundary $\Gamma_{\rm c}$, which enables their extension to infinity by a constant. We do not place such a requirement on the *inner* continuum boundary because $\Gamma_{\rm core}$ is an artificial boundary. There we will employ *virtual continuum* boundary controls belonging to the space $\boldsymbol{\Lambda}^{\rm c} := \Lambda^{\rm c}/\mathbb{R}^d$ where

$$\Lambda^{\rm c} := \left\{ \lambda_{\rm c} : \mathcal{N}_h \cap \Gamma_{\rm core} \to \mathbb{R}^d \right\} \tag{1.31}$$

Since $\Gamma_{\rm core}$ represents a curve, we can define the piecewise linear interpolant of $\lambda_{\rm c} \in \Lambda_{\rm c}$ with respect to $\mathcal{N}_h \cap \Gamma_{\rm core}$ by $I\lambda_c(\xi) = \lambda_c(\xi)$ for all $\xi \in \mathcal{N}_h \cap \Gamma_{\rm core}$. Again, if $\lambda_{\rm c}$ is constant, the $I\lambda_{\rm c}$ is as well so that this operator is well defined on $\boldsymbol{\Lambda}^{\rm c}$. Henceforth, we will always identify elements of $\boldsymbol{\Lambda}^{\rm c}$ with their piecewise linear interpolant on $\Gamma_{\rm core}$ without explicitly using I.

The restricted continuum energy functional on $\boldsymbol{\mathcal{U}}_h^{\rm c}$ is then

$$\tilde{\mathcal{E}}^{\rm c}(\boldsymbol{u}^{\rm c}) := \int_{\Omega_{\rm c}} W(\nabla \boldsymbol{u}^{\rm c}(x)) \, dx = \sum_{T \in \mathcal{T}_h} W(\nabla \boldsymbol{u}^{\rm c}(x)) \, |T| \, . \tag{1.32}$$

Given $\lambda_{\rm c} \in \boldsymbol{\Lambda}^{\rm c}$, we consider the following restricted continuum problem

$$\boldsymbol{u}^{\rm c} = \arg\min_{\boldsymbol{\mathcal{U}}_h^{\rm c}} \tilde{\mathcal{E}}^{\rm c}(\boldsymbol{w}^{\rm c}) \quad \text{such that} \quad \boldsymbol{u}^{\rm c} = \lambda_{\rm c} \quad \text{on} \quad \Gamma_{\rm core}. \tag{1.33}$$

An appropriate space of test functions for (1.33) is $\boldsymbol{\mathcal{U}}_{h,0}^{\rm c} := \mathcal{U}_{h,0}^{\rm c}/\mathbb{R}^d$, where

$$\mathcal{U}_{h,0}^{\rm c} := \left\{ u^{\rm c} \in \mathcal{U}_h^{\rm c} : \exists\, K \in \mathbb{R}^d, u^{\rm c}|_{\Gamma_{\rm core}} = K \right\}. \tag{1.34}$$

Thus, the Euler-Lagrange equation for (1.33) is given by: seek $\boldsymbol{u}^{\rm c} \in \boldsymbol{\mathcal{U}}_h^{\rm c}$ such that

$$\begin{aligned} \langle \delta\tilde{\mathcal{E}}^{\rm c}(\boldsymbol{u}^{\rm c}), \boldsymbol{v}^{\rm c} \rangle = 0 \quad \forall \boldsymbol{v}^{\rm c} \in \boldsymbol{\mathcal{U}}_{h,0}^{\rm c}, \\ \boldsymbol{u}^{\rm c} = \lambda_{\rm c} \quad \text{on} \quad \Gamma_{\rm core}. \end{aligned} \tag{1.35}$$

The following lemma is an analogue of Lemma 1.6.

Lemma 1.7. *The restricted continuum energy functional $\tilde{\mathcal{E}}^{\rm c}$ is four times continuously Frechet differentiable on $\boldsymbol{\mathcal{U}}_h^{\rm c}$ with derivatives bounded uniformly in the parameter R_c. Moreover, $\delta^2\tilde{\mathcal{E}}^{\rm c}$ is Lipschitz continuous with Lipschitz bound independent of R_c.*

1.2.3. *Continuum Error*

This section estimates the error between the restricted continuum and atomistic solutions. We refer to this error as the *continuum error*. We will first define an operator taking functions in $\boldsymbol{\mathcal{U}}$ to functions in $\boldsymbol{\mathcal{U}}_h^{\rm c}$. This will yield a representation of $\boldsymbol{u}^\infty$ in $\boldsymbol{\mathcal{U}}_h^{\rm c}$ which we can input into the variational equation (1.35) to obtain the consistency error.

To this end, let η be a smooth bump function equal to 1 on $B_{3/4}(0)$ and vanishing off of $B_1(0)$. Given $R > 0$ and an annulus $A_R := B_R \backslash B_{3/4R}$, we follow [9, 14] to define an operator $T_R : \boldsymbol{\mathcal{U}} \to \boldsymbol{\mathcal{U}}_\Omega$ according to

$$T_R \boldsymbol{u}(x) = \eta(x/R)\big(\tilde{I}\boldsymbol{u} - \textstyle\fint_{A_R} \tilde{I}\boldsymbol{u}\, dx\big). \tag{1.36}$$

Above, $\fint_U f\, dx = \frac{1}{|U|}\int f\, dx$ is the average value of f. We then set

$$\Pi_h \boldsymbol{u} = I_h\left((T_{r_{\rm c}}\boldsymbol{u})\,|_{\Omega_{\rm c}} \right). \tag{1.37}$$

We will use $\Pi_h \boldsymbol{u}^\infty$ in (1.35) to obtain the consistency error. The following lemma estimates the error of this operator over $\Omega_{\rm c}$. We note that the proof below is standard and is similar to, e.g., [30, Lemma 2.1]. Moreover, $r_{\rm core} \lesssim R_{\rm core} \lesssim r_{\rm core}$ and $r_{\rm c} \lesssim R_{\rm c} \lesssim r_{\rm c}$ so that estimates in terms of $R_{\rm core}$ and $R_{\rm c}$ can be phrased in terms of $r_{\rm core}$ and $r_{\rm c}$ and vice versa.

Lemma 1.8.

$$\|\nabla \Pi_h \boldsymbol{u}^\infty - \nabla \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})} \lesssim R_{\rm core}^{-d/2-1} + R_{\rm c}^{-d/2} \tag{1.38}$$

Proof. We first estimate the error by

$$\|\nabla I_h T_{r_{\rm c}}\boldsymbol{u}^\infty - \nabla \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})} \le \|\nabla I_h T_{r_{\rm c}}\boldsymbol{u}^\infty - \nabla T_{r_{\rm c}}\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})} + \|\nabla T_{r_{\rm c}}\boldsymbol{u}^\infty - \nabla \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})} \tag{1.39}$$

We can easily estimate the second term:

$$\begin{aligned} &\|\nabla T_{r_{\rm c}}\boldsymbol{u}^\infty - \nabla \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})} \\ &\lesssim \left\| \tfrac{1}{r_{\rm c}} \nabla\eta(x/r_{\rm c})\big(\tilde{I}\boldsymbol{u}^\infty - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}^\infty\, dx\big) + [\eta(x/r_{\rm c}) - 1]\nabla\tilde{I}\boldsymbol{u}^\infty \right\|_{L^2(\Omega_{\rm c})} \\ &\lesssim \frac{1}{r_{\rm c}} \left\| \nabla\eta(x/r_{\rm c})\big(\tilde{I}\boldsymbol{u}^\infty - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}^\infty\, dx\big) \right\|_{L^2(A_{r_{\rm c}})} + \|(\eta(x/r_{\rm c}) - 1)\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\mathbb{R}^d \backslash B_{3r_{\rm c}/4})} \\ &\lesssim \|\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(A_{r_{\rm c}})} + \|\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\mathbb{R}^d \backslash B_{3r_{\rm c}/4})} \lesssim \|\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\mathbb{R}^d \backslash B_{3r_{\rm c}/4})}. \end{aligned} \tag{1.40}$$

In the second to last inequality, we have used the Poincare inequality. Employing the decay rates in Theorem 1.4, we obtain

$$\|\nabla T_{r_c}\boldsymbol{u}^\infty - \nabla \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \lesssim R_c^{-d/2}. \tag{1.41}$$

Similarly, the first term of (1.39) can be estimated by first using standard finite element approximation results for smooth functions, the definition of T_{r_c}, the fact that $h/r_c \le 1$, and the Poincare inequality.

$$\begin{aligned}
\|\nabla I_h T_{r_c}\boldsymbol{u}^\infty - \nabla T_{r_c}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} &\lesssim \|h\nabla^2 T_{r_c}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \\
&\lesssim \big\|h\nabla^2\big(\eta(x/r_c)(\tilde{I}\boldsymbol{u}^\infty - \textstyle\fint_{A_{r_c}} \tilde{I}\boldsymbol{u}^\infty\,dx)\big)\big\|_{L^2(\Omega_c)} \\
&= \frac{1}{r_c}\big\|(h/r_c)\nabla^2\eta(x/r_c)(\tilde{I}\boldsymbol{u}^\infty - \textstyle\fint_{A_{r_c}} \tilde{I}\boldsymbol{u}^\infty\,dx)\big\|_{L^2(A_{r_c})} + \|\nabla\tilde{I}\boldsymbol{u}^\infty\nabla\eta(x/r_c)\|_{L^2(A_{r_c})} \\
&\quad + \|h\eta(x/r_c)\nabla^2\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \\
&\lesssim \|\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(A_{r_c})} + \frac{1}{r_c}\|h\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(A_{r_c})} + \|h\nabla^2\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \\
&\lesssim \|\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(A_{r_c})} + \|h\nabla^2\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)}.
\end{aligned} \tag{1.42}$$

A straightforward application of the regularity estimates in Theorem 1.4 and the conditions on $h(x)$ in Assumption E give

$$\|\nabla I_h T_{r_c}\boldsymbol{u}^\infty - \nabla T_{r_c}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \lesssim R_c^{-d/2} + R_{\mathrm{core}}^{-d/2-1}. \tag{1.43}$$

Combining (1.41) and (1.43) and keeping only the leading order terms yields (1.38). □

The following Lemma provides information about the stability of the Hessian of $\tilde{\mathcal{E}}^c$ at $\Pi_h\boldsymbol{u}^\infty$.

Lemma 1.9. *There exists $R^*_{\mathrm{core}} > 0$ and $\gamma_c > 0$ such that for all $R_{\mathrm{core}} \ge R^*_{\mathrm{core}}$ (and all continuum partitions $\mathcal{T}_h$ satisfying the assumptions in this section),*

$$\gamma_c\|\nabla\boldsymbol{v}^c\|^2_{L^2(\Omega_c)} \le \big\langle\delta^2\tilde{\mathcal{E}}^c(\Pi_h\boldsymbol{u}^\infty)\boldsymbol{v}^c, \boldsymbol{v}^c\big\rangle \quad \forall\,\boldsymbol{v}^c \in \boldsymbol{\mathcal{U}}^c_{h,0}.$$

Proof. For $\boldsymbol{u} \in \boldsymbol{\mathcal{U}}$ define

$$\mathcal{E}^a_{\mathrm{hom}}(\boldsymbol{u}) := \sum_{\xi\in\mathbb{Z}^d} V(D\boldsymbol{u}).$$

From [9, Proposition 2.6] and Assumption D, we deduce that

$$\langle\delta^2\mathcal{E}^a_{\mathrm{hom}}(\boldsymbol{0})\boldsymbol{v}, \boldsymbol{v}\rangle \ge \gamma_a\|\nabla I\boldsymbol{v}\|^2_{L^2(\mathbb{R}^d)} \quad \forall\,\boldsymbol{v} \in \boldsymbol{\mathcal{U}}_0, \tag{1.44}$$

while [31, Lemma 5.2] implies

$$\langle\delta^2\mathcal{E}^c(0)\boldsymbol{v}, \boldsymbol{v}\rangle \ge \gamma_a\|\nabla\boldsymbol{v}\|^2_{L^2(\mathbb{R}^d)} \qquad \forall v \in H^1_0(\mathbb{R}^d).$$

Furthermore, extending $\boldsymbol{v}^c \in \mathcal{U}^c_{h,0}$ by a constant to all of $\mathbb{R}^d$ yields

$$\begin{aligned}
\langle\delta^2\tilde{\mathcal{E}}^c(\Pi_h\boldsymbol{u}^\infty)\boldsymbol{v}^c, \boldsymbol{v}^c\rangle &= \langle\delta^2\mathcal{E}^c(\Pi_h\boldsymbol{u}^\infty)\boldsymbol{v}^c, \boldsymbol{v}^c\rangle - \langle\delta^2\mathcal{E}^c(\boldsymbol{0})\boldsymbol{v}^c, \boldsymbol{v}^c\rangle + \langle\delta^2\mathcal{E}^c(\boldsymbol{0})\boldsymbol{v}^c, \boldsymbol{v}^c\rangle \\
&\ge -\big|\langle\delta^2\tilde{\mathcal{E}}^c(\Pi_h\boldsymbol{u}^\infty)\boldsymbol{v}^c, \boldsymbol{v}^c\rangle - \langle\delta^2\mathcal{E}^c(\boldsymbol{0})\boldsymbol{v}^c, \boldsymbol{v}^c\rangle\big| + \langle\delta^2\mathcal{E}^c(\boldsymbol{0})\boldsymbol{v}^c, \boldsymbol{v}^c\rangle \\
&\gtrsim -\|\nabla\Pi_h\boldsymbol{u}^\infty\|_{L^\infty(\Omega_c)}\cdot\|\nabla\boldsymbol{v}^c\|^2_{L^2(\Omega_c)} + \gamma_a\|\nabla\boldsymbol{v}^c\|^2_{L^2(\Omega_c)},
\end{aligned} \tag{1.45}$$

The final bound is a consequence of the Lipschitz continuity of W. Next,

$$
\begin{aligned}
\|\nabla \Pi_h \boldsymbol{u}^\infty\|_{L^\infty(\Omega_{\rm c})} &\leq \|\nabla T_{r_{\rm c}} \boldsymbol{u}^\infty\|_{L^\infty(\Omega_{\rm c})} \\
&= \|\nabla\big[\eta(x/r_{\rm c})\big(\tilde{I}\boldsymbol{u} - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}\,dx\big)\big]\|_{L^\infty(\Omega_{\rm c})} \\
&= \|\nabla(\eta(x/r_{\rm c}))\big(\tilde{I}\boldsymbol{u} - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}\,dx\big) + \eta(x/r_{\rm c})\nabla\big(\tilde{I}\boldsymbol{u} - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}\,dx\big)\|_{L^\infty(\Omega_{\rm c})} \\
&\leq \|\nabla(\eta(x/r_{\rm c}))\big(\tilde{I}\boldsymbol{u} - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}\,dx\big)\|_{L^\infty(A_{r_{\rm c}})} + \|\eta(x/r_{\rm c})\nabla\big(\tilde{I}\boldsymbol{u} - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}\,dx\big)\|_{L^\infty(\Omega_{\rm c})} \\
&\lesssim \frac{1}{r_{\rm c}}\|\big(\tilde{I}\boldsymbol{u} - \textstyle\fint_{A_{r_{\rm c}}} \tilde{I}\boldsymbol{u}\,dx\big)\|_{L^\infty(A_{r_{\rm c}})} + \|\nabla\tilde{I}\boldsymbol{u}\|_{L^\infty(\Omega_{\rm c})} \\
&\lesssim \|\nabla\tilde{I}\boldsymbol{u}\|_{L^\infty(A_{r_{\rm c}})} + \|\nabla\tilde{I}\boldsymbol{u}\|_{L^\infty(\Omega_{\rm c})} \\
&\lesssim \|\nabla\tilde{I}\boldsymbol{u}\|_{L^\infty(\Omega_{\rm c})}.
\end{aligned}
$$

Using this result in (1.45) together with (1.10) yields

$$
\langle \delta^2\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty)\boldsymbol{v}^{\rm c}, \boldsymbol{v}^{\rm c}\rangle \;\gtrsim\; (-\|\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^\infty(\Omega_{\rm c})} + \gamma_{\rm a})\|\nabla\boldsymbol{v}^{\rm c}\|^2_{L^2(\Omega_{\rm c})} \;\gtrsim\; (-(R_{\rm core})^{-d} + \gamma_{\rm a})\|\nabla\boldsymbol{v}^{\rm c}\|^2_{L^2(\Omega_{\rm c})}.
$$

Choosing $R^*_{\rm core}$ such that $-(R^*_{\rm core})^{-d} + \gamma_{\rm a} \geq \gamma_{\rm a}/2$ completes the proof with $\gamma_{\rm c} := \gamma_{\rm a}/2$. □

For the proof of existence of a solution to the restricted continuum problem, we rely on the following quantitative version of the inverse function theorem [19, 25].

Theorem 1.10 (Inverse Function Theorem)**.** *Let X and Y be Banach spaces with $f : X \to Y$ a continuously differentiable function on an open set U containing x_0. Let $y_0 = f(x_0)$ with $\|y_0\|_Y < \eta$. Furthermore, suppose that $\delta f(x_0)$ is invertible such that $\|\delta f(x_0)^{-1}\|_{\mathcal{L}(Y,X)} < \sigma$, $B_{2\eta\sigma}(x_0) \subset U$, δf is Lipschitz continuous on $B_{2\eta\sigma}(x_0)$ with Lipschitz constant L, and $2L\eta\sigma^2 < 1$. Then there exists a unique continuously differentiable function $g : B_\eta(y_0) \to B_{2\eta\sigma}(x_0)$ such that*

$$
g(y_0) = x_0 \quad \text{and} \quad f(g(y)) = y \quad \forall y \in B_\eta(y_0)\,.
$$

In particular, there exists $\bar{x} = g(0) \in X$ such that $f(\bar{x}) = 0$ and

$$
\|g(y_0) - g(0)\|_X = \|x_0 - \bar{x}\|_X < 2\eta\sigma,
$$

Theorem 1.11 (Continuum Error)**.** *Let $\lambda^\infty_{\rm c} := \boldsymbol{u}^\infty|_{\Gamma_{\rm core}}$. There exists $R^*_{\rm core} > 0$ such that for all $R_{\rm core} \geq R^*_{\rm core}$, the variational problem*

$$
\langle \delta\tilde{\mathcal{E}}^{\rm c}(\boldsymbol{u}), \boldsymbol{v}^{\rm c}\rangle = 0 \quad \forall\, \boldsymbol{v}^{\rm c} \in \boldsymbol{\mathcal{U}}^{\rm c}_{h,0} \quad \text{subject to} \quad \boldsymbol{u} = \lambda^\infty_{\rm c} \quad \text{on} \quad \Gamma_{\rm core}, \tag{1.46}
$$

has a solution $\boldsymbol{u}^{\rm con}$ such that

$$
\|\nabla\boldsymbol{u}^{\rm con} - \nabla I\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})} \lesssim R_{\rm core}^{-d/2-1} + R_{\rm c}^{-d/2} \tag{1.47}
$$

Furthermore, there exists $\gamma'_{\rm c}$ such that

$$
\big\langle \delta^2\tilde{\mathcal{E}}^{\rm c}(\boldsymbol{u}^{\rm con})\boldsymbol{v}^{\rm c}, \boldsymbol{v}^{\rm c}\big\rangle \geq \gamma'_{\rm c}\|\nabla\boldsymbol{v}^{\rm c}\|^2_{L^2(\Omega_{\rm c})}. \tag{1.48}
$$

Proof. The proof uses ideas from [14, 31]. We employ Theorem 1.10 by linearizing $f = \delta\tilde{\mathcal{E}}^{\rm c}(\cdot)$ about $x_0 = \Pi_h\boldsymbol{u}^\infty$. Let $R^*_{\rm core}$ be as in Lemma 1.9. Then $\delta^2\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty)^{-1}$ exists and is bounded by $\gamma_{\rm c}^{-1}$ for all $R_{\rm core} \geq R^*_{\rm core}$. Moreover,

$\delta^2\tilde{\mathcal{E}}^{\rm c}$ is Lipschitz continous by Lemma 1.7. It remains to estimate the residual

$$\sup_{\boldsymbol{v}^{\rm c}\in\boldsymbol{\mathcal{U}}^{\rm c}_{h,0},\boldsymbol{v}^{\rm c}\neq\boldsymbol{0}} \frac{\langle\delta\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty),\boldsymbol{v}^{\rm c}\rangle}{\|\boldsymbol{v}^{\rm c}\|_{L^2(\Omega_{\rm c})}}. \tag{1.49}$$

This task requires an atomistic version of the stress. Following [31], let $\zeta(x)$ be the nodal basis function at 0 on the atomistic partition $\mathcal{T}_{\rm a}$, i.e., $\zeta(0)=1$ and $\zeta(\xi)=0$ for $0\neq\xi\in\mathbb{Z}^d$. This allows us to write the interpolant as $Iv(x)=\sum_{\xi\in\mathbb{Z}^d} v(\xi)\zeta(x-\xi)$. Further define the "quasi-interpolant," v^*, by

$$v^*(x) := (Iv*\zeta)(x),$$

and note that $v^*\in W^{3,\infty}_{\rm loc}$ [28,31]. Letting $\chi_{\xi,\rho}(x) := \int_0^1 \zeta(\xi+t\rho-x)\,dt$, the atomistic stress, $\mathsf{S}^{\rm a}(\boldsymbol{u},x)$, is then defined by

$$\int_{\mathbb{R}^d} \mathsf{S}^{\rm a}(\boldsymbol{u},x) : \nabla I\boldsymbol{v} := \langle\delta\mathcal{E}^{\rm a}(\boldsymbol{u}),\boldsymbol{v}^*\rangle = \int_{\mathbb{R}^d}\sum_{\xi\in\mathbb{Z}^d}\sum_{\rho\in\mathcal{R}}\chi_{\xi,\rho}V_{\xi,\rho}(D\boldsymbol{u})\otimes\rho : \nabla I\boldsymbol{v}. \tag{1.50}$$

See [14,31] for further details.

We now estimate the residual (1.49). Fix an element $\boldsymbol{v}^{\rm c}\in\boldsymbol{\mathcal{U}}^{\rm c}_{h,0}$, and assume it has been extended to all of $\mathbb{R}^d$. Let $\boldsymbol{w}^{\rm c}=S_{\rm a}\boldsymbol{v}^{\rm c}$ where $S_{\rm a}$ is the Scott-Zhang interpolant onto $\mathcal{T}_{\rm a}$. Note that $I\boldsymbol{w}^{\rm c}=IS_{\rm a}\boldsymbol{v}^{\rm c}=S_{\rm a}\boldsymbol{v}^{\rm c}$ for these choices.

We now subtract $0=\langle\delta\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty),\boldsymbol{w}^{{\rm c},*}\rangle$ from the numerator of (1.49):

$$\begin{aligned}
&\langle\delta\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty),\boldsymbol{v}^{\rm c}\rangle\\
&= \langle\delta\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty),\boldsymbol{v}^{\rm c}\rangle - \langle\delta\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty),\boldsymbol{w}^{{\rm c},*}\rangle\\
&= \langle\delta\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty)-\delta\tilde{\mathcal{E}}^{\rm c}(\tilde{I}\boldsymbol{u}^\infty),\boldsymbol{v}^{\rm c}\rangle + \langle\delta\tilde{\mathcal{E}}^{\rm c}(\tilde{I}\boldsymbol{u}^\infty),\boldsymbol{v}^{\rm c}-S_{\rm a}\boldsymbol{v}^{\rm c}\rangle + (\langle\delta\tilde{\mathcal{E}}^{\rm c}(\tilde{I}\boldsymbol{u}^\infty),S_{\rm a}\boldsymbol{v}^{\rm c}\rangle - \langle\delta\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty),\boldsymbol{w}^{{\rm c},*}\rangle)\\
&=: E_1+E_2+E_3.
\end{aligned}$$

In the above, we have used the notation $\langle\delta\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty),w\rangle := \int_{\Omega_{\rm c}} W'(\nabla\Pi_h\boldsymbol{u}^\infty):\nabla w$ for an arbitrary $w\in H^1(\Omega_{\rm c})$.

E_1 can be easily estimated:

$$\begin{aligned}
\langle\delta\tilde{\mathcal{E}}^{\rm c}(\Pi_h\boldsymbol{u}^\infty)-\delta\tilde{\mathcal{E}}^{\rm c}(\tilde{I}\boldsymbol{u}^\infty),\boldsymbol{v}^{\rm c}\rangle &\lesssim \|\nabla\Pi_h\boldsymbol{u}^\infty-\nabla\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)}\|\nabla\boldsymbol{v}^{\rm c}\|_{L^2(\Omega_c)}\\
&\lesssim (R_{\rm core}^{-d/2-1}+R_{\rm c}^{-d/2})\|\nabla\boldsymbol{v}^{\rm c}\|_{L^2(\Omega_c)} \quad \text{by Lemma 1.8.}
\end{aligned}$$

We estimate E_2 by integrating by parts

$$\begin{aligned}
\langle\delta\tilde{\mathcal{E}}^{\rm c}(\tilde{I}\boldsymbol{u}^\infty),\boldsymbol{v}^{\rm c}-S_{\rm a}\boldsymbol{v}^{\rm c}\rangle &= \int_{\Omega_{\rm c}} W'(\nabla\tilde{I}\boldsymbol{u}^\infty):\nabla(\boldsymbol{v}^{\rm c}-S_{\rm a}\boldsymbol{v}^{\rm c})\\
&= \int_{\Omega_{\rm c}} {\rm div}W'(\nabla\tilde{I}\boldsymbol{u}^\infty)\cdot(\boldsymbol{v}^{\rm c}-S_{\rm a}\boldsymbol{v}^{\rm c})\\
&\leq \|{\rm div}W'(\nabla\tilde{I}\boldsymbol{u}^\infty)\|_{L^2(\Omega_{\rm c})}\cdot\|\boldsymbol{v}^{\rm c}-S_{\rm a}\boldsymbol{v}^{\rm c}\|_{L^2(\Omega_{\rm c})}\\
&\lesssim \|\nabla^2\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})}\|\nabla\boldsymbol{v}^{\rm c}\|_{L^2(\Omega_{\rm c})},\\
&\lesssim R_{\rm core}^{-d/2-1}\|\nabla\boldsymbol{v}^{\rm c}\|_{L^2(\Omega_{\rm c})},
\end{aligned}$$

where we have used the chain rule, bounded the second derivatives of $\tilde{I}\boldsymbol{u}^\infty$ by $\|\nabla^2\tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_{\rm c})}$, utilized the interpolation estimate (4) for $S_{\rm a}$, and applied the decay rates of Theorem 1.4.

We estimate E_3 by observing

$$\begin{aligned}
E_3 &= \int_{\Omega_c} W'(\nabla \tilde{I}\boldsymbol{u}^\infty) : \nabla S_a \boldsymbol{v}^c - \int_{\Omega_c} \mathsf{S}^a(\boldsymbol{u}^\infty, x) : \nabla I \boldsymbol{w}^c \\
&= \int_{\Omega_c} \big(W'\big(\nabla \tilde{I}\boldsymbol{u}^\infty\big) - \mathsf{S}^a(\boldsymbol{u}^\infty, x)\big) : \nabla S_a \boldsymbol{v}^c. \\
&\le \|W'(\nabla \tilde{I}\boldsymbol{u}^\infty) - \mathsf{S}^a(\boldsymbol{u}^\infty, x)\|_{L^2(\Omega_c)} \|\nabla S_a \boldsymbol{v}^c\|_{L^2(\Omega_c)} \\
&\le \|W'(\nabla \tilde{I}\boldsymbol{u}^\infty) - \mathsf{S}^a(\boldsymbol{u}^\infty, x)\|_{L^2(\Omega_c)} \|\boldsymbol{v}^c\|_{L^2(\Omega_c)},
\end{aligned}$$

where in the last step we used the stability of the Scott-Zhang interpolant. One may then modify the arguments in [31, Lemma 4.5, Equations (4.22)–(4.24)] to prove that[6]

$$E_3 \lesssim \big(\|\nabla^3 \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} + \|\nabla^2 \tilde{I}\boldsymbol{u}^\infty\|^2_{L^4(\Omega_c)}\big)\|\boldsymbol{v}^c\|_{L^2(\Omega_c)},$$

and using the regularity theorem, Theorem 1.4, shows $E_3 \lesssim R_{\rm core}^{-d/2-2}\|\boldsymbol{v}^c\|_{L^2(\Omega_c)}$.

Combining the bounds on all E_i yields the residual estimate

$$\sup_{\boldsymbol{v}^c \in \boldsymbol{\mathcal{U}}_h^c, \boldsymbol{v}^c \neq \boldsymbol{0}} \frac{\langle \delta \tilde{\mathcal{E}}^c(\Pi_h \boldsymbol{u}^\infty), \boldsymbol{v}^c \rangle}{\|\boldsymbol{v}^c\|_{L^2(\Omega_c)}} \lesssim R_{\rm core}^{-d/2-1} + R_c^{-d/2}. \tag{1.51}$$

The stability result of Lemma 1.9 in conjunction with (1.51) and the inverse function theorem implies the existence of $\boldsymbol{u}^{\rm con}$ satisfying (1.46) and

$$\|\nabla \boldsymbol{u}^{\rm con} - \nabla \Pi_h \boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \lesssim R_{\rm core}^{-d/2-1} + R_c^{-d/2}. \tag{1.52}$$

Observe that

$$\|\nabla \boldsymbol{u}^{\rm con} - \nabla I \boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \le \|\nabla \boldsymbol{u}^{\rm con} - \nabla \Pi_h \boldsymbol{u}^\infty\|_{L^2(\Omega_c)} + \|\nabla \Pi_h \boldsymbol{u}^\infty - \nabla \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} + \|\nabla \tilde{I}\boldsymbol{u}^\infty - \nabla I \boldsymbol{u}^\infty\|_{L^2(\Omega_c)}$$

Hence, combining (1.52) and Lemma 1.8 yields

$$\|\nabla \boldsymbol{u}^{\rm con} - \nabla I \boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \lesssim R_{\rm core}^{-d/2-1} + R_c^{-d/2} + \|\nabla \tilde{I}\boldsymbol{u}^\infty - \nabla I \boldsymbol{u}^\infty\|_{L^2(\Omega_c)}.$$

Since $\tilde{I}$ is in H^2 and $I\boldsymbol{u}^\infty = I\tilde{I}\boldsymbol{u}^\infty$, standard finite element approximation theory and the decay estimates in Theorem 1.4 give

$$\|\nabla \tilde{I}\boldsymbol{u}^\infty - \nabla I \boldsymbol{u}^\infty\|_{L^2(\Omega_c)} = \|\nabla \tilde{I}\boldsymbol{u}^\infty - \nabla I \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \lesssim \|\nabla^2 \tilde{I}\boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \lesssim R_{\rm core}^{-d/2-1}.$$

The last inequalities imply the desired estimate (1.47).

To prove the inequality (1.48), note that

$$\begin{aligned}
\big\langle \delta^2 \tilde{\mathcal{E}}(\boldsymbol{u}^{\rm con})\boldsymbol{v}^c, \boldsymbol{v}^c \big\rangle &= \big\langle \big(\delta^2 \tilde{\mathcal{E}}(\boldsymbol{u}^{\rm con}) - \delta^2 \tilde{\mathcal{E}}(\Pi_h \boldsymbol{u}^\infty)\big)\boldsymbol{v}^c, \boldsymbol{v}^c \big\rangle + \big\langle \delta^2 \tilde{\mathcal{E}}(\Pi_h \boldsymbol{u}^\infty)\boldsymbol{v}^c, \boldsymbol{v}^c \big\rangle \\
&\gtrsim -\|\nabla \boldsymbol{u}^{\rm con} - \nabla \Pi_h \boldsymbol{u}^\infty\|_{L^2(\Omega_c)} \|\nabla v^c\|^2_{L^2(\Omega_c)} + \gamma_c \|\nabla v^c\|^2_{L^2(\Omega_c)} \\
&\gtrsim (\gamma_c - R_{\rm core}^{-d/2-1} + R_c^{-d/2})\|\nabla v^c\|^2_{L^2(\Omega_c)}.
\end{aligned}$$

□

[6]The difference is that our choice of $\tilde{I}u$ is not the same as the smooth interpolant used there.

1.3. **The AtC Coupled Problem**

We couple the restricted atomistic and continuum subproblems by minimizing the H^1 semi-norm of the difference between their solutions, i.e. our AtC formulation seeks an optimal solution $(u^{\rm a}, u^{\rm c}) \in \mathcal{U}^{\rm a} \times \mathcal{U}_h^{\rm c}$, $(\lambda_{\rm a}, \lambda_{\rm c}) \in \Lambda^a \times \Lambda^c$ of the constrained optimization problem:

$$\min_{\{u^{\rm a}, u^{\rm c}, \lambda^{\rm a}, \lambda^{\rm c}\}} \|\nabla I u^{\rm a} - \nabla u^{\rm c}\|_{L^2(\Omega_{\rm o})} \quad \text{subject to}$$
$$\begin{cases} \langle \delta\tilde{\mathcal{E}}^{\rm a}(u^{\rm a}), v^{\rm a}\rangle = 0 \quad \forall\, v^{\rm a} \in \mathcal{U}_0^{\rm a} \\ u^{\rm a} = \lambda_{\rm a} \quad \text{on}\, \partial_{\rm a}\mathcal{L}_{\rm a} \end{cases} ; \begin{cases} \langle \delta\tilde{\mathcal{E}}^{\rm c}(u^{\rm c}), v^{\rm c}\rangle = 0 \quad \forall\, v^{\rm c} \in \mathcal{U}_{h,0}^{\rm c} \\ u^{\rm c} = 0 \quad \text{on}\, \Gamma_{\rm c} \quad \text{and} \quad u^{\rm c} = \lambda_{\rm c} \quad \text{on}\, \Gamma_{\rm core} \end{cases} ; \int_{\Omega_{\rm o}} (Iu^{\rm a} - u^{\rm c})\, dx = 0 \tag{1.53}$$

Alternatively, we may pose the AtC problem on quotient spaces:

$$\min_{\{\boldsymbol{u}^{\rm a}, \boldsymbol{u}^{\rm c}, \lambda^{\rm a}, \lambda^{\rm c}\}} \|\nabla I \boldsymbol{u}^{\rm a} - \nabla \boldsymbol{u}^{\rm c}\|_{L^2(\Omega_{\rm o})} \quad \text{subject to}$$
$$\begin{cases} \langle \delta\tilde{\mathcal{E}}^{a}(\boldsymbol{u}^{\rm a}), \boldsymbol{v}^{\rm a}\rangle = 0 \quad \forall\, \boldsymbol{v}^{\rm a} \in \boldsymbol{\mathcal{U}}_0^{\rm a} \\ \boldsymbol{u}^{\rm a} = \lambda_{\rm a} \quad \text{on}\, \partial_{\rm a}\boldsymbol{\mathcal{L}}_{\rm a} \end{cases} , \quad \begin{cases} \langle \delta\tilde{\mathcal{E}}^{c}(\boldsymbol{u}^{\rm c}), \boldsymbol{v}^{\rm c}\rangle = 0 \quad \forall\, \boldsymbol{v}^{\rm c} \in \boldsymbol{\mathcal{U}}_{h,0}^{\rm c} \\ \boldsymbol{u}^{\rm c} = \lambda_{\rm c} \quad \text{on}\, \Gamma_{\rm core} \end{cases} \tag{1.54}$$

It is easy to see that (1.53) and (1.54) are equivalent in the sense that every minimizer $(u^{\rm a}, u^{\rm c})$ of the former generates an equivalence class $(\boldsymbol{u}^{\rm a}, \boldsymbol{u}^{\rm c})$ that is a minimizer of the latter and vice versa. Indeed, if $(u^{\rm a}, u^{\rm c})$ solves (1.53) then for all $(v^{\rm a}, v^{\rm c}) \in \mathcal{U}^{\rm a} \times \mathcal{U}_h^{\rm c}$,

$$\|\nabla I\boldsymbol{u}^{\rm a} - \nabla \boldsymbol{u}^{\rm c}\|_{L^2(\Omega_{\rm o})} = \|\nabla I u^{\rm a} - \nabla u^{\rm c}\|_{L^2(\Omega_{\rm o})} \le \|\nabla I v^{\rm a} - \nabla v^{\rm c}\|_{L^2(\Omega_{\rm o})} = \|\nabla I\boldsymbol{v}^{\rm a} - \nabla \boldsymbol{v}^{\rm c}\|_{L^2(\Omega_{\rm o})}.$$

Thus, $(\boldsymbol{u}^{\rm a}, \boldsymbol{u}^{\rm c})$ is a minimizer of (1.54). The reverse statement follows by the same argument.

Notwithstanding the equivalence of the two problems, (1.54) is more convenient for the analysis and so we will study the existence of AtC solutions $(\boldsymbol{u}_{\rm a}^{\rm atc}, \boldsymbol{u}_{\rm c}^{\rm atc})$ in quotient spaces. Our main result is as follows.

Theorem 1.12 (Existence and Error Estimate)**.** *Let* $\boldsymbol{u}_{\rm a}^\infty := \boldsymbol{u}^\infty|_{\mathcal{L}_{\rm a}}$ *and* $\boldsymbol{u}_{\rm c}^\infty := \boldsymbol{u}^\infty|_{\mathcal{L}_{\rm c}}$*. There exists* $R_{\rm core}^*$ *such that for all* $R_{\rm core} \ge R_{\rm core}^*$*, the minimization problem* (1.54) *has a solution* $(\boldsymbol{u}_{\rm a}^{\rm atc}, \boldsymbol{u}_{\rm c}^{\rm atc})$ *and*

$$\|\nabla\left(I\boldsymbol{u}_{\rm a}^{\rm atc} - I\boldsymbol{u}_{\rm a}^\infty\right)\|_{L^2(\Omega_{\rm a})}^2 + \|\nabla\left(\boldsymbol{u}_{\rm c}^{\rm atc} - I\boldsymbol{u}_{\rm c}^\infty\right)\|_{L^2(\Omega_{\rm c})}^2 \lesssim R_{\rm core}^{-d/2-1} + R_{\rm c}^{-d/2}. \tag{1.55}$$

We prove this result in the remainder of the paper.

2. Error Analysis

To carry out the analysis of the AtC problem we switch to an equivalent reduced space formulation of (1.54) and apply the inverse function theorem.

2.1. **Reduced space formulation of the AtC problem**

Given $\lambda_{\rm a} \in \boldsymbol{\Lambda}^{\bf a}$ and $\lambda_{\rm c} \in \boldsymbol{\Lambda}^{\bf c}$, there exist solutions of atomistic and continuum restricted problems (1.23) and (1.33) which we use to define mappings $\boldsymbol{U}^{\rm a} : \boldsymbol{\Lambda}^{\rm a} \to \boldsymbol{\mathcal{U}}^{\rm a}$, and $\boldsymbol{U}^{\rm c} : \boldsymbol{\Lambda}^{\rm c} \to \boldsymbol{\mathcal{U}}_h^{\rm c}$, respectively in Theorems 2.3 and 2.4. Using these mappings, we can eliminate the states from (1.54) and obtain an equivalent unconstrained minimization problem in terms of the virtual controls only:

$$\left(\lambda_{\rm a}^{\rm atc}, \lambda_{\rm c}^{\rm atc}\right) = \underset{(\lambda_{\rm a}, \lambda_{\rm c}) \in \boldsymbol{\Lambda}^{\rm a} \times \boldsymbol{\Lambda}^{\rm c}}{\arg\min}\; J(\lambda_{\rm a}, \lambda_{\rm c}), \tag{2.1}$$

where J is defined as

$$J\left(\lambda_{\rm a}, \lambda_{\rm c}\right) = \frac{1}{2}\|\nabla I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}) - \nabla \boldsymbol{U}^{\rm c}(\lambda_{\rm c})\|_{L^2(\Omega_{\rm o})}^2. \tag{2.2}$$

The Euler-Lagrange equation of (2.1) is given by

$$\langle \delta J(\lambda_{\rm a},\lambda_{\rm c}),(\mu_{\rm a},\mu_{\rm c})\rangle \;=\; 0, \quad \forall\,(\mu_{\rm a},\mu_{\rm c})\in \mathbf{\Lambda}^{\rm a}\times\mathbf{\Lambda}^{\rm c}, \tag{2.3}$$

and the first variation of J is

$$\langle \delta J(\lambda_{\rm a},\lambda_{\rm c}),(\mu_{\rm a},\mu_{\rm c})\rangle = \left(\nabla\left(\boldsymbol{I}\boldsymbol{U}^{\rm a}(\lambda_{\rm a})-\boldsymbol{U}^{\rm c}(\lambda_{\rm c})\right),\nabla\left(I\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a})[\mu_{\rm a}]-\delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c})[\mu_{\rm c}]\right)\right)_{L^2(\Omega_{\rm o})}. \tag{2.4}$$

In terms of the reduced problem, the AtC error (1.55) assumes the form

$$\|\nabla\left(\boldsymbol{I}\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\rm atc})-\boldsymbol{I}\boldsymbol{u}_{\rm a}^{\infty}\right)\|^2_{L^2(\Omega_{\rm a})}+\|\nabla\left(\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^{\rm atc})-\boldsymbol{I}\boldsymbol{u}_{\rm c}^{\infty}\right)\|^2_{L^2(\Omega_{\rm c})}. \tag{2.5}$$

Analysis of (2.5) requires several problem-dependent norms. Solutions of linearized problems on $\Omega_{\rm a}$ and $\Omega_{\rm c}$ define these norms. Let $\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\infty})[\cdot]:\mathbf{\Lambda^a}\to\mathcal{U}^{\rm a}$ be the solution to the linearized problem[7]

$$\begin{aligned}\left\langle \delta^2\tilde{\mathcal{E}}^a(\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\infty}))\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\infty})[\mu_{\rm a}],\boldsymbol{v}^{\rm a}\right\rangle &= 0 \quad \forall \boldsymbol{v}^{\rm a}\in\boldsymbol{\mathcal{U}}^{\rm a}_0,\\ \delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\infty})[\mu_{\rm a}] &= \mu_{\rm a} \quad \text{on}\,\partial_{\rm a}\mathcal{L}_{\rm a},\end{aligned} \tag{2.6}$$

and $\delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^{\infty})[\cdot]:\mathbf{\Lambda^c}\to\mathcal{U}^{\rm c}$ be the solution to a similar continuum linearized problem

$$\begin{aligned}\left\langle \delta^2\tilde{\mathcal{E}}^c(\boldsymbol{u}^{\rm con})\delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^{\infty})[\mu_{\rm c}],\boldsymbol{v}^{\rm c}\right\rangle &= 0 \quad \forall\,\boldsymbol{v}^{\rm c}\in\boldsymbol{\mathcal{U}}^{\rm c}_{h,0},\\ \delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^{\infty})[\mu_{\rm c}] &= \mu_{\rm c} \quad \text{on} \quad \Gamma_{\rm core}.\end{aligned} \tag{2.7}$$

It is easy to see that

$$\|\mu_{\rm a}\|_{\mathbf{\Lambda}^{\rm a}} := \|\nabla I\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\infty})[\mu_{\rm a}]\|_{L^2(\Omega_{\rm a})} \quad \text{and} \quad \|\mu_{\rm c}\|_{\mathbf{\Lambda}^{\rm c}} := \|\nabla\delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^{\infty})[\mu_{\rm c}]\|_{L^2(\Omega_{\rm c})},$$

define norms norms on $\mathbf{\Lambda}^{\rm a}$, and $\mathbf{\Lambda}^{\rm c}$, respectively, while their sum

$$\|(\mu_{\rm a},\mu_{\rm c})\|^2_{\rm err} := \;\|\mu_{\rm a}\|^2_{\mathbf{\Lambda}^{\rm a}}+\|\mu_{\rm c}\|^2_{\mathbf{\Lambda}^{\rm c}} \tag{2.8}$$

is a norm on $\mathbf{\Lambda}^{\rm a}\times\mathbf{\Lambda}^{\rm c}$. In Section 3 we shall prove

$$\|(\mu_{\rm a},\mu_{\rm c})\|_{\rm op} := \|\nabla\left(I\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\infty})[\mu_{\rm a}]-\delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^{\infty})[\mu_{\rm c}]\right)\|_{L^2(\Omega_{\rm o})} \tag{2.9}$$

is a norm equivalent to 2.8. We state this result below for further reference within this section.

Theorem 2.1 (Norm Equivalence)**.** *There exists $R^*_{\rm core}>0$ such that for all $R_{\rm core}\geq R^*_{\rm core}$,*

$$\|\cdot\|_{\rm op}\lesssim\;\|\cdot\|_{\rm err}\lesssim\;\|\cdot\|_{\rm op}. \tag{2.10}$$

2.2. The Inverse Function Theorem framework

We consider the first order optimality condition (2.3) for (2.1), and apply the inverse function theorem, Theorem 1.10, with $f=\delta J$ and $X=\mathbf{\Lambda}^{\rm a}\times\mathbf{\Lambda}^{\rm c}$ equipped with the $\|\cdot\|_{\rm op}$ norm. To apply the theorem, we must prove there exist L,η,σ such that

$$\sup_{(\lambda_{\rm a},\lambda_{\rm c})\text{ near }(\lambda_{\rm a}^{\infty},\lambda_{\rm c}^{\infty})}\|\delta^3J(\lambda_{\rm a},\lambda_{\rm c})\|\leq L\,,\quad \|\delta J(\lambda_{\rm a}^{\infty},\lambda_{\rm c}^{\infty})\|\leq\eta,\quad \text{and}\quad \|(\delta^2J(\lambda_{\rm a}^{\infty},\lambda_{\rm c}^{\infty}))^{-1}\|\leq\sigma.$$

[7]We show subsequently that $\boldsymbol{U}^{\rm a}$ is differentiable, and $\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^{\infty})[\cdot]$ is the Gateaux derivative of $\boldsymbol{U}^{\rm a}$ at $\lambda_{\rm a}^{\infty}$.

Each of these results requires differentiability of the functional J, which in turn requires differentiability of the functions $\boldsymbol{U}^{\mathrm{a}}$ and $\boldsymbol{U}^{\mathrm{c}}$. We prove the necessary differentiability results and boundedness of the third derivative of J in Section 2.2.1. The second result is a consistency error estimate and is proven in Section 2.2.2 while the final estimate is a stability result proven in Section 2.2.3.

2.2.1. *Regularity*

We use the following version of the implicit function theorem to obtain regularity results for $\boldsymbol{U}^{\mathrm{a}}$ and $\boldsymbol{U}^{\mathrm{c}}$. It can be obtained by adapting the proof of the implicit function theorem in [11] to Banach spaces and by tracking the constants involved.

Theorem 2.2 (Implicit Function Theorem)**.** *Let X, Y, and Z be Banach spaces with $U \subset X \times Y$ an open set. Let $f : X \times Y \to Z$ be continuously differentiable with $(x_0, y_0) \in U$ satisfying $f(x_0, y_0) = 0$. Suppose that $\delta_y f(x_0, y_0) : Y \to Z$ is a bounded, invertible linear transformation with $\left\|(\delta_y f(x_0, y_0))^{-1}\right\| =: \theta$. Also set $\phi := \|\delta_x f(x_0, y_0)\|$ and*

$$\sigma := \max\{1 + \theta\phi, \theta\}.$$

If there exists η such that

(1) $B_{2\eta\sigma}((x_0, y_0)) \subset U$
(2) $\|\delta f(x_1, y_1) - \delta f(x_2, y_2)\| \le \frac{1}{2\eta\sigma^2}\|(x_1, y_1) - (x_2, y_2)\|$ *for all* $(x_1, y_1), (x_2, y_2) \in B_{2\eta\sigma}((x_0, y_0))$,

then there is a unique continuously differentiable function $g : B_\eta(x_0) \to B_{2\eta\sigma}(y_0)$ such that $g(x_0) = y_0$ and $f(x, g(x)) = 0$ for all $x \in B_\eta(x_0)$. The derivative of g is

$$\delta g(x) = -\left[\delta_y f(x, g(x))^{-1}\right]\left[\delta_x f(x, g(x))\right].$$

Moreover, if f is C^k, then g is C^k, and derivatives of g can be bounded in terms of derivatives of f and $\delta_y f(x_0, g(x_0))^{-1}$.

Theorem 2.3 (Regularity of $\boldsymbol{U}^{\mathrm{a}}$)**.** *Under Assumptions C and D, there exists $R^*_{\mathrm{core}} > 0$ such that for all $R_{\mathrm{core}} \ge R^*_{\mathrm{core}}$, there exists a mapping $\boldsymbol{U}^{\mathrm{a}} : \boldsymbol{\Lambda}^{\mathbf{a}} \to \boldsymbol{\mathcal{U}}^{\mathrm{a}}$ such that $\boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}})$ solves (1.23) and which is C^3 on an open ball V centered at $\lambda^\infty_{\mathrm{a}}$ in $\boldsymbol{\Lambda}^{\mathrm{a}}$. The radius of V is independent of R_{core}, and the derivatives of $\boldsymbol{U}^{\mathrm{a}}$ are also bounded uniformly in $R_{\mathrm{core}} \ge R^*_{\mathrm{core}}$.*

Proof. We apply Theorem 2.2 with $X = \boldsymbol{\Lambda}^{\mathrm{a}}$, $Y = \boldsymbol{\mathcal{U}}^{\mathrm{a}}_0$, $Z = (\boldsymbol{\mathcal{U}}^{\mathrm{a}}_0)^*$, $U = X \times Y$, and

$$f(\lambda_{\mathrm{a}}, \boldsymbol{v}^{\mathrm{a}}) := \delta\tilde{\mathcal{E}}^{\mathrm{a}}\left(h(\lambda_{\mathrm{a}}, \boldsymbol{v}^{\mathrm{a}})\right),$$

where h is an auxiliary function $X \times Y \to \boldsymbol{\mathcal{U}}^{\mathrm{a}}$ defined by (recall $\delta\boldsymbol{U}^{a}(\lambda^\infty_{\mathrm{a}})[\mu^{\mathrm{a}}]$ solves (2.6))

$$h(\lambda_{\mathrm{a}}, \boldsymbol{v}^{\mathrm{a}}) = \boldsymbol{v}^{\mathrm{a}} + \boldsymbol{u}^\infty_{\mathrm{a}} + \delta\boldsymbol{U}^{\mathrm{a}}(\lambda^\infty_{\mathrm{a}})\left[\lambda_{\mathrm{a}} - \lambda^\infty_{\mathrm{a}}\right].$$

Because h is affine, f is C^k provided that $\tilde{\mathcal{E}}^{\mathrm{a}}$ is C^{k+1} on $\boldsymbol{\mathcal{U}}^{\mathrm{a}}$. Hence, Theorem 1.6 implies f is C^3. For the point (x_0, y_0), we take the point $(\lambda^\infty_{\mathrm{a}}, \boldsymbol{0})$ so that $h(x_0, y_0) = \boldsymbol{u}^\infty_{\mathrm{a}}$. The chain rule shows

$$\delta_y f(x_0, y_0) = \delta^2\tilde{\mathcal{E}}^{\mathrm{a}}\left(h(x_0, y_0)\right) \circ \delta_y h(x_0, y_0).$$

In conjunction with $\delta_y h(x_0, y_0)[\boldsymbol{v}^{\mathrm{a}}] = \boldsymbol{v}^{\mathrm{a}}$, it follows that $\delta_y f(x_0, y_0) : Y \to Z$ is given by

$$\langle \delta_y f(x_0, y_0)\boldsymbol{v}^{\mathrm{a}}, \boldsymbol{w}^{\mathrm{a}}\rangle = \langle \delta^2\tilde{\mathcal{E}}^{\mathrm{a}}\left(\boldsymbol{u}^\infty_{\mathrm{a}}\right)\boldsymbol{v}^{\mathrm{a}}, \boldsymbol{w}^{\mathrm{a}}\rangle.$$

Since both $\boldsymbol{v}^{\mathrm{a}}$ and $\boldsymbol{w}^{\mathrm{a}}$ are elements of $\boldsymbol{\mathcal{U}}^{\mathrm{a}}_0$ they can be extended by a constant to all of $\mathbb{Z}^d$ while keeping the norm of their gradient the same. Then using Assumption D, we find

$$\langle \delta_y f(x_0, y_0)\boldsymbol{v}^{\mathrm{a}}, \boldsymbol{v}^{\mathrm{a}}\rangle = \langle \delta^2\tilde{\mathcal{E}}^{\mathrm{a}}\left(\boldsymbol{u}^\infty_{\mathrm{a}}\right)\boldsymbol{v}^{\mathrm{a}}, \boldsymbol{v}^{\mathrm{a}}\rangle = \langle \delta^2\mathcal{E}^{\mathrm{a}}\left(\boldsymbol{u}^\infty\right)\boldsymbol{v}^{\mathrm{a}}, \boldsymbol{v}^{\mathrm{a}}\rangle \ge \gamma_{\mathrm{a}}\|\nabla I\boldsymbol{v}^{\mathrm{a}}\|^2_{L^2(\mathbb{R}^d)} = \gamma_{\mathrm{a}}\|\nabla I\boldsymbol{v}^{\mathrm{a}}\|^2_{L^2(\Omega_{\mathrm{a}})}.$$

This shows $\delta_y f(x_0, y_0)$ is coercive, and consequently that $\delta_y f(x_0, y_0)^{-1}$ exists with norm bounded by $\theta := \gamma_{\mathrm{a}}$. Using again the chain rule, we obtain

$$\delta_x f(x_0, y_0) = \delta^2 \tilde{\mathcal{E}}^{\mathrm{a}} \left(h\left(x_0, y_0\right)\right) \circ \delta_x h\left(x_0, y_0\right) = 0$$

so that $\phi = \|\delta_x f(x_0, y_0)\| = 0$.

Next, observe that h is Lipschitz on its entire domain with Lipschitz constant 1, and $\delta^2 \tilde{\mathcal{E}}^{\mathrm{a}}$ is Lipschitz with some Lipschitz constant M, as guaranteed by Theorem 1.6. As a result, δf is Lipschitz with Lipschitz constant M. Now we may choose η small enough so that $\frac{1}{2\eta\sigma^2} \leq M$, which means both conditions (1) and (2) in the statement of implicit function theorem are fulfilled. This allows us to deduce the existence of an implicit function $g : B_\eta(\lambda_{\mathrm{a}}^\infty) \to B_{2\eta\sigma}(\mathbf{0})$, which we use to define a mapping $\boldsymbol{U}^{\mathrm{a}}$ via

$$\boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}) = h\left(\lambda_{\mathrm{a}}, g(\lambda_{\mathrm{a}})\right) = g(\lambda_{\mathrm{a}}) + \boldsymbol{u}^\infty + \delta \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^\infty)\left[\lambda_{\mathrm{a}} - \lambda^\infty\right].$$

Since f is C^3, the implicit function theorem ensures g is also C^3. Thus $\boldsymbol{U}^{\mathrm{a}}$ is C^3. The radius of V is η, which is clearly independent of R_{core}, and the uniform bounds on the derivatives of $\boldsymbol{U}^{\mathrm{a}}$ follow by noting derivatives of f correspond to derivatives of the restricted atomistic energy (which is uniformly bounded by Theorem 1.6) and using the final remark in the statement of the implicit function theorem. □

We note that the Gateaux derivative, $\delta \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}})[\mu_{\mathrm{a}}]$, of $\boldsymbol{U}^{\mathrm{a}}$ at λ_{a} in the direction of μ_{a} solves the problem

$$\begin{aligned} \langle \delta^2 \tilde{\mathcal{E}}^a(\boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}))\delta \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}})[\mu_{\mathrm{a}}], \boldsymbol{v}^{\mathrm{a}}\rangle = 0 \quad \forall\, \boldsymbol{v}^{\mathrm{a}} \in \boldsymbol{\mathcal{U}}_0^{\mathrm{a}}, \\ \delta \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}})[\mu_{\mathrm{a}}] = \mu_{\mathrm{a}} \quad \text{on} \quad \partial_{\mathrm{a}}\mathcal{L}_{\mathrm{a}}, \end{aligned} \tag{2.11}$$

thus justifying our usage of notation in the proof.

With only minor modifications, the proof of Theorem 2.3 can be adapted to establish the regularity of $\boldsymbol{U}^{\mathrm{c}}$.

Theorem 2.4 (Regularity of $\boldsymbol{U}^{\mathrm{c}}$)**.** *There exists $R_{\mathrm{core}}^* > 0$ such that for all $R_{\mathrm{core}} \geq R_{\mathrm{core}}^*$, there exists a mapping $\boldsymbol{U}^{\mathrm{c}} : \boldsymbol{\Lambda}^{\mathbf{c}} \to \boldsymbol{\mathcal{U}}^{\mathrm{c}}$ such that $\boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}})$ solves 1.33 and which is C^3 on an open ball V centered at $\lambda_{\mathrm{c}}^\infty$ in $\boldsymbol{\Lambda}^{\mathrm{c}}$. The derivatives of $\boldsymbol{U}^{\mathrm{c}}$ are bounded uniformly in R_{core}, and the radius of V is independent of R_{core}.*

Combining the above results we obtain an upper bound on Hessian of the atomistic mapping

$$\|\delta^2 \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^\infty)[\mu_{\mathrm{a}}, \nu_{\mathrm{a}}]\|_{\boldsymbol{\mathcal{U}}^{\mathrm{a}}} \lesssim \|\mu_{\mathrm{a}}\|_{\boldsymbol{\Lambda}^{\mathrm{a}}} \cdot \|\nu_{\mathrm{a}}\|_{\boldsymbol{\Lambda}^{\mathrm{a}}}, \tag{2.12}$$

and a similar bound for the Hessian of the continuum mapping

$$\|\delta^2 \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^\infty)[\mu_{\mathrm{c}}, \nu_{\mathrm{c}}]\|_{\boldsymbol{\mathcal{U}}^{\mathrm{c}}} \lesssim \|\mu_{\mathrm{c}}\|_{\boldsymbol{\Lambda}^{\mathrm{c}}} \cdot \|\nu_{\mathrm{c}}\|_{\boldsymbol{\Lambda}^{\mathrm{c}}}. \tag{2.13}$$

The proof of Theorem 1.12 relies on a stability result that enables the application of the inverse function theorem. This stability result requires the following auxiliary lemma.

Lemma 2.5. *There exists R_{core}^* such that for all $R_{\mathrm{core}} \geq R_{\mathrm{core}}^*$ and all $\mu_{\mathrm{a}}, \nu_{\mathrm{a}} \in \boldsymbol{\Lambda}^{\mathrm{a}}$ and all $\mu_{\mathrm{c}}, \nu_{\mathrm{c}} \in \boldsymbol{\Lambda}^{\mathrm{c}}$,*

$$\|\nabla \left(I\delta^2 \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^\infty)[\mu_{\mathrm{a}}, \nu_{\mathrm{a}}] - \delta^2 \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^\infty)[\mu_{\mathrm{c}}, \nu_{\mathrm{c}}]\right)\|_{L^2(\Omega_{\mathrm{o}})} \lesssim \|(\mu_{\mathrm{a}}, \mu_{\mathrm{c}})\|_{\mathrm{op}} \cdot \|(\nu_{\mathrm{a}}, \nu_{\mathrm{c}})\|_{\mathrm{op}}. \tag{2.14}$$

Proof. The triangle inequality implies

$$\|\nabla \left(I\delta^2 \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^\infty)[\mu_{\mathrm{a}}, \nu_{\mathrm{a}}] - \delta^2 \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^\infty)[\mu_{\mathrm{c}}, \nu_{\mathrm{c}}]\right)\|_{L^2(\Omega_{\mathrm{o}})} \leq \|\nabla I\delta^2 \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^\infty)[\mu_{\mathrm{a}}, \nu_{\mathrm{a}}]\|_{L^2(\Omega_{\mathrm{a}})} + \|\nabla \delta^2 \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^\infty)[\mu_{\mathrm{c}}, \nu_{\mathrm{c}}]\|_{L^2(\Omega_{\mathrm{c}})}.$$

We then utilize (2.12)–(2.13) to bound the right hand side and apply the norm equivalence theorem, Theorem 2.1, to obtain

$$\begin{aligned} \|\nabla\left(I\delta^2\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a},\nu_{\rm a}]-\delta^2\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c},\nu_{\rm c}]\right)\| &\lesssim \|\mu_{\rm a}\|_{\boldsymbol{\Lambda}^{\rm a}}\cdot\|\nu_{\rm a}\|_{\boldsymbol{\Lambda}^{\rm a}}+\|\mu_{\rm c}\|_{\boldsymbol{\Lambda}^{\rm c}}\cdot\|\nu_{\rm c}\|_{\boldsymbol{\Lambda}^{\rm c}} \\ &\leq \left(\|\mu_{\rm a}\|_{\boldsymbol{\Lambda}^{\rm a}}+\|\mu_{\rm c}\|_{\boldsymbol{\Lambda}^{\rm c}}\right)\left(\|\nu_{\rm a}\|_{\boldsymbol{\Lambda}^{\rm a}}+\|\nu_{\rm c}\|_{\boldsymbol{\Lambda}^{\rm c}}\right) \\ &\lesssim \|(\mu_{\rm a},\mu_{\rm c})\|_{\rm op}\cdot\|(\mu_{\rm a},\mu_{\rm c})\|_{\rm op}. \end{aligned} \tag{2.15}$$

□

We proceed to establish regularity of the reduced space functional J.

Theorem 2.6 (Regularity of J)**.** *Let $V^{\rm a}$ and $V^{\rm c}$ be the neighborhoods of $\lambda_{\rm a}^\infty$ and $\lambda_{\rm c}^\infty$ in $\boldsymbol{\Lambda}_{\rm a}$ and $\boldsymbol{\Lambda}_{\rm c}$ on which $\boldsymbol{U}^{\rm a}$ and $\boldsymbol{U}^{\rm c}$ are C^3. Then J is C^3 on $V^{\rm a}\times V^{\rm c}$ and its $\ell^{\rm th}$ derivatives can be bounded by derivatives of $\boldsymbol{U}^{\rm a}$ and $\boldsymbol{U}^{\rm c}$ of order at most ℓ.*

Proof. Theorems 2.3–2.4 guarantee that $\boldsymbol{U}^{\rm a}$ and $\boldsymbol{U}^{\rm c}$ are C^3 on $V^{\rm a}$ and $V^{\rm c}$. Moreover, the interpolant I is a linear operator so $\lambda^{\rm a}\mapsto I\boldsymbol{U}^{\rm a}(\lambda^{\rm a})$ will also be C^3 on $V^{\rm a}$. The assertion of the theorem then follows from the fact that $J=\|\nabla I\boldsymbol{U}^{\rm a}(\lambda_{\rm a})-\nabla\boldsymbol{U}^{\rm c}(\lambda_{\rm c})\|^2_{L^2(\Omega_{\rm o})}$ is a composition of a quadratic form and the C^3 functions $I\boldsymbol{U}^{\rm a}(\lambda^{\rm a})$ and $\boldsymbol{U}^{\rm c}(\lambda^{\rm c})$. □

2.2.2. *Consistency*

The consistency error measures by how much $\boldsymbol{u}^\infty$ fails to satisfy the approximate problem, which in this case is the reduced space formulation (2.1). Thus, we seek an upper bound for

$$\|\delta J(\lambda_{\rm a}^\infty,\lambda_{\rm c}^\infty)\|_{\rm op} = \sup_{\|(\mu_{\rm a},\mu_{\rm c})\|_{\rm op}=1}\left|\left(\nabla\left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)-\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right),\nabla\left(I\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}]-\delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}]\right)\right)_{L^2(\Omega_{\rm o})}\right|. \tag{2.16}$$

Theorem 2.7 (Consistency Error)**.** *There exists $R^*_{\rm core}>0$ such that for all $R_{\rm core}\geq R^*_{\rm core}$, we have*

$$\|\delta J(\lambda_{\rm a}^\infty,\lambda_{\rm c}^\infty)\|_{\rm op}\lesssim R_{\rm core}^{-d/2-1}+R_{\rm c}^{-d/2}. \tag{2.17}$$

Proof. Applying the Cauchy-Schwarz inequality to (2.16) yeields

$$\begin{aligned} &\|\delta J(\lambda_{\rm a}^\infty,\lambda_{\rm c}^\infty)\|_{\rm op} \\ &\quad\leq \sup_{\|(\mu_{\rm a},\mu_{\rm c})\|_{\rm op}=1}\|\nabla\left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)-\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})}\|\nabla\left(I\delta\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}]-\delta\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}]\right)\|_{L^2(\Omega_{\rm o})}. \\ &\quad= \|\nabla\left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)-\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})}. \end{aligned} \tag{2.18}$$

Note that $\lambda_{\rm a}^\infty$ and $\lambda_{\rm c}^\infty$ are traces of the exact atomistic solution and so,

$$\|\nabla\left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)-\boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})}=\|\nabla I\boldsymbol{u}_{\rm a}^\infty-\nabla\boldsymbol{u}^{\rm con}\|_{L^2(\Omega_{\rm o})}$$

is the simply the continuum error made by replacing the atomistic model with the continuum model on $\Omega_{\rm o}$. Thus, (2.17) follows directly from (1.47) in Theorem 1.11. □

2.2.3. *Stability*

In this section we prove that the bilinear form $\langle\delta^2 J(\lambda_{\rm a}^\infty,\lambda_{\rm c}^\infty)\cdot,\cdot\rangle$ is coercive.

Theorem 2.8. *There exists $R^*_{\rm core}$ such that for each $R_{\rm core}\geq R^*_{\rm core}$*

$$\langle\delta^2 J(\lambda_{\rm a}^\infty,\lambda_{\rm c}^\infty)(\mu_{\rm a},\mu_{\rm c}),(\mu_{\rm a},\mu_{\rm c})\rangle\geq\ \tfrac{1}{2}\|(\mu_{\rm a},\mu_{\rm c})\|^2_{\rm op},\quad\forall\,(\mu_{\rm a},\mu_{\rm c})\in\boldsymbol{\Lambda}^{\rm a}\times\boldsymbol{\Lambda}^{\rm c}. \tag{2.19}$$

Proof. The Hessian of J is given by

$$\begin{aligned}\langle \delta^2 J(\lambda_{\rm a}^\infty, \lambda_{\rm c}^\infty)(\mu_{\rm a}, \mu_{\rm c}), (\mu_{\rm a}, \mu_{\rm c})\rangle = \ & \|\nabla \left(I\delta \boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}] - \delta \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}]\right)\|_{L^2(\Omega_{\rm o})}^2 \\ + \left(\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right), \nabla \left(I\delta^2 \boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}, \mu_{\rm a}] - \delta^2 \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}, \mu_{\rm c}]\right)\right)_{L^2(\Omega_{\rm o})}. \end{aligned} \tag{2.20}$$

Using the definition of $\|\cdot\|_{\rm op}$, this is equivalent to

$$\begin{aligned}&\langle \delta^2 J(\lambda_{\rm a}^\infty, \lambda_{\rm c}^\infty)(\mu_{\rm a}, \mu_{\rm c}), (\mu_{\rm a}, \mu_{\rm c})\rangle = \\ &\quad \|(\mu_{\rm a}, \mu_{\rm c})\|_{\rm op}^2 + \left(\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right), \nabla \left(I\delta^2 \boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}, \mu_{\rm a}] - \delta^2 \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}, \mu_{\rm c}]\right)\right)_{L^2(\Omega_{\rm o})}. \end{aligned} \tag{2.21}$$

Lemma 2.5 implies the existence of $R_{\rm core}^{*,1}$ and $C_{\rm stab}$ such that for all $R_{\rm core} \geq R_{\rm core}^{*,1}$,

$$\|\nabla \left(I\delta^2 \boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}, \mu_{\rm a}] - \delta^2 \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}, \mu_{\rm c}]\right)\|_{L^2(\Omega_{\rm o})} \leq \ C_{\rm stab}\|(\mu_{\rm a}, \mu_{\rm c})\|_{\rm op}^2. \tag{2.22}$$

We then have that

$$\begin{aligned}&\left(\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right), \nabla \left(I\delta^2 \boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}, \mu_{\rm a}] - \delta^2 \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}, \mu_{\rm c}]\right)\right)_{L^2(\Omega_{\rm o})} \\ &\quad \geq \ -\|\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})} \cdot \|\nabla \left(I\delta^2 \boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty)[\mu_{\rm a}, \mu_{\rm a}] - \delta^2 \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)[\mu_{\rm c}, \mu_{\rm c}]\right)\|_{L^2(\Omega_{\rm o})} \\ &\quad \geq \ -C_{\rm stab}\|\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})} \cdot \|(\mu_{\rm a}, \mu_{\rm c})\|_{\rm op}^2. \end{aligned}$$

This implies

$$\begin{aligned}\langle \delta^2 J(\lambda_{\rm a}^\infty, \lambda_{\rm c}^\infty)(\mu_{\rm a}, \mu_{\rm c}), (\mu_{\rm a}, \mu_{\rm c})\rangle &\geq \ \|(\mu_{\rm a}, \mu_{\rm c})\|_{\rm op}^2 - C_{\rm stab}\|\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})} \cdot \|(\mu_{\rm a}, \mu_{\rm c})\|_{\rm op}^2 \\ &= \ \left(1 - C_{\rm stab}\|\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})}\right)\|(\mu_{\rm a}, \mu_{\rm c})\|_{\rm op}^2, \end{aligned}$$

where $\|\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})}$ is the continuum error. By Theorem 1.11, there exists $R_{\rm core}^{*,2}$ such that for all $R_{\rm core} \geq R_{\rm core}^{*,2}$,

$$\left(1 - C_{\rm stab}\|\nabla \left(I\boldsymbol{U}^{\rm a}(\lambda_{\rm a}^\infty) - \boldsymbol{U}^{\rm c}(\lambda_{\rm c}^\infty)\right)\|_{L^2(\Omega_{\rm o})}\right) \geq 1/2.$$

Taking $R_{\rm core}^* = \max\left\{R_{\rm core}^{*,1}, R_{\rm core}^{*,2}\right\}$ completes the proof. □

2.2.4. *Error Estimate*

Having proven regularity of J, a consistency estimate, and a stability result, we are now in a position to prove our main error result, Theorem 1.12. This will be a consequence of following theorem providing important information about the AtC formulation.

Theorem 2.9. *There exists $R_{\rm core}^* > 0$ such that for all $R_{\rm core} \geq R_{\rm core}^*$, the reduced space problem* (2.1) *has a solution $(\lambda_{\rm a}^{\rm atc}, \lambda_{\rm c}^{\rm atc})$, such that*

$$\|(\lambda_{\rm a}^\infty, \lambda_{\rm c}^\infty) - (\lambda_{\rm a}^{\rm atc}, \lambda_{\rm c}^{\rm atc})\|_{\rm op} \lesssim \ R_{\rm core}^{-d/2-1} + R_{\rm c}^{-d/2}. \tag{2.23}$$

Proof. We apply the inverse function theorem, Theorem 1.10, with $f = \delta J$, $X = \boldsymbol{\Lambda}^{\rm a} \times \boldsymbol{\Lambda}^{\rm c}$ endowed with the norm $\|\cdot\|_{\rm op}$, $Y = (\boldsymbol{\Lambda}^{\rm a} \times \boldsymbol{\Lambda}^{\rm c})^*$ endowed with the dual norm $\|\cdot\|_{{\rm op}^*}$, and $x_0 = (\lambda_{\rm a}^\infty, \lambda_{\rm c}^\infty)$. Let $R_{\rm core}^*$ be the maximum of the $R_{\rm core}^*$ guaranteed to exist in Theorems 2.3, 2.4, 2.7 and, 2.8. Noting that $\|f(x_0)\|_{{\rm op}^*}$ is the consistency error defined in Section 2.2.2, Theorem 2.7, implies the bound

$$\|f(x_0)\|_{{\rm op}^*} \lesssim R_{\rm core}^{-d/2-1} + R_{\rm c}^{-d/2} =: \eta.$$

Observe also that $\delta f(x_0) = \delta^2 J(\lambda_{\rm a}^\infty, \lambda_{\rm c}^\infty)$ and the existence of a coercivity constant, $\sigma := 1/2$, from Section 2.2.3 implies $\|\delta f(x_0)^{-1}\| < \sigma^{-1} = 2$.

Furthermore, Theorems 2.3 and 2.4 provide constants η_{a} and η_{c} such that $\boldsymbol{U}^{\mathrm{a}}$ and $\boldsymbol{U}^{\mathrm{c}}$ are C^3 on $B_{\eta_{\mathrm{a}}}(\lambda_{\mathrm{a}}^{\infty})$ and $B_{\eta_{\mathrm{c}}}(\lambda_{\mathrm{c}}^{\infty})$ respectively. By Theorem 2.6, $\delta^3 J$ is bounded by derivatives of $\boldsymbol{U}^{\mathrm{a}}$ and $\boldsymbol{U}^{\mathrm{c}}$ of order at most 3. Furthermore, Theorems 2.3 and 2.4 state that derivatives of $\boldsymbol{U}^{\mathrm{a}}$ and $\boldsymbol{U}^{\mathrm{c}}$ are uniformly bounded in R_{core}. We may therefore conclude that the third derivative of J is also uniformly bounded in R_{core}. This implies $\delta f = \delta^2 J$ is Lipschitz on $B_{\eta_{\mathrm{a}}}(\lambda_{\mathrm{a}}^{\infty}) \times B_{\eta_{\mathrm{c}}}(\lambda_{\mathrm{c}}^{\infty})$ with a Lipschitz constant that we denote by L.

The bound $2L\eta(2)^2 < 1$ holds since the consistency error η may be made small for R_{core}^* large enough. Analogously, $B_{4\eta}(\lambda_{\mathrm{a}}^{\infty}, \lambda_{\mathrm{c}}^{\infty}) \subset B_{\eta_{\mathrm{a}}}(\lambda_{\mathrm{a}}^{\infty}) \times B_{\eta_{\mathrm{c}}}(\lambda_{\mathrm{c}}^{\infty})$ for small enough η. Theorem 1.10, can now be invoked to deduce the existence of a minimizer, $(\lambda_{\mathrm{a}}^{\mathrm{atc}}, \lambda_{\mathrm{c}}^{\mathrm{atc}}) \in B_{4\eta}(\lambda_{\mathrm{a}}^{\infty}, \lambda_{\mathrm{c}}^{\infty})$ of J, satisfying the stated bounds (2.23). ◻

We now provide a proof of Theorem 1.12, which is our main result.

Proof of Theorem 1.12. Let R_{core}^* be the maximum of the R_{core}^* from Theorem 2.9 and Theorem 2.1 so there exists $(\lambda_{\mathrm{a}}^{\mathrm{atc}}, \lambda_{\mathrm{c}}^{\mathrm{atc}})$ satisfying (2.23). Furthermore, $(\boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^{\mathrm{atc}}), \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\mathrm{atc}}))$ solve the minimization problem (1.54). Hence,

$$\begin{aligned}
&\|\nabla\left(I\boldsymbol{u}_{\mathrm{a}}^{\infty} - I\boldsymbol{u}_{\mathrm{a}}^{\mathrm{atc}}\right)\|_{L^2(\Omega_{\mathrm{a}})}^2 + \|\nabla\left(I\boldsymbol{u}_{\mathrm{c}}^{\infty} - \boldsymbol{u}_{\mathrm{c}}^{\mathrm{atc}}\right)\|_{L^2(\Omega_{\mathrm{c}})}^2 \\
&= \|\nabla I\left(\boldsymbol{u}^{\infty} - \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^{\mathrm{atc}})\right)\|_{L^2(\Omega_{\mathrm{a}})}^2 + \|\nabla\left(I\boldsymbol{u}^{\infty} - \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\mathrm{atc}})\right)\|_{L^2(\Omega_{\mathrm{c}})}^2 \\
&= \|\nabla\left(\boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^{\infty}) - \boldsymbol{U}^{\mathrm{a}}(\lambda_{a}^{\mathrm{atc}})\right)\|_{L^2(\Omega_{\mathrm{a}})}^2 + \|\nabla\left(I\boldsymbol{u}^{\infty} - \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\infty}) + \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\infty}) - \boldsymbol{U}^{\mathrm{c}}(\lambda_{c}^{\mathrm{atc}})\right)\|_{L^2(\Omega_{\mathrm{c}})}^2 \\
&\leq \|\nabla I\left(\boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^{\infty}) - \boldsymbol{U}^{\mathrm{a}}(\lambda_{\mathrm{a}}^{\mathrm{atc}})\right)\|_{L^2(\Omega_{\mathrm{a}})}^2 + \|\nabla\left(I\boldsymbol{u}^{\infty} - \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\infty})\right)\|_{L^2(\Omega_{\mathrm{c}})}^2 + \|\nabla\left(\boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\infty}) - \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\mathrm{atc}})\right)\|_{L^2(\Omega_{\mathrm{c}})}^2
\end{aligned} \tag{2.24}$$

The second term above is the continuum error. To handle the remaining terms we recall that $\boldsymbol{U}^{\mathrm{a}}$ and $\boldsymbol{U}^{\mathrm{c}}$ are Lipschitz on $B_{\eta_{\mathrm{a}}}(\lambda_{\mathrm{a}}^{\infty})$ and $B_{\eta_{\mathrm{c}}}(\lambda_{\mathrm{c}}^{\infty})$ by virtue of $\delta\boldsymbol{U}^{\mathrm{a}}$ and $\delta\boldsymbol{U}^{\mathrm{c}}$ being uniformly bounded on these sets. Then, using norm-equivalence (2.10), Theorem 1.11 and Theorem 2.9 yields

$$\begin{aligned}
&\|\nabla\left(I\boldsymbol{u}^{\infty} - I\boldsymbol{u}_{\mathrm{a}}^{\mathrm{atc}}\right)\|_{L^2(\Omega_{\mathrm{a}})}^2 + \|\nabla\left(I\boldsymbol{u}^{\infty} - \boldsymbol{u}_{\mathrm{c}}^{\mathrm{atc}}\right)\|_{L^2(\Omega_{\mathrm{c}})}^2 \\
&\lesssim \|\lambda_{\mathrm{a}}^{\infty} - \lambda_{\mathrm{a}}^{\mathrm{atc}}\|_{\boldsymbol{\Lambda}^{\mathrm{a}}}^2 + \|\nabla\left(I\boldsymbol{u}^{\infty} - \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\infty})\right)\|_{L^2(\Omega_{\mathrm{c}})}^2 + \|\lambda_{\mathrm{c}}^{\infty} - \lambda_{\mathrm{c}}^{\mathrm{atc}}\|_{\boldsymbol{\Lambda}^{\mathrm{c}}}^2 \\
&= \|(\lambda_{\mathrm{a}}^{\infty}, \lambda_{\mathrm{c}}^{\infty}) - (\lambda_{\mathrm{a}}^{\mathrm{atc}}, \lambda_{\mathrm{c}}^{\mathrm{atc}})\|_{\mathrm{err}}^2 + \|\nabla\left(I\boldsymbol{u}^{\infty} - \boldsymbol{U}^{\mathrm{c}}(\lambda_{\mathrm{c}}^{\infty})\right)\|_{L^2(\Omega_{\mathrm{c}})}^2 \lesssim R_{\mathrm{core}}^{-d-2} + R_{\mathrm{c}}^{-d}.
\end{aligned} \tag{2.25}$$

Taking square roots completes the proof. ◻

3. Norm Equivalence

The main result of this section is the norm equivalence result stated in Theorem 2.1. We recall that the finite element mesh $\mathcal{T}_h$ is subject to a minimum angle condition for some $\beta > 0$.

Theorem 3.1. *There exists $C, R_{\mathrm{core}}^* > 0$ such that for all domains $\Omega_{\mathrm{a}}, \Omega_{\mathrm{c}}$ and meshes $\mathcal{T}_h$ constructed according to the guidelines of Section 1.2 (in particular $\psi_{\mathrm{a}} R_{\mathrm{core}} = R_{\mathrm{a}}$) with $R_{\mathrm{core}} \geq R_{\mathrm{core}}^*$, there holds*

$$\|(\mu_{\mathrm{a}}, \mu_{\mathrm{c}})\|_{\mathrm{err}} \leq C\|(\mu_{\mathrm{a}}, \mu_{\mathrm{c}})\|_{\mathrm{op}} \quad \forall(\mu_{\mathrm{a}}, \mu_{\mathrm{c}}) \in \boldsymbol{\Lambda}^{\mathrm{a}} \times \boldsymbol{\Lambda}^{\mathrm{c}}. \tag{3.1}$$

Equivalently, for all $(\boldsymbol{w}^{\mathrm{a}}, \boldsymbol{w}^{\mathrm{c}}) \in \boldsymbol{\mathcal{U}}^{\mathrm{a}} \times \boldsymbol{\mathcal{U}}_h^{\mathrm{c}}$ such that

$$\langle \delta^2 \tilde{\mathcal{E}}^a(\boldsymbol{u}_{\mathrm{a}}^{\infty})\boldsymbol{w}^{\mathrm{a}}, \boldsymbol{v}^{\mathrm{a}}\rangle = 0 \quad \forall\, \boldsymbol{v}^{\mathrm{a}} \in \boldsymbol{\mathcal{U}}_0^{\mathrm{a}} \qquad \textit{and} \tag{3.2}$$

$$\langle \delta^2 \tilde{\mathcal{E}}^c(\boldsymbol{u}^{\mathrm{con}})\boldsymbol{w}^{\mathrm{c}}, \boldsymbol{v}^{\mathrm{c}}\rangle = 0 \quad \forall\, \boldsymbol{v}^{\mathrm{c}} \in \boldsymbol{\mathcal{U}}_{h,0}^{\mathrm{c}} \tag{3.3}$$

we have

$$\|\nabla I\boldsymbol{w}^{\mathrm{a}}\|_{L^2(\Omega_{\mathrm{a}})}^2 + \|\nabla \boldsymbol{w}^{\mathrm{c}}\|_{L^2(\Omega_{\mathrm{c}})}^2 \leq C\|\nabla\left(I\boldsymbol{w}^{\mathrm{a}} - \boldsymbol{w}^{\mathrm{c}}\right)\|_{L^2(\Omega_{\mathrm{o}})}^2 \tag{3.4}$$

Equivalence of (3.1) and (3.4) follows directly from definitions of $\|\cdot\|_{\rm err}$, $\|\cdot\|_{\rm op}$, $\boldsymbol{U}^{\rm a}$, and $\boldsymbol{U}^{\rm c}$. Our assumptions imply that $R_{\rm core}$ and $R_{\rm a}$ are of the same order and grow at the same rate while $R_{\rm c}/R_{\rm core}$ getting large implies $R_{\rm c}$ grows at a faster rate than $R_{\rm a}$ and $R_{\rm core}$.

In Section 3.1 we show that proving Theorem 3.1 reduces to proving the following result.

Theorem 3.2. *There exists $R^*_{\rm core} > 0$ such that for all domains $\Omega_{\rm a}, \Omega_{\rm c}$ and meshes $\mathcal{T}_h$ constructed according to the guidelines of Section 1.2 (in particular $\psi_{\rm a} R_{\rm core} = R_{\rm a}$) with $R_{\rm core} \geq R^*_{\rm core}$,*

$$\sup_{\boldsymbol{w}^{\rm a}, \boldsymbol{w}^{\rm c} \neq 0} \frac{(\nabla I \boldsymbol{w}^{\rm a}, \nabla \boldsymbol{w}^{\rm c})}{\|\nabla (I\boldsymbol{w}^{\rm a})\|_{L^2(\Omega_{\rm o})} \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}} < 1, \tag{3.5}$$

for all $(\boldsymbol{w}^{\rm a}, \boldsymbol{w}^{\rm c}) \in \boldsymbol{\mathcal{U}}^{\rm a} \times \boldsymbol{\mathcal{U}}^{\rm c}_h$ such that

$$\langle \delta^2 \tilde{\mathcal{E}}^{\rm a}(\boldsymbol{u}^\infty_{\rm a}) \boldsymbol{w}^{\rm a}, \boldsymbol{v}^{\rm a} \rangle = 0 \quad \forall \boldsymbol{v}^{\rm a} \in \boldsymbol{\mathcal{U}}^{\rm a}_0,$$
$$\langle \delta^2 \tilde{\mathcal{E}}^{\rm c}(\boldsymbol{u}^{\rm con}) \boldsymbol{w}^{\rm c}, \boldsymbol{v}^{\rm c} \rangle = 0 \quad \forall \boldsymbol{v}^{\rm c} \in \boldsymbol{\mathcal{U}}^{\rm c}_{h,0}.$$

We prove Theorem 3.2 in Section 3.2 by using extension results from Theorems A.1–A.2. The latter allow us to bound solutions to the atomistic and continuum subproblems in terms of the solution on $\Omega_{\rm o}$ only.

3.1. Reduction

In this section we prove Theorem 3.2. The first step in showing that Theorem 3.2 implies Theorem 3.1 is to bound solutions of the atomistic and continuum problem in terms of their values over the overlap region. The proof of this as well as the proof of Theorem 3.1 will be a proof by contradiction involving scaled versions of (3.2) and (3.3). We distinguish objects in the scaled domain by using a tilde accent, i.e. $\tilde{\mathcal{L}}_{{\rm a},n} = \epsilon_n \mathcal{L}_a$.

In each proof, we will consider sequences $R^{*,n}_{\rm core} \to \infty$ and $R_{{\rm c},n} \to \infty$ with $R_{{\rm c},n}/R^{*,n}_{\rm core} \to \infty$. Given $\boldsymbol{w}^{\rm a}_n$ and $\boldsymbol{w}^{\rm c}_n$, we will then set $\varepsilon_n = 1/R_{{\rm core},n}$, and scale by ε_n to obtain functions $\tilde{\boldsymbol{w}}^{\rm c}_n(\varepsilon_n x) = \boldsymbol{w}^{\rm c}_n(x)$ and $\tilde{\boldsymbol{w}}^{\rm a}_n(\varepsilon_n x) = \boldsymbol{w}^{\rm a}_n(x)$. Thus, each $\tilde{\boldsymbol{w}}^{\rm a}_n$ is defined on $\tilde{\Omega}_{\rm a} := \epsilon_n \Omega_{{\rm a},n}$. Note also that the domains $\tilde{\Omega}_{\rm core} := \epsilon_n \Omega_{{\rm core},n}$ and $\tilde{\Omega}_{\rm a}$ have fixed radii of 1 and $\psi_{\rm a}$ respectively. The domains in the sequence $\{\Omega_{{\rm c},n}\}$ have fixed inner boundaries but their outer boundaries tend to infinity. Since each $w^{\rm c}_n$ is constant on the outer boundary of $\Omega_{{\rm c},n}$, we may extend each of them outside of this region to infinity to obtain functions defined on $\tilde{\Omega}_{\rm c} := \mathbb{R}^n \backslash \tilde{\Omega}_{\rm core}$.

The functions $\tilde{\boldsymbol{w}}^{\rm a}_n$ and $\tilde{\boldsymbol{w}}^{\rm c}_n$ now satisfy scaled versions of (3.2) and (3.3) in which the displacement spaces are parametrized by n in the obvious manner: $\tilde{\boldsymbol{\mathcal{U}}}^{\rm a}_n, \tilde{\boldsymbol{\mathcal{U}}}^{\rm a}_{0,n}, \tilde{\boldsymbol{\mathcal{U}}}^{\rm c}_{h,n}$, and $\tilde{\boldsymbol{\mathcal{U}}}^{\rm c}_{h,0,n}$. For clarity, we introduce several new notations. We use $V_{\xi,\rho}$ to denote the partial derivative of V_ξ with respect to finite difference $D_\rho u$ and $V_{\xi,\rho\tau}$ to denote second derivatives. We further define scaled finite differences and finite difference stencils for $\xi \in \tilde{\mathcal{L}}_{{\rm a},n}$ and $\rho \in \mathcal{R}$ by

$$D_{\epsilon_n \rho} \tilde{\boldsymbol{u}}(\xi) = \frac{\tilde{\boldsymbol{u}}(\xi + \epsilon_n \rho) - \tilde{\boldsymbol{u}}(\xi)}{\epsilon_n} \quad \text{and} \quad D_{\epsilon_n} \tilde{\boldsymbol{u}}(\xi) = (D_{\epsilon_n \rho} \tilde{\boldsymbol{u}}(\xi))_{\rho \in \mathcal{R}}.$$

The norm (1.26) scales to

$$\|D_{\epsilon_n} \tilde{\boldsymbol{v}}\|^2_{\ell^2_{\epsilon_n}(\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n})} = \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} \sup_{\rho \in \mathcal{R}} |D_{\epsilon_n \rho} \tilde{\boldsymbol{v}}|^2 \epsilon_n^d, \tag{3.6}$$

for which there continues to hold

$$\|D_{\epsilon_n} \tilde{\boldsymbol{v}}\|_{\ell^2_{\epsilon_n}(\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n})} \lesssim \|\nabla I_n \tilde{\boldsymbol{v}}\|_{L^2(\tilde{\Omega}_{{\rm a},n})}.$$

The function $\tilde{\boldsymbol{w}}^{\rm a}_n$ satisfies the following scaled variational equation:

$$\begin{aligned} &\sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} \sum_{\rho,\tau \in \mathcal{R}} V_{\xi,\rho\tau}(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{a,n}(\xi)) \cdot D_{\epsilon_n \rho} \tilde{\boldsymbol{w}}^{\rm a}_n, D_{\epsilon_n \tau} \tilde{\boldsymbol{v}}^{\rm a} \epsilon^d = 0 \quad \forall \boldsymbol{v}^{\rm a} \in \tilde{\boldsymbol{\mathcal{U}}}^{\rm a}_{0,n} \\ \equiv &\sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{a,n}(\xi)) : D_{\epsilon_n} \tilde{\boldsymbol{w}}^{\rm a}_n : D_{\epsilon_n} \tilde{\boldsymbol{v}}^{\rm a} \epsilon_n^d = 0 \quad \forall \tilde{\boldsymbol{v}}^{\rm a} \in \tilde{\boldsymbol{\mathcal{U}}}^{\rm a}_{0,n}. \end{aligned} \tag{3.7}$$

It will be convenient to express (3.7) as an integral for $\tilde{\boldsymbol{v}}^{\rm a}$ for which $D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}$ vanishes on $\tilde{\mathcal{L}}_{{\rm a},n}\backslash\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}$ and on a neighborhood of the origin. This requires an additional tool. The cell, ς_ξ, based on $\xi \in \tilde{\mathcal{L}}_n$ is

$$\varsigma_\xi := \left\{ x \in \mathbb{R}^d : 0 \le x_i - \xi_i < \epsilon_n, i = 1, \dots, d \right\}.$$

Let $\bar{I}_n$ be a piecewise constant interpolation operator defined by

$$\bar{I}_n f(x) := f(\xi) \quad \text{where}\, x \in \varsigma_\xi.$$

Then for such a $\tilde{\boldsymbol{v}}^{\rm a}$ and for n large enough such that $D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}$ vanishes on a neighborhood of the origin,

$$\begin{aligned}
\sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{a,n}(\xi)) : D_{\epsilon_n}\tilde{\boldsymbol{w}}^{\rm a}_n : D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}\epsilon_n^d &= \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{a,n}(\xi)) : D_{\epsilon_n}\tilde{\boldsymbol{w}}^{\rm a}_n : D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}\,\mathrm{vol}(\varsigma_\xi\cap\tilde{\Omega}_{\rm a}) \\
&= \sum_{\xi\in\tilde{\mathcal{L}}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{a,n}(\xi)) : D_{\epsilon_n}\tilde{\boldsymbol{w}}^{\rm a}_n : D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}\,\mathrm{vol}(\varsigma_\xi\cap\tilde{\Omega}_{\rm a}) \\
&= \int_{\tilde{\Omega}_{{\rm a},n}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{a,n}) : \bar{I}_n D_{\epsilon_n}\tilde{\boldsymbol{w}}^{\rm a}_n : \bar{I}_n D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}\,dx \\
&= \int_{\tilde{\Omega}_{\rm a}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{a,n}) : \bar{I}_n D_{\epsilon_n}\tilde{\boldsymbol{w}}^{\rm a}_n : \bar{I}_n D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}\,dx
\end{aligned} \tag{3.8}$$

Observe that we have replaced V''_ξ with V'' in the integral since $D_{\epsilon_n}\tilde{\boldsymbol{v}}^{\rm a}$ is assumed to vanish where $V \neq V_\xi$.

Similarly, $\tilde{\boldsymbol{w}}^{\rm c}_n$ satisfies an analogous scaled version f (3.9):

$$\int_{\tilde{\Omega}_{{\rm c},n}} \sum_{\rho,\tau\in\mathcal{R}} \langle V_{,\rho\tau}\left(\epsilon_n\nabla\tilde{\boldsymbol{u}}^{\rm con}_n\mathcal{R}\right)\nabla_\rho\tilde{\boldsymbol{w}}^{\rm c}_n, \nabla_\tau\tilde{\boldsymbol{v}}^{\rm c}\rangle\,dx \equiv \int_{\tilde{\Omega}_{{\rm c},n}} W''(\epsilon_n\nabla\tilde{\boldsymbol{u}}^{\rm con}_n) : \nabla\tilde{\boldsymbol{w}}^{\rm c}_n : \nabla\tilde{\boldsymbol{v}}^{\rm c}_n\,dx = 0 \quad \forall\tilde{\boldsymbol{v}}^{\rm c}\in\tilde{\boldsymbol{\mathcal{U}}}^{\rm c}_{h,0,n}. \tag{3.9}$$

Further define the fourth order tensor, $\mathbb{C} = W''(0)$ and note that

$$(\mathbb{C} : \mathsf{G}) : \mathsf{F} := \sum_{\rho,\tau\in\mathcal{R}} V_{,\rho\tau}(0)\mathsf{G}\rho\cdot\mathsf{F}\tau = (V''(0) : (\mathsf{F}\mathcal{R})) : (\mathsf{G}\mathcal{R}).$$

We bound solutions of the atomistic and continuum problem in terms of their values over the overlap region.

Lemma 3.3. *Suppose that $\boldsymbol{w}^{\rm a}$ and $\boldsymbol{w}^{\rm c}$ are such that equations* (3.2) *and* (3.3) *hold. Then, there exists $R^*_{\rm core} > 0$ such that*

$$\|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm a})} \lesssim \|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm o})} \qquad \textit{and} \tag{3.10}$$

$$\|\nabla\boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm c})} \lesssim \|\nabla\boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}. \tag{3.11}$$

for all domains $\Omega_{\rm a}, \Omega_{\rm c}$ and continuum meshes $\mathcal{T}_h$ constructed according to the guidelines of Section 1.2 (in particular $\psi_{\rm a}R_{\rm core} = R_{\rm a}$) with $R_{\rm core} \ge R^*_{\rm core}$.

Proof. Assume that (3.10)–(3.11) do not hold. Then, there exists a sequence $R^{*,n}_{\rm core} \to \infty$, with corresponding sequences $R_{\rm core,n} \ge R^{*,n}_{\rm core}$, $R_{{\rm c},n}$, $\Omega_{{\rm a},n}, \Omega_{{\rm c},n}$, $\mathcal{T}_{h,n}$, $\boldsymbol{w}^{\rm c}_n$ and $\boldsymbol{w}^{\rm a}_n$, such that $R_{{\rm core},n} \to \infty$, $R_{{\rm c},n} \to \infty$, $R_{{\rm c},n}/R_{\rm core,n} = R^\kappa_{\rm core,n} \to \infty$ with

$$\frac{\|\nabla I_n\boldsymbol{w}^{\rm a}_n\|_{L^2(\Omega_{\rm a})}}{\|\nabla I_n\boldsymbol{w}^{\rm a}_n\|_{L^2(\Omega_{{\rm o},n})}} \to \infty, \qquad \frac{\|\nabla\boldsymbol{w}^{\rm c}_n\|_{L^2(\Omega_{\rm c})}}{\|\nabla\boldsymbol{w}^{\rm c}_n\|_{L^2(\Omega_{{\rm o},n})}} \to \infty. \tag{3.12}$$

After scaling the lattice, the domains, and the functions by $\epsilon_n := \frac{1}{R_{\rm core,n}}$ we find from (3.12) that

$$\frac{\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm a})}}{\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm o})}} \to \infty. \tag{3.13}$$

Extend $I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}}$ to $\mathbb{R}^d$ using the extension operator R from Theorem A.2. Then we have

$$\|\nabla(R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}}))\|_{L^2(\tilde\Omega_{\rm a})} \leq \; C(\tilde\Omega_{\rm o})\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm o})}.$$

Moreover, $R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}}) = I_n \tilde{\boldsymbol{w}}_n^{\rm a}$ on $\partial_{\rm a}\tilde{\mathcal{L}}_{\rm a}$. Let $S_{{\rm a},n}$ be the Scott-Zhang interpolant operator from $H^1(\tilde\Omega_{\rm a})$ to

$$\left\{ u \in {\rm C}(\tilde\Omega_{\rm a}) : u|_\tau \in \mathcal{P}_1(\tau) \quad \forall \tau \in \tilde{\mathcal{T}}_{{\rm a},n} \right\}.$$

Then $S_{{\rm a},n}R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})$ defines an atomistic function in $\boldsymbol{\mathcal{U}}_n^{\rm a}$, which is equal to $\tilde{\boldsymbol{w}}_n^{\rm a}$ on $\partial_{\rm a}\tilde\Omega_{\rm a}$ since $R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})$ is piecewise linear on $\tilde\Omega_{\rm o}$ and due to the projection property of $S_{{\rm a},n}$. This implies that $\tilde{\boldsymbol{z}}_n^{\rm a} := S_{{\rm a},n}R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})|_{\tilde\Omega_{\rm a}} - \tilde{\boldsymbol{w}}_n^{\rm a} \in \tilde{\boldsymbol{\mathcal{U}}}_{0,n}^{\rm a}$ and that $\tilde{\boldsymbol{z}}_n^{\rm a}$ solves the problem

$$\langle \delta^2 \tilde{\mathcal{E}}_n^{\rm a}(\tilde{\boldsymbol{u}}_{{\rm a},n}^\infty)\tilde{\boldsymbol{z}}_n^{\rm a}, \tilde{\boldsymbol{v}}_n^{\rm a}\rangle = \langle \delta^2 \tilde{\mathcal{E}}^{\rm a}(\boldsymbol{u}_{\rm a}^\infty) S_{{\rm a},n}R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})|_{\tilde\Omega_{\rm a}}, \tilde{\boldsymbol{v}}_n^{\rm a}\rangle \quad \forall\, \tilde{\boldsymbol{v}}_n^{\rm a} \in \tilde{\boldsymbol{\mathcal{U}}}_{0,n}^{\rm a}.$$

Thus, taking $\tilde{\boldsymbol{v}}_n^{\rm a} = \tilde{\boldsymbol{z}}_n^{\rm a}$, using (1.28), and the stability of the Scott-Zhang interpolant (see **P.3** or [4, Theorem 4.8.16]), we see that

$$\|\nabla I_n \tilde{\boldsymbol{z}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm a})} \lesssim \|\nabla S_{{\rm a},n}R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})|_{\tilde\Omega_{\rm a}}\|_{L^2(\tilde\Omega_{\rm a})} \lesssim \|\nabla R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})\|_{L^2(\tilde\Omega_{\rm a})} \leq C(\tilde\Omega_{\rm o})\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm o})}.$$

This and the definition of $\boldsymbol{z}_n^a$ imply

$$\|\nabla S_{{\rm a},n}R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})|_{\tilde\Omega_{\rm a}} - \nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm a})} \lesssim \; C(\tilde\Omega_{\rm o})\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm o})},$$

which further leads to

$$\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm a})} \lesssim \; C(\tilde\Omega_{\rm o})\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm o})} + \|\nabla R(I_n \tilde{\boldsymbol{w}}_n^{\rm a}|_{\tilde\Omega_{\rm o}})\|_{L^2(\tilde\Omega_{\rm a})} \leq \; 2C(\tilde\Omega_{\rm o})\|\nabla I_n \tilde{\boldsymbol{w}}_n^{\rm a}\|_{L^2(\tilde\Omega_{\rm o})},$$

a contradiction to (3.13). This establishes (3.10).

A similar argument utilizing the Scott-Zhang interpolant on $\tilde\Omega$ with mesh $\tilde{\mathcal{T}}_{h,n}$ yields (3.11). □

Proof of Theorem 3.1. According to Lemma 3.3 if $\boldsymbol{w}^{\rm a}$ and $\boldsymbol{w}^{\rm c}$ satisfy equations (3.2) and (3.3) then

$$\|\nabla(I\boldsymbol{w}^{\rm a})\|_{L^2(\Omega_{\rm a})}^2 + \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm c})}^2 \lesssim \; \|\nabla(I\boldsymbol{w}^{\rm a})\|_{L^2(\Omega_{\rm o})}^2 + \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}^2.$$

Consequently, to prove (3.4) in Theorem 3.1 it suffices to show that

$$\|\nabla(I\boldsymbol{w}^{\rm a})\|_{L^2(\Omega_{\rm o})}^2 + \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}^2 \lesssim \|\nabla(I\boldsymbol{w}^{\rm a} - \boldsymbol{w}^{\rm c})\|_{L^2(\Omega_{\rm o})}^2.$$

This result is a direct consequence of Theorem 3.2 since

$$\begin{aligned}
\|\nabla(I\boldsymbol{w}^{\rm a} - \boldsymbol{w}^{\rm c})\|_{L^2(\Omega_{\rm o})}^2 \;&=\; \|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm o})}^2 + \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}^2 - 2\left(\nabla I\boldsymbol{w}^{\rm a}, \nabla \boldsymbol{w}^{\rm c}\right)_{L^2(\Omega_{\rm o})} \\
&\geq\; \|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm o})}^2 + \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}^2 - 2c\|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm o})}\|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})} \quad \text{for some } 0 < c < 1 \text{ by Theorem 3.2} \\
&\geq\; \|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm o})}^2 + \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}^2 - c\|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm o})}^2 - c\|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}^2 \\
&=\; (1-c)\left(\|\nabla I\boldsymbol{w}^{\rm a}\|_{L^2(\Omega_{\rm o})}^2 + \|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}^2\right).
\end{aligned}$$

□

For clarity we break the proof Theorem 3.2 into several intermediate steps.

3.2. Proof of Theorem 3.2

The proof is by contradiction. To this end we start with the following

Conjecture 1. *For all $R^*_{\rm core} > 0$, there exist domains $\Omega_{\rm a}, \Omega_{\rm c}$ and a continuum mesh $\mathcal{T}_h$ constructed according to the guidelines of Section 1.2 with $R_{\rm core} \geq R^*_{\rm core}$ and $R_{\rm c}/R_{\rm core} = R^{\kappa}_{\rm core}$ and*

$$\sup_{\boldsymbol{w}^{\rm a},\boldsymbol{w}^{\rm c}\neq 0} \frac{(\nabla I\boldsymbol{w}^{\rm a}, \nabla \boldsymbol{w}^{\rm c})}{\|\nabla(I\boldsymbol{w}^{\rm a})\|_{L^2(\Omega_{\rm o})}\|\nabla \boldsymbol{w}^{\rm c}\|_{L^2(\Omega_{\rm o})}} = 1, \tag{3.14}$$

where $\boldsymbol{w}^{\rm a}$ and $\boldsymbol{w}^{\rm c}$ satisfy

$$\begin{aligned} \langle \delta^2 \tilde{\mathcal{E}}^{\rm a}(\boldsymbol{u}^\infty_{\rm a})\boldsymbol{w}^{\rm a}, \boldsymbol{v}^{\rm a}\rangle = 0 \quad \forall \boldsymbol{v}^{\rm a} \in \boldsymbol{\mathcal{U}}^{\rm a}_0, \\ \langle \delta^2 \tilde{\mathcal{E}}^{\rm c}(\boldsymbol{u}^{\rm con})\boldsymbol{w}^{\rm c}, \boldsymbol{v}^{\rm c}\rangle = 0 \quad \forall \boldsymbol{v}^{\rm c} \in \boldsymbol{\mathcal{U}}^{\rm c}_{h,0}. \end{aligned}$$

Conjecture 1 implies the existence of sequences $R^{*;n}_{\rm core} \to \infty$, $R_{{\rm core},n} \to \infty$, $R_{{\rm c},n} \to \infty$, $R_{{\rm c},n}/R_{\rm core,n} \to \infty$, a corresponding sequence of grids $\mathcal{T}_{h,n}$ with a minimum angle at least β, and associated sequences $\boldsymbol{w}^{\rm c}_n$, $\boldsymbol{w}^{\rm a}_n$, such that

$$\frac{(\nabla I\boldsymbol{w}^{\rm a}_n, \nabla \boldsymbol{w}^{\rm c}_n)}{\|\nabla(I\boldsymbol{w}^{\rm a}_n)\|_{L^2(\Omega_{\rm o})}\|\nabla \boldsymbol{w}^{\rm c}_n\|_{L^2(\Omega_{\rm o})}} \to 1. \tag{3.15}$$

We will show (3.15) yields a contradiction in four steps. In the first step, we will scale the lattice by $\varepsilon_n = 1/R_{{\rm core},n}$ to define sequences of functions $\tilde{\boldsymbol{w}}^{\rm a}_n$ having a common domain of definition and $\tilde{\boldsymbol{w}}^{\rm c}_n$ having a common domain of definition. This will allow us to extract weak limits of these sequences. The second step will show these limits satisfy the homogeneous Cauchy-Born equation. In the third step, we show weak convergence combined with satisfying atomistic and finite element equations implies the limit and inner product commute. This will yield a contradiction in the final, fourth step of the proof.

Step 1:

Recall that we use the tilde accent for objects on the scaled domains. Let I_n be the piecewise interpolant onto the lattice $\tilde{\mathcal{L}}_n$, and normalize $\tilde{\boldsymbol{w}}^{\rm a}_n$ and $\tilde{\boldsymbol{w}}^{\rm c}_n$ to functions $\bar{\boldsymbol{w}}^{\rm a}_n$ and $\bar{\boldsymbol{w}}^{\rm c}_n$ such that

$$\|\nabla(I_n\bar{\boldsymbol{w}}^{\rm a}_n)\|_{L^2(\tilde{\Omega}_{\rm o})} = 1, \quad \text{and} \quad \|\nabla\bar{\boldsymbol{w}}^{\rm c}_n\|_{L^2(\tilde{\Omega}_{\rm o})} = 1. \tag{3.16}$$

Due to this property and our hypothesis (3.15), we have that

$$(\nabla I_n\bar{\boldsymbol{w}}^{\rm a}_n, \nabla\bar{\boldsymbol{w}}^{\rm c}_n)_{L^2(\tilde{\Omega}_{\rm o})} \to 1. \tag{3.17}$$

Moreover, $\nabla I_n\bar{\boldsymbol{w}}^{\rm a}_n$ is a bounded sequence in $L^2(\tilde{\Omega}_{\rm a})$ since

$$\|\nabla I_n\bar{\boldsymbol{w}}^{\rm a}_n\|_{L^2(\tilde{\Omega}_{\rm a})} = \|\nabla I_n\tilde{\boldsymbol{w}}^{\rm a}_n\|_{L^2(\tilde{\Omega}_{\rm a})}/\|\nabla I_n\tilde{\boldsymbol{w}}^{\rm a}_n\|_{L^2(\tilde{\Omega}_{\rm o})} \lesssim \|\nabla I_n\tilde{\boldsymbol{w}}^{\rm a}_n\|_{L^2(\tilde{\Omega}_{\rm o})}/\|\nabla I_n\tilde{\boldsymbol{w}}^{\rm a}_n\|_{L^2(\tilde{\Omega}_{\rm o})} = 1,$$

after using the scaled version of Lemma 3.3. Similarly, $\nabla\bar{\boldsymbol{w}}^{\rm c}_n$ is bounded in $L^2(\tilde{\Omega}_{\rm c})$. Meanwhile, $\bar{\boldsymbol{w}}^{\rm a}_n$ and $\bar{\boldsymbol{w}}^{\rm c}_n$ will still satisfy the variational equalities (3.7) and (3.9) by linearity.

For each n, we let $I_n\bar{w}^{\rm a}_n$ be the element in the equivalence class of $\bar{\boldsymbol{w}}^{\rm a}_n$ with mean value 0 over $\tilde{\Omega}_a$. The resulting sequence is bounded in $H^1(\tilde{\Omega}_{\rm a})$ and so it has a weakly convergent subsequence, which we denote again by $I_n\bar{w}_n^{\rm a}$. Let $\bar{w}_0^{\rm a} \in H^1(\tilde{\Omega}_{\rm a})$ be the weak limit. By the compactness of the embedding $H^1(\tilde{\Omega}_{\rm a}) \subset L^2(\tilde{\Omega}_{\rm a})$ it follows that $I_n\bar{w}_n^{\rm a} \to \bar{w}_0^{\rm a}$ in $L^2(\tilde{\Omega}_{\rm a})$. Similarly, the functions $\bar{\boldsymbol{w}}_n^{\rm c}$ form a bounded sequence on the Hilbert space,

$$\boldsymbol{H}^1(\tilde{\Omega}_{\rm c}) := \left\{u^{\rm c} \in H^1_{\rm loc}(\tilde{\Omega}_{\rm c}) : \nabla u^{\rm c} \in L^2(\tilde{\Omega}_{\rm c})\right\} \backslash \mathbb{R}^d. \tag{3.18}$$

Thus, we can extract a weakly convergent subsequence, still denoted by $\bar{\boldsymbol{w}}_n^{\rm c}$, with limit $\bar{\boldsymbol{w}}_0^{\rm c} \in \boldsymbol{H}^1(\tilde{\Omega}_{\rm c})$, i.e, $\bar{\boldsymbol{w}}_n^{\rm c} \rightharpoonup \bar{\boldsymbol{w}}_0^{\rm c}$ in $\boldsymbol{H}^1(\tilde{\Omega}_{\rm c})$. This implies $\nabla\bar{\boldsymbol{w}}_0^{\rm c} \rightharpoonup \nabla\bar{\boldsymbol{w}}_0^{\rm c}$ in $L^2(\tilde{\Omega}_{\rm c})$.

We call a continuum mesh *fully resolved* if $T \in \tilde{\mathcal{T}}_{h,n}$ with $T^\circ \cap \tilde{\Omega}_{\rm o,ex} \neq \emptyset$ implies $T \in \tilde{\mathcal{T}}_{{\rm a},n}$ and vice-versa. For the remainder of the proof we shall assume that the finite element mesh is fully resolved beyond the overlap region $\Omega_{\rm o}$. We recall that $\Omega_{{\rm a},n} = \psi_{\rm a}\Omega_{\rm core,n}$, $\tilde{\Omega}_{\rm a} = \frac{1}{R_{\rm core,n}}\Omega_{{\rm a},n}$, and $\tilde{\Omega}_{\rm o} := \frac{1}{R_{\rm core,n}}\Omega_{{\rm o},n}$. Define $\tilde{\Omega}_{\rm o,ex}$ by

$$\tilde{\Omega}_{\rm o,ex} := \epsilon_n(2\psi_{\rm a}\Omega_{\rm core,n}\backslash\Omega_{\rm core,n}).$$

The purpose of $\tilde{\Omega}_{\rm o,ex}$ is to have a domain of definition common to all continuum elements which extends slightly beyond $\tilde{\Omega}_{\rm o}$.

Let $\bar{w}_n^{\rm c}$ and $\bar{w}_0^{\rm c}$ be equivalence class elements having zero mean over $\tilde{\Omega}_{\rm o,ex}$. Then $\bar{w}_n^{\rm c}$ is bounded in $H^1(\tilde{\Omega}_{\rm o,ex})$ and converges weakly to some $\bar{w}^{\rm c} \in H^1(\tilde{\Omega}_{\rm o,ex})$. But since the restriction operator from $L^2(\tilde{\Omega}_{\rm c})$ to $L^2(\tilde{\Omega}_{\rm o,ex})$ is continuous with respect to the strong topology and hence the weak topology, we must have $\nabla\bar{w} = \nabla\bar{w}_0^{\rm c}$ on $\tilde{\Omega}_{\rm o,ex}$ so the two functions differ a.e by a constant on $\tilde{\Omega}_{\rm o,ex}$. Since both $\bar{w}_0^{\rm c}$ and $\bar{w}^{\rm c}$ have mean value 0 over $\tilde{\Omega}_{\rm o,ex}$, the two functions are in fact equal on $\tilde{\Omega}_{\rm o,ex}$. Thus $\bar{w}_n^{\rm c}$ converges weakly to $\bar{w}_0^{\rm c}$ in $H^1(\tilde{\Omega}_{\rm o,ex})$. The strong convergence $\bar{w}_n^{\rm c} \to \bar{w}_0^{\rm c}$ in $L^2(\tilde{\Omega}_{\rm o,ex})$ follows from the compactness of the embedding $H^1(\tilde{\Omega}_{\rm o,ex}) \hookrightarrow L^2(\tilde{\Omega}_{\rm o,ex})$.

In summary, we have established the following result.

Lemma 3.4. *There exist sequences $\bar{w}_n^{\rm a} \in H^1(\tilde{\Omega}_{\rm a})$ and $\bar{w}_n^{\rm c} \in L^2_{\rm loc}(\tilde{\Omega}_{\rm c})$ and with $\nabla\bar{w}_n^{\rm c} \in L^2(\tilde{\Omega}_{\rm c})$ which satisfy the variational equalities* (3.7) *and* (3.9) *such that*

$$I_n\bar{w}_n^{\rm a} \rightharpoonup \bar{w}_0^{\rm a} \quad in \quad H^1(\tilde{\Omega}_{\rm a}), \qquad I_n\bar{w}_n^{\rm a} \to \bar{w}_0^{\rm a} \quad in \quad L^2(\tilde{\Omega}_{\rm a}), \tag{3.19}$$

$$\nabla\bar{w}_n^{\rm c} \rightharpoonup \nabla\bar{w}_0^{\rm c} \quad in \quad L^2(\tilde{\Omega}_{\rm c}), \qquad \bar{w}_n^{\rm c} \rightharpoonup \bar{w}_0^{\rm c} \quad in \quad H^1(\tilde{\Omega}_{\rm o,ex}), \qquad \bar{w}_n^{\rm c} \to \bar{w}_0^{\rm c} \quad in \quad L^2(\tilde{\Omega}_{\rm o,ex}). \tag{3.20}$$

Step 2:

Theorem 3.5. *The functions $\bar{w}_0^{\rm a}$ and $\bar{w}_0^{\rm c}$ satisfy the linear homogeneous Cauchy-Born elasticity equations*

$$\int_{\tilde{\Omega}_a} (\mathbb{C} : \nabla\bar{w}_0^{\rm a}) : \nabla v = 0 \quad \forall v \in H^1_0(\tilde{\Omega}_{\rm a}) \tag{3.21}$$

$$\int_{\tilde{\Omega}_{\rm c}} (\mathbb{C} : \nabla\bar{w}_0^{\rm c}) : \nabla v = 0 \quad \forall v \in H^1_0(\tilde{\Omega}_{\rm c}). \tag{3.22}$$

We break the proof into several lemmas. We start with the atomistic case (3.21) where special care must be exercised near the defect at the origin.

Lemma 3.6. *Let $\tilde{N}$ be any neighborhood of the origin with $\tilde{N} \subset \tilde{\Omega}_{\rm a}$ and set $\tilde{\Omega}' := \tilde{\Omega}_{\rm a}\backslash\tilde{N}$. Then $\bar{w}_0^{\rm a}$ satisfies*

$$\int_{\tilde{\Omega}'} (\mathbb{C} : \nabla\bar{w}_0^{\rm a}) : \nabla v = 0 \quad \forall v \in H^1_0(\tilde{\Omega}'). \tag{3.23}$$

The key result in proving Lemma 3.6 is the auxiliary Lemma 3.7.

Lemma 3.7. *Let Ω be a bounded quasiconvex region of $\mathbb{R}^d$ satisfying the assumptions of Theorem A.1 with $\Omega_1 \subset\subset \Omega$. Set $\mathcal{L}_{n,1} = \Omega_1 \cap \mathcal{L}_n$, and suppose v_n is piecewise linear with respect to $\mathcal{L}_n$ and $v_n \rightharpoonup v_0$ in $H^1(\Omega)$. For $r \in \mathcal{R}$, $\bar{I}_n D_{\varepsilon_n r} v_n \rightharpoonup \nabla_r v_0$ in $L^2(\Omega_1)$.*

Proof of Lemma 3.7. We prove the Lemma for $v_0 = 0$ and then reduce the general case $v_0 \neq 0$ to this setting.
Case 1 ($v_0 = 0$). Take $\varphi \in C_0^\infty(\Omega_1)$, and note since $v_n \rightharpoonup 0$ in H^1, $v_n \to 0$ strongly in L^2. Then

$$\begin{aligned}
&\limsup_{n\to\infty} \left|(\bar{I}_n D_{\varepsilon_n r} v_n, \varphi)_{L^2(\Omega_1)}\right| \\
&= \limsup_{n\to\infty} \left| \int_{\Omega_1} \bar{I}_n D_{\varepsilon_n r} v_n(x)\varphi(x)\,dx \right| = \limsup_{n\to\infty} \left| \sum_{\xi\in\Omega_1} \int_{\varsigma_\xi\cap\Omega_1} \bar{I}_n D_{\varepsilon_n r} v_n(x)\varphi(x)\,dx \right| \\
&= \limsup_{n\to\infty} \left| \sum_{\xi\in\Omega_1} \int_{\varsigma_\xi\cap\Omega_1} D_{\varepsilon_n r} v_n(\xi)(\varphi(\xi) + \nabla\varphi(\xi)\tau_{\xi,x})\,dx \right| \quad \text{for } \tau_{\xi,x} \in \operatorname{conv}(\xi, x). \qquad (3.24) \\
&\le \underbrace{\limsup_{n\to\infty} \left| \sum_{\xi\in\Omega_1} D_{\varepsilon_n r} v_n(\xi)\varphi(\xi)\operatorname{vol}(\varsigma_\xi\cap\Omega_1) \right|}_{T_1} + \underbrace{\limsup_{n\to\infty} \left| \sum_{\xi\in\Omega_1} \int_{\varsigma_\xi\cap\Omega_1} D_{\varepsilon_n r} v_n(\xi)\nabla\varphi(\xi)\tau_{\xi,x}\,dx \right|}_{T_2}.
\end{aligned}$$

We first estimate T_2 by noting

$$\begin{aligned}
T_2 &\le \sum_{\xi\in\Omega_1} \int_{\varsigma_\xi\cap\Omega_1} |D_{\varepsilon_n r} v_n(\xi)||\nabla\varphi(\xi)\tau_{\xi,x}|\,dx \\
&\le \sum_{\xi\in\Omega_1} \Big(\int_{\varsigma_\xi\cap\Omega_1} |D_{\varepsilon_n r} v_n(\xi)|^2\,dx \Big)^{1/2} \Big(\int_{\varsigma_\xi\cap\Omega_1} |\nabla\varphi(\xi)\tau_{\xi,x}|^2\,dx \Big)^{1/2} \\
&\le \Big(\sum_{\xi\in\Omega_1} \int_{\varsigma_\xi\cap\Omega_1} |D_{\varepsilon_n r} v_n(\xi)|^2\,dx \Big)^{1/2} \Big(\sum_{\xi\in\Omega_1} \int_{\varsigma_\xi\cap\Omega_1} |\nabla\varphi(\xi)\tau_{\xi,x}|^2\,dx \Big)^{1/2} \\
&\le \Big(\sum_{\xi\in\Omega_1} |D_{\varepsilon_n r} v_n(\xi)|^2 \operatorname{vol}(\varsigma_\xi\cap\Omega_1) \Big)^{1/2} \Big(\sum_{\xi\in\Omega_1} \int_{\varsigma_\xi\cap\Omega_1} \|\nabla\varphi\|_{L^\infty}^2 \epsilon_n^2\,dx \Big)^{1/2} \\
&\lesssim \epsilon_n \Big(\sum_{\xi\in\Omega_1} |D_{\varepsilon_n r} v_n(\xi)|^2 \operatorname{vol}(\varsigma_\xi\cap\Omega_1) \Big)^{1/2} \le \epsilon_n \Big(\sum_{\xi\in\Omega_1} \sup_{r\in\mathcal{R}} |D_{\varepsilon_n r} v_n(\xi)|^2 \operatorname{vol}(\varsigma_\xi\cap\Omega_1) \Big)^{1/2} \lesssim \epsilon_n \|\nabla v_n\|_{L^2(\Omega)}.
\end{aligned}$$

To estimate T_1 we shift the finite difference operator onto $\varphi(\xi)\operatorname{vol}(\varsigma_\xi\cap\Omega_1)$ and recall that $\varphi \in \mathcal{C}_0^\infty(\Omega_1)$.

$$\begin{aligned}
T_1 &= \sum_{\xi\in\Omega_1} D_{\varepsilon_n r} v_n(\xi)\varphi(\xi)\operatorname{vol}(\varsigma_\xi\cap\Omega_1) = \sum_{\xi\in\Omega_1} v_n(\xi) D_{-\varepsilon_n r}(\varphi(\xi)\operatorname{vol}(\varsigma_\xi\cap\Omega_1)) \\
&= \sum_{\xi\in\Omega_1} v_n(\xi)(D_{-\varepsilon_n r}(\varphi(\xi))\operatorname{vol}(\varsigma_\xi\cap\Omega_1) + \varphi(\xi+\epsilon_n r) D_{-\varepsilon_n r}\operatorname{vol}(\varsigma_\xi\cap\Omega_1)) \\
&= \sum_{\xi\in\Omega_1} v_n(\xi) D_{-\varepsilon_n r}(\varphi(\xi))\operatorname{vol}(\varsigma_\xi\cap\Omega_1) \\
&\le \Big(\sum_{\xi\in\Omega_1} |v_n(\xi)|^2 \operatorname{vol}(\varsigma_\xi\cap\Omega_1) \Big)^{1/2} \Big(\sum_{\xi\in\Omega_1} |D_{-\varepsilon_n r}\varphi(\xi)|^2 \operatorname{vol}(\varsigma_\xi\cap\Omega_1) \Big)^{1/2} \\
&\lesssim \|\bar{I}_n v_n\|_{L^2(\Omega_1)} \|\nabla I_n \varphi\|_{L^2(\Omega_1)}. \qquad (3.25)
\end{aligned}$$

Consider a micro-simplex T of $\mathcal{L}_n$ with nodes $\mathcal{N}(T)$ belonging to cell ς_ξ and a a reference simplex $\hat{T}$ with nodes $\mathcal{N}(\hat{T})$. If $\hat{f}$ is the pullback of a function f on T, then

$$\|\bar{I}_n v_n\|_{L^2(T)} = |T|^{1/2} \cdot |v_n(\xi)| \le |T|^{1/2} \sup_{\zeta\in\mathcal{N}(T)} |v_n(\zeta)| = |T|^{1/2} \sup_{\hat{\zeta}\in\mathcal{N}(\hat{T})} |\hat{v}_n(\hat{\zeta})| \lesssim |T|^{1/2} \|\hat{v}_n\|_{L^2(\hat{T})} = \|v_n\|_{L^2(T)}$$

Summing over all elements gives

$$\|\bar{I}_n v_n\|_{L^2(\Omega_1)} \leq \|v_n\|_{L^2(\Omega)},$$

and using this in (3.25) yields

$$T_1 \lesssim \|v_n\|_{L^2(\Omega)} \|\nabla I_n \varphi\|_{L^2(\Omega_1)}. \tag{3.26}$$

Because v_n converges weakly to 0 in $H^1(\Omega)$, v_n converges strongly to 0 in $L^2(\Omega)$. Moreover, because φ is smooth, $\|\nabla I_n \varphi\|_{L^2(\Omega_1)}$ converges to $\|\nabla \varphi\|_{L^2(\Omega_1)}$. Employing (3.25) and (3.26) in (3.24) shows

$$\limsup_{n\to\infty} \left| (\bar{I}_n D_{\varepsilon_n r} v_n, \varphi)_{L^2(\Omega_1)} \right| = 0.$$

Case 2 ($v_0 \neq 0$). We reduce this case to the previous one. Let η_R be a standard mollifier on a ball of radius R, and define

$$v_{0,R}(x) := (\eta_R * v_0)(x) = \int_\Omega \eta_R(x-y) v_0(y) \mathrm{d}y,$$

for x in $\Omega^R := \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) > R\}$. From standard properties of mollifiers, it follows that

$$\lim_{R\to 0} \nabla v_{0,R} = \nabla v_0 \quad \text{in} \quad H^1_{\mathrm{loc}}(\Omega). \tag{3.27}$$

Moreover, since $v_{0,R}$ is smooth, for any fixed R,

$$\lim_{n\to\infty} I_n v_{0,R} \to v_{0,R} \quad \text{in}\, H^1_{\mathrm{loc}}(\Omega) \quad (R > 0). \tag{3.28}$$

Now fix Ω_2 such that $\Omega_1 \subset\subset \Omega_2 \subset\subset \Omega$. For each integer $m > 0$, set $\alpha_m := \frac{1}{m}$ and define R_{α_m} by requiring

$$\|\nabla v_{0,R_{\alpha_m}} - \nabla v_0\|_{H^1(\Omega_2)} \leq \alpha_m/2.$$

By (3.28), for each integer m (or index $\alpha_m = \frac{1}{m}$), there exists an integer N_{α_m} such that

$$\|\nabla I_n v_{0,R_{\alpha_m}} - \nabla v_{0,R_{\alpha_m}}\|_{H^1(\Omega_2)} \leq \alpha_m/2 \quad \forall n \geq N_{\alpha_m}.$$

In particular,

$$\|\nabla I_{N_{\alpha_m}} v_{0,R_{\alpha_m}} - \nabla v_{0,R_{\alpha_m}}\|_{H^1(\Omega_2)} \leq \alpha_m/2.$$

Thus

$$\|\nabla I_{N_{\alpha_m}} v_{0,R_{\alpha_m}} - \nabla v_0\|_{H^1(\Omega_2)} \leq \|\nabla I_{N_{\alpha_m}} v_{0,R_{\alpha_m}} - \nabla v_{0,R_{\alpha_m}}\|_{H^1(\Omega_2)} + \|\nabla v_{0,R_{\alpha_m}} - \nabla v_0\|_{H^1(\Omega_2)} \leq \alpha_m \to 0. \tag{3.29}$$

Next note that $v_{0,R}$ is smooth so $D_{\epsilon_n r} v_{0,R} \to \nabla_r v_{0,R}$ uniformly on compact subsets of Ω and hence in $H^1_{\rm loc}(\Omega)$. Furthermore,

$$\|\bar{I}_n D_{\epsilon_n r} v_{0,R} - D_{\epsilon_n r} v_{0,R}\|^2_{L^2(\Omega_2)} = \int_{\Omega_2} |\bar{I}_n D_{\epsilon_n r} v_{0,R} - D_{\epsilon_n r} v_{0,R}|^2 \, dx$$

$$= \sum_{\xi \in \Omega_2} \int_{\varsigma_\xi \cap \Omega_2} |D_{\epsilon_n r} v_{0,R}(\xi) - D_{\epsilon_n r} v_{0,R}(x)|^2 \, dx$$

$$= \sum_{\xi \in \Omega_2} \int_{\varsigma_\xi \cap \Omega_2} |D_{\epsilon_n r} v_{0,R}(\xi) - D_{\epsilon_n r} v_{0,R}(\xi) + D_{\epsilon_n r} \nabla v_{0,R}(\xi)(\tau_{\xi,x})|^2 \, dx \quad \text{for } \tau_{\xi,x} \in \operatorname{conv}(\xi, x).$$

$$\leq \epsilon_n^2 \sum_{\xi \in \Omega_2} \int_{\varsigma_\xi \cap \Omega_2} |D_{\epsilon_n r} \nabla v_{0,R}(\xi)|^2 \, dx \lesssim \epsilon_n^2 \|\nabla^2 v_{0,R}\|^2_{L^2(\Omega_2)} \to 0.$$

Thus, as $n \to \infty$, we have that

$$\|\bar{I}_n D_{\varepsilon_n r} v_{0,R} - \nabla_r v_{0,R}\|_{L^2(\Omega_2)} \leq \|\bar{I}_n D_{\varepsilon_n r} v_{0,R} - D_{\varepsilon_n r} v_{0,R}\|_{L^2(\Omega_2)} + \|D_{\varepsilon_n r} v_{0,R} - \nabla_r v_{0,R}\|_{L^2(\Omega_2)} \to 0. \tag{3.30}$$

As before, we may assume

$$\|\bar{I}_n D_{\varepsilon_n r} v_{0,R_{\alpha_m}} - \nabla_r v_{0,R_{\alpha_m}}\|_{L^2(\Omega_2)} \leq \alpha_m/2 \quad \forall \quad n \geq \ N_{\alpha_m}.$$

In particular,

$$\|\bar{I}_{N_{\alpha_m}} D_{\varepsilon_{N_{\alpha_m}} r} v_{0,R_{\alpha_m}} - \nabla_r v_{0,R_{\alpha_m}}\|_{L^2(\Omega_2)} \leq \alpha_m/2.$$

Therefore

$$\begin{aligned} &\|\bar{I}_{N_{\alpha_m}} D_{\varepsilon_{N_{\alpha_m}} r} v_{0,R_{\alpha_m}} - \nabla_r v_0\|_{L^2(\Omega_2)} \leq \\ &\quad \|\bar{I}_{N_{\alpha_m}} D_{\varepsilon_{N_{\alpha_m}} r} v_{0,R_{\alpha_m}} - \nabla_r v_{0,R_{\alpha_m}}\|_{L^2(\Omega_2)} + \|\nabla_r v_{0,R_{\alpha_m}} - \nabla_r v_0\|_{L^2(\Omega_2)} \leq \alpha_m \to 0. \end{aligned} \tag{3.31}$$

Next let $\hat{v}_m := v_{N_{\alpha_m}} - v_{0,R_{\alpha_m}}$. By assumption, $v_{N_{\alpha_m}}$ converges weakly to ∇v_0. From (3.29), we see $\nabla I_{N_{\alpha_m}} v_{0,R_{\alpha_m}}$ converges strongly, whence weakly, to ∇v_0 on Ω_2. Consequently, $\nabla I_{N_{\alpha_m}} \hat{v}_m$ converges weakly to 0 on Ω_2. From case (1), $\bar{I}_{N_{\alpha_m}} D_{\varepsilon_{N_{\alpha_m}} r} \hat{v}_m \rightharpoonup 0$ in $L^2(\Omega_1)$. But $\bar{I}_{N_{\alpha_m}} D_{\varepsilon_{N_{\alpha_m}} r} v_{0,R_{\alpha_m}} \to \nabla_r v_0$ by (3.31) implying $\bar{I}_{N_{\alpha_m}} D_{\varepsilon_{N_{\alpha_m}} r} v_0 \rightharpoonup \nabla_r v_0$. Since this argument can be applied to any subsequence of $\bar{I}_n D_{\varepsilon_n r} v_n$, by the Urysohn property [41], we have $\bar{I}_n D_{\varepsilon_n r} v_n \rightharpoonup \nabla_r v_0$ in $L^2(\Omega_1)$. □

Proof of Lemma 3.6. First, notice that it is enough to test (3.23) with $v \in C_0^\infty(\tilde{\Omega}_{\rm a} \setminus \tilde{N})$, i.e., for $\operatorname{supp}(v) \subset\subset \tilde{\Omega}_{\rm a}$, $0 \notin \operatorname{supp}(v)$. Since v has compact support inside $\tilde{\Omega}_{\rm a} \setminus \tilde{N}$, $D_{\epsilon_n \rho} v(\xi)$ vanishes on $\tilde{\mathcal{L}}_{{\rm a},n} \backslash \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}$ for all n large enough and $\rho \in \mathcal{R}$. We may therefore rewrite (3.7) with $\bar{w}_n^{\rm a}$ using the integral formulation introduced in (3.8)

$$0 = \int_{\tilde{\Omega}_{\rm a}} \bar{I}_n V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}) : \bar{I}_n D_{\epsilon_n} \bar{w}_n^{\rm a} : \bar{I}_n D_{\epsilon_n} v \, dx. \tag{3.32}$$

We have that $\nabla \bar{w}_n^{\rm a} \rightharpoonup \nabla \bar{w}_0^{\rm a}$ on $\tilde{\Omega}_{\rm a}$. Taking Ω_1 with supp $\subset\subset \Omega_1 \subset\subset \tilde{\Omega}_{\rm a}$, from Lemma 3.7 it follows that

$$\bar{I}_n D_{\epsilon_n r} \bar{w}_n^{\rm a} \rightharpoonup (\nabla_r \bar{w}_0^{\rm a}) \quad \text{on } \Omega_1 \text{ for all } r \in \mathcal{R}. \tag{3.33}$$

Because v is smooth, (3.30) implies

$$\bar{I}_n D_{\epsilon_n r} v^{\mathrm{a}} \to (\nabla_r v) \quad \text{for all } r \in \mathcal{R}. \tag{3.34}$$

According to Assumption D there exists a local minimum $\boldsymbol{u}^\infty$ of $\mathcal{E}^{\mathrm{a}}$ such that

$$|\nabla I \boldsymbol{u}^\infty(\xi)| \lesssim |\xi|^{-d} \quad \text{for } \xi \notin \Omega_{\mathrm{core}}. \tag{3.35}$$

After scaling the lattice by ϵ_n we get a sequence of global solutions $\tilde{\boldsymbol{u}}_n^\infty(\xi) = \boldsymbol{u}^\infty(\xi/\epsilon_n)$ for $\xi \in \tilde{\mathcal{L}}_n$. Thus, for $x \neq 0$ and large enough n there holds $x \notin \epsilon_n \Omega_{\mathrm{core}} = \tilde{\Omega}_{\mathrm{core},n}$. As a result, since $d > 1$ it follows that

$$|\nabla(I_n \tilde{\boldsymbol{u}}_n^\infty(x))| = \frac{1}{\epsilon_n} |(\nabla I_n \boldsymbol{u}_n^\infty)(x/\epsilon_n)| \lesssim \frac{1}{\epsilon_n} |x/\epsilon_n|^{-d} = \epsilon_n^{d-1} |x|^{-d} \to 0 \tag{3.36}$$

uniformly as $\epsilon_n \to 0$. This also implies

$$|\epsilon_n \bar{I}_n D_{\epsilon_n} \tilde{\boldsymbol{u}}_{\mathrm{a},n}^\infty(x)| \to 0 \qquad \text{uniformly as } \epsilon_n \to 0 \text{ on } \tilde{\Omega}_{\mathrm{a}} \backslash \tilde{N};$$

whence

$$\bar{I}_n V''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}_{\mathrm{a},n}^\infty(x)) = V''(\epsilon_n \bar{I}_n D_{\epsilon_n} \tilde{\boldsymbol{u}}_{\mathrm{a},n}^\infty(x)) \to 0 \quad \text{uniformly as } \epsilon_n \to 0 \text{ on } \tilde{\Omega}_{\mathrm{a}} \backslash \tilde{N}.$$

Hence, taking the limit of (3.32), and using (3.33), (3.34), and the fact that the "dual pairing" (:) of a weakly convergent and a strongly convergent sequence converges to the dual pairing of the limits, we obtain

$$\begin{aligned} 0 &= \lim_{n\to\infty} \int_{\tilde{\Omega}_{\mathrm{a}}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}_{\mathrm{a}}^\infty) : \bar{I}_n D_{\epsilon_n} \bar{w}_n^{\mathrm{a}} : \bar{I}_n D_{\epsilon_n} v \, dx \\ &= \lim_{n\to\infty} \int_{\tilde{\Omega}_{\mathrm{a}}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}_{\mathrm{a}}^\infty) : \bar{I}_n D_{\epsilon_n} v : \bar{I}_n D_{\epsilon_n} \bar{w}_n^{\mathrm{a}} \, dx \\ &= \int_{\tilde{\Omega}_{\mathrm{a}}} V''(\mathbf{0}) : \nabla_{\mathcal{R}} \bar{w}_0^{\mathrm{a}} : \nabla_{\mathcal{R}} v \, dx = \int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla v \, dx. \end{aligned}$$

$\square$

Proof of Theorem 3.5. Our first task is to prove (3.21). By density, it suffices to prove the theorem for $v \in \mathrm{C}_0^\infty(\tilde{\Omega}_{\mathrm{a}})$. Let η_R be the standard mollifier defined by $\eta_R(x) = \frac{1}{R^d}\eta(x/R)$ Let

$$\chi_R = \begin{cases} 1 & \text{if} \quad |x| < 2R \\ 0 & \text{if} \quad |x| \geq 2R, \end{cases}$$

be the indicator function of B_R, and set

$$\varphi_R(x) := (\eta_R * \chi_R)(x)$$

so that it is a smooth bump function. Recall that $\varphi_R(x)$ is of class C^∞ and satisfies

$$0 \leq \varphi_R(x) \leq 1, \quad \text{and} \quad \begin{cases} \varphi_R(x) = 1 & \text{for} \quad |x| < R, \\ \varphi_R(x) = 0 & \text{for} \quad |x| \geq 3R, \end{cases}$$

Thus, $v-\varphi_R v$ is smooth and vanishes on $B_R(0)$. By Theorem 3.6,

$$
\begin{aligned}
0 &= \int_{\tilde{\Omega}_{\mathrm{a}}\setminus B_R(0)} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla (v-\varphi_R v) = \int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla (v-\varphi_R v) \\
&= \int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla v - \int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla(\varphi_R v) = \int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla v - \int_{B_{3R}(0)} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla(\varphi_R v).
\end{aligned}
$$

This implies

$$
\int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla v = \int_{B_{3R}(0)} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla(\varphi_R v). \tag{3.37}
$$

Also note

$$
\Big| \int_{B_{3R}(0)} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla(\varphi_R v) \Big| \leq \; \|\mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}}\|_{L^2(B_{3R}(0))} \|\nabla(\varphi_R v)\|_{L^2(B_{3R}(0))}. \tag{3.38}
$$

Moreover,

$$
\begin{aligned}
\|\nabla(\varphi_R v)\|_{L^2(B_{3R}(0))} &\leq \|\varphi_R \nabla v\|_{L^2(B_{3R}(0))} + \left\| v \nabla \varphi_R^{\top} \right\|_{L^2(B_{3R}(0))} \\
&\leq \|\nabla v\|_{L^2(B_{3R}(0))} + \|v\|_{L^2(B_{3R}(0))} \|\nabla \varphi_R\|_{L^2(B_{3R}(0))}.
\end{aligned} \tag{3.39}
$$

Furthermore,

$$
\begin{aligned}
\|\nabla \varphi_R\|^2_{L^2(B_{3R}(0))} &= \sum_{i=1}^d \int\limits_{L^2(B_{3R}(0))} \left|\tfrac{\partial \varphi_R}{\partial x_i}\right|^2 dx = \sum_{i=1}^d \int\limits_{L^2(B_{3R}(0))} \left|\tfrac{\partial \eta_R}{\partial x_i} * \chi_R\right|^2 dx \\
&= \sum_{i=1}^d \left\|\tfrac{\partial \eta_R}{\partial x_i} * \chi_R\right\|^2_{L^2(B_{3R}(0))} \leq \sum_{i=1}^d \left\|\tfrac{\partial \eta_R}{\partial x_i}\right\|^2_{L^1(B_{3R}(0))} \|\chi_R\|^2_{L^2(B_{3R}(0))} \quad \text{by Youngs's Inequality} \\
&= \sum_{i=1}^d \Big(\int\limits_{B_{3R}(0)} \left|\tfrac{\partial \eta_R}{\partial x_i}\, dx\right| \Big)^2 \cdot \Big(\int\limits_{B_{3R}(0)} |\chi_R|^2\, dx \Big) \leq \sum_{i=1}^d \Big(\int\limits_{B_{3R}(0)} \left|\tfrac{1}{R^{d+1}} \tfrac{\partial \eta}{\partial x_i}(x/R)\right| dx \Big)^2 \cdot \Big(\int\limits_{B_{3R}(0)} 1\, dx \Big) \\
&= \sum_{i=1}^d \Big(\int\limits_{B_3(0)} \left|\tfrac{1}{R} \tfrac{\partial \eta}{\partial x_i}(x)\right| dx \Big)^2 \cdot \Big(\int\limits_{B_{3R}(0)} 1 dx \Big) \lesssim R^{d-2}.
\end{aligned}
$$

Thus for $d \geq 3, \|\nabla \varphi_R\|_{L^2(B_{3R}(0))} \to 0$ and for $d=2$, $\|\nabla \varphi_R\|_{L^2(B_{3R}(0))}$ is uniformly bounded in R. Since v is fixed, $\|v\|_{L^2(B_{3R}(0))} \to 0$ as $R \to 0$ and taking $R \to 0$ in (3.38) and using (3.37) and (3.39) shows

$$
\begin{aligned}
\Big| \int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla v \Big| &= \lim_{R\to 0} \Big| \int_{B_{3R}(0)} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}} : \nabla(\varphi_R v) \Big| \\
&\leq \lim_{R\to 0} \|\mathbb{C} : \nabla \bar{w}_0^{\mathrm{a}}\|_{L^2(B_{3R}(0))} \big(\|\nabla v\|_{L^2(B_{3R}(0))} + \|v\|_{L^2(B_{3R}(0))} \|\nabla \varphi_R\|_{L^2(B_{3R}(0))} \big) = 0
\end{aligned} \tag{3.40}
$$

so long as $d \geq 2$, which proves (3.21). The $d=1$ is special since the atomistic region becomes disconnected when a neighborhood of the origin is deleted. To remedy this, additional constraints for each connected overlap region are required so the above arguments need to be carried out twice.

Next, we establish the continuum analogue for Theorem 3.5: the function $\bar{w}_0^{\mathrm{c}}$ satisfies

$$
\int_{\tilde{\Omega}_c} \mathbb{C} : \nabla \bar{w}_0^{\mathrm{c}} : \nabla v = 0 \quad \forall\, v \in H_0^1(\tilde{\Omega}_{\mathrm{c}}). \tag{3.41}
$$

We prove (3.41) for $v \in \mathrm{C}_0^\infty(\tilde{\Omega}_{\mathrm{c}})$; the general case follows by density. Interpolation of v on each finite element grid $\tilde{\mathcal{T}}_{h,n} = \epsilon_n \mathcal{T}_{h,n}$ yields a sequence, v_n^{c}, which converges to v in $H^1_{\mathrm{loc}}(\tilde{\Omega}_{\mathrm{c}})$. For large enough n (once $\tilde{\Omega}_{\mathrm{c},n}$ contains the support of v), we have

$$0 = \int_{\tilde{\Omega}_{\mathrm{c},n}} W''(\epsilon_n \nabla \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx = \int\limits_{\mathrm{supp(v)}} W''(\epsilon_n \nabla \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx. \tag{3.42}$$

Summarizing, v_n^{c} converges to v strongly on $H^1(\mathrm{supp}(v))$ and $\bar{w}_n^{\mathrm{c}} \rightharpoonup \bar{w}_0^{\mathrm{c}}$. Moreover

$$\begin{aligned}
0 = & \lim_{n\to\infty} \int\limits_{\mathrm{supp}(v)} W''(\epsilon_n \nabla \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx \\
= & \lim_{n\to\infty} \int\limits_{\mathrm{supp}(v)} (W''(\epsilon_n \nabla \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) - W''(\epsilon_n \nabla I_n \tilde{\boldsymbol{u}}_n^{\infty})) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx \\
& \quad + \lim_{n\to\infty} \int\limits_{\mathrm{supp}(v)} W''(\epsilon_n \nabla I_n \tilde{\boldsymbol{u}}_n^{\infty}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx \\
\lesssim & \lim_{n\to\infty} \epsilon_n \|\nabla \tilde{\boldsymbol{u}}_n^{\mathrm{con}} - \nabla I_n \tilde{\boldsymbol{u}}_n^{\infty}\|_{L^2(\tilde{\Omega}_{\mathrm{c},n})} \|\nabla \bar{w}_n^{\mathrm{c}}\|_{L^2(\tilde{\Omega}_{\mathrm{c},n})} \|\nabla v_n^{\mathrm{c}}\|_{L^2(\tilde{\Omega}_{\mathrm{c},n})} \\
& \quad + \lim_{n\to\infty} \int\limits_{\mathrm{supp}(v)} W''(\epsilon_n \nabla I_n \tilde{\boldsymbol{u}}_n^{\infty}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx \\
= & \lim_{n\to\infty} \int\limits_{\mathrm{supp}(v)} W''(\epsilon_n \nabla I_n \tilde{\boldsymbol{u}}_n^{\infty}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx
\end{aligned} \tag{3.43}$$

Reasoning as in the atomistic case, $W''(\epsilon_n \nabla I_n \tilde{\boldsymbol{u}}_n^{\infty})$ converges uniformly to $W''(0)$. Thus, we have a duality pairing of a strongly and weakly convergent sequence, which converges to the pairing of the limits:

$$0 = \lim_{n\to\infty} \int\limits_{\mathrm{supp}(v)} W''(\epsilon_n \nabla I_n \tilde{\boldsymbol{u}}_n^{\infty}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla v_n^{\mathrm{c}}\, dx = \int\limits_{\mathrm{supp}(v)} W''(0) : \nabla \bar{w}_0^{\mathrm{c}} : \nabla v\, dx$$

□

Step 3:

With the convergence properties of Step 1 and limiting equations of Step 2, we shall prove

Theorem 3.8. *Let $\bar{w}_n^{\mathrm{a}}$ and $\nabla \bar{w}_n^{\mathrm{c}}$ be as defined in Step 1. Then*

$$(\nabla I \bar{w}_n^{\mathrm{a}}, \nabla \bar{w}_n^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})} \to (\nabla \bar{w}_0^{\mathrm{a}}, \nabla \bar{w}_0^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})}\,. \tag{3.44}$$

Proof of Theorem 3.8. Split $\tilde{\Omega}_{\mathrm{o}}$ into an inner part, A_1, and an outer part, A_2 such that $\tilde{\Omega}_{\mathrm{o}} = A_1 \cup A_2$ and A_1 and A_2 have disjoint interiors. Specifically, let $\lfloor x \rfloor$ be the greatest integer less than x and set

$$\begin{aligned}
A_1 &:= (\lfloor \psi_{\mathrm{a}}/2 \rfloor \tilde{\Omega}_{\mathrm{core}}) \backslash \tilde{\Omega}_{\mathrm{core}} \\
A_2 &:= \tilde{\Omega}_{\mathrm{o}} \backslash A_1.
\end{aligned}$$

From (3.46) of Lemma 3.9 below, we see that

$$\|\nabla \left(\bar{w}_n^{\mathrm{c}} - \bar{w}_0^{\mathrm{c}}\right)\|_{L^2(A_2)} \to 0.$$

and (3.57) of Lemma 3.10 below gives,

$$\|\nabla\left(I_n\bar{w}_n^{\mathrm{a}}-\bar{w}_0^{\mathrm{a}}\right)\|_{L^2(A_1)}\to 0.$$

Using these two results along with the weak convergence properties of Lemma 3.4—namely, $\bar{w}_n^{\mathrm{c}}\rightharpoonup\bar{w}_0^{\mathrm{c}}$ on A_1 and $\bar{w}_n^{\mathrm{a}}\rightharpoonup\bar{w}_0^{\mathrm{a}}$ on A_2—yields

$$\begin{aligned}(\nabla I_n\bar{w}_n^{\mathrm{a}},\nabla\bar{w}_n^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})} &= (\nabla I_n\bar{w}_n^{\mathrm{a}},\nabla\bar{w}_n^{\mathrm{c}})_{L^2(A_1)}+(\nabla I_n\bar{w}_n^{\mathrm{a}},\nabla\bar{w}_n^{\mathrm{c}})_{L^2(A_2)}\\ &\to (\nabla\bar{w}_0^{\mathrm{a}},\nabla\bar{w}_0^{\mathrm{c}})_{L^2(A_1)}+(\nabla\bar{w}_0^{\mathrm{a}},\nabla\bar{w}_0^{\mathrm{c}})_{L^2(A_2)}=(\nabla\bar{w}_0^{\mathrm{a}},\nabla\bar{w}_0^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})}.\end{aligned} \tag{3.45}$$

□

In the preceding, we have made reference to the following lemma, which we now prove.

Lemma 3.9. *Let $\bar{w}_n^{\mathrm{c}}$ and $\bar{w}_0^{\mathrm{c}}$ be as defined in Lemma 3.4. Then*

$$\|\nabla\left(\bar{w}_n^{\mathrm{c}}-\bar{w}_0^{\mathrm{c}}\right)\|_{L^2(A_2)}\to 0. \tag{3.46}$$

Proof. Recall that each element of the continuum sequence satisfies a variational equality of the form

$$\int_{\tilde{\Omega}_{\mathrm{c},n}} W''(\epsilon_n\nabla\tilde{\boldsymbol{u}}_n^{\mathrm{con}}):\nabla\bar{w}_n^{\mathrm{c}}:\nabla v_n^{\mathrm{c}}\,dx = 0 \quad \forall\, v^{\mathrm{c}}\in\tilde{\boldsymbol{\mathcal{U}}}_{h,0,n}^{\mathrm{c}}. \tag{3.47}$$

According to Theorem 3.6 the function $\bar{w}_0^{\mathrm{c}}$ satisfies a variational equality of the form

$$\int_{\tilde{\Omega}_{\mathrm{c}}} W''(0):\bar{w}_0^{\mathrm{c}}:v_0^{\mathrm{c}}\,dx=0 \quad \forall\, v_0^{\mathrm{c}}\in H_0^1(\tilde{\Omega}_{\mathrm{c}}), \tag{3.48}$$

which corresponds to a linear elliptic system. From elliptic regularity, $\bar{w}_0^{\mathrm{c}}$ belongs to $H^2_{\mathrm{loc}}(\tilde{\Omega}_{\mathrm{c}})$. Recalling that mesh is fully resolved on $\tilde{\Omega}_{\mathrm{o,ex}}$, it follows that

$$\hat{w}_n^{\mathrm{c}}:=I_n\bar{w}_0^{\mathrm{c}}\to\bar{w}_0^{\mathrm{c}} \quad \text{in } H^1(A_2). \tag{3.49}$$

The goal is now to show

$$\|\nabla\left(\hat{w}_n^{\mathrm{c}}-\bar{w}_n^{\mathrm{c}}\right)\|_{L^2(A_2)}\to 0, \tag{3.50}$$

which will further imply (3.46).

Let η be a smooth bump function with compact support in $\tilde{\Omega}_{\mathrm{o,ex}}$ and equal to 1 on A_2. Thus $\eta^2(\hat{w}_n^{\mathrm{c}} - \bar{w}_n^{\mathrm{c}})$ can be extended by 0 to get a sequence of functions well defined on all of $\tilde{\Omega}_{\mathrm{c}}$. Also set $z_n := \hat{w}_n^{\mathrm{c}} - \bar{w}_n^{\mathrm{c}}$. We have

$$\begin{aligned}
\int_{A_2} |\nabla z_n|^2 \, dx &\le \int_{\tilde{\Omega}_{\mathrm{o,ex}}} |\nabla(\eta z_n)|^2 \, dx \lesssim \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla(\eta z_n) : \nabla(\eta z_n) \, dx \\
&= \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \eta \nabla z_n : \eta \nabla z_n + 2W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \eta \nabla z_n : \left(z_n \nabla \eta^\top\right) dx \\
&\quad + \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \left(z_n \nabla \eta^\top\right) : \left(z_n \nabla \eta^\top\right) dx \\
&= \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \hat{w}_n^{\mathrm{c}} : \eta^2 \nabla z_n + 2W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \hat{w}_n^{\mathrm{c}} : \left(\eta z_n \nabla \eta^\top\right) dx \\
&\quad - \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \eta^2 \nabla z_n + 2W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \left(\eta z_n \nabla \eta^\top\right) dx \\
&\quad + \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \left(z_n \nabla \eta^\top\right) : \left(z_n \nabla \eta^\top\right) dx.
\end{aligned} \tag{3.51}$$

Since $I_n\left(\eta^2 z_n\right) \in \tilde{\boldsymbol{\mathcal{U}}}_{h,0,n}^{\mathrm{c}}$ has support in $\tilde{\Omega}_{\mathrm{o,ex}}$, using (3.47) we can write the second integral above as

$$\begin{aligned}
&\int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \eta^2 \nabla z_n + 2W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \eta z_n \nabla \eta^\top \, dx \\
&\quad = \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \eta^2 \nabla z_n + 2W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \eta z_n \nabla \eta^\top \, dx \\
&\qquad - \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla I_n\left(\eta^2 z_n\right) dx \\
&\quad = \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla\left(\eta^2 z_n - I_n\left(\eta^2 z_n\right)\right) dx.
\end{aligned} \tag{3.52}$$

Using this result in (3.51) produces

$$\begin{aligned}
\int_{A_2} |\nabla z_n|^2 \, dx &\lesssim \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \hat{w}_n^{\mathrm{c}} : \eta^2 \nabla z_n + 2W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \hat{w}_n^{\mathrm{c}} : \left(\eta z_n \nabla \eta^\top\right) dx \\
&- \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \nabla \bar{w}_n^{\mathrm{c}} : \nabla\left(\eta^2 z_n - I_n\left(\eta^2 z_n\right)\right) dx + \int_{\tilde{\Omega}_{\mathrm{o,ex}}} W''(\epsilon_n \tilde{\boldsymbol{u}}_n^{\mathrm{con}}) : \left(z_n \nabla \eta^\top\right) : \left(z_n \nabla \eta^\top\right) dx.
\end{aligned} \tag{3.53}$$

Hence,

$$\int_{A_2} |\nabla z_n|^2\, dx \lesssim \int_{\tilde\Omega_{\rm o,ex}} W''(\epsilon_n \tilde{\boldsymbol u}_n^{\rm con}) : \nabla\eta \hat w_n^{\rm c} : \eta\nabla z_n\, dx + \|\eta z_n \nabla\eta^\top\|_{L^2({\rm supp}(\eta))} + \|\nabla\left(\eta^2\left(z_n\right) - I_n\left(\eta^2 z_n\right)\right)\|_{L^2(\tilde\Omega_{\rm o,ex})} + \|z_n\nabla\eta^\top\|^2_{L^2({\rm supp}(\eta))}. \tag{3.54}$$

Since z_n converges weakly to 0 in H^1 and hence strongly in L^2, both $\|\eta z_n \nabla\eta^\top\|_{L^2({\rm supp}(\eta))}$ and $\|z_n\nabla\eta^\top\|^2_{L^2({\rm supp}(\eta))}$ go to zero in (3.54). Moreover, $\nabla\hat w_n^{\rm c} \to \nabla\bar w_0^{\rm c}$ by construction and $\nabla z_n \rightharpoonup 0$ so reasoning as we did just after (3.43)

$$\int_{\tilde\Omega_{\rm o,ex}} W''(\epsilon_n \tilde{\boldsymbol u}_n^{\rm con}) : \nabla\eta \hat w_n^{\rm c} : \eta\nabla z_n\, dx \to 0. \tag{3.55}$$

Finally, to show

$$\|\nabla\left(\eta^2 z_n - I_n\left(\eta^2 z_n\right)\right)\|_{L^2(\tilde\Omega_{\rm o,ex})} \to\ 0, \tag{3.56}$$

observe that $\eta^2 z_n - I_n\left(\eta^2 z_n\right)$ vanishes outside a neighborhood $N_\delta \subset\subset \tilde\Omega_{\rm o,ex}$ of ${\rm supp}(\eta)$. Then

$$\begin{aligned}\|\nabla\left(\eta^2 z_n - I_n\left(\eta^2 z_n\right)\right)\|^2_{L^2(N_\delta)} &= \int_{N_\delta} \left|\nabla\left(\eta^2 z_n - I_n\left(\eta^2 z_n\right)\right)\right|^2\, dx \\ &\le \sum_{\substack{T\in\mathcal{T}_{h,n}\\ T\cap N_\delta\neq\emptyset}} \int_T \left|\nabla\left(\eta^2 z_n - I_n\left(\eta^2 z_n\right)\right)\right|^2\, dx \lesssim \sum_{\substack{T\in\mathcal{T}_{h,n}\\ T\cap N_\delta\neq\emptyset}} |T|^2 \|\nabla^2\left(\eta^2 z_n\right)\|^2_{L^2(T)},\end{aligned}$$

where the last line follows from the Bramble-Hilbert lemma and scaling. Because z_n is piecewise linear its second derivatives vanish on all T. Using the uniform boundedness of η and its derivatives then yields

$$\|\nabla^2(\eta^2 z_n)\|^2_{L^2(T)} = \int_T \left|\nabla^2(\eta^2 z_n)\right|^2 dx \lesssim \int_T |z_n|^2\, dx + \int_T |\nabla(z_n)|^2\, dx.$$

Choose N'_δ such that $\bigcup_{\substack{T\in\mathcal{T}_{h,n}\\ T\cap N_\delta\neq\emptyset}} \subset N'_\delta \subset\subset \tilde\Omega_{\rm o,ex}$. Then

$$\begin{aligned}\|\nabla\left(\eta^2 z_n - I_n\left(\eta^2 z_n\right)\right)\|^2_{L^2(N_\delta)} &\lesssim \max_{\substack{T\in\mathcal{T}_{h,n}\\ T\cap N_\delta\neq\emptyset}} |T|^2 \Big(\sum_{\substack{T\in\mathcal{T}_{h,n}\\ T\cap N_\delta\neq\emptyset}} \int_T |z_n|^2 + |\nabla z_n|^2\, dx\Big) \\ &\lesssim \max_{\substack{T\in\mathcal{T}_{h,n}\\ T\cap N_\delta\neq\emptyset}} |\epsilon_n|^2 \left(\|z_n\|_{L^2(N'_\delta)} + \|\nabla z_n\|_{L^2(N'_\delta)}\right).\end{aligned}$$

Now note that $\|z_n\|_{L^2(N'_\delta)} = \|\hat w_n^{\rm c} - \bar w_n^{\rm c}\|_{L^2(N'_\delta)} \to 0$ by construction of $\hat w_n^{\rm c}$ while $\|\nabla z_n\|_{L^2(N'_\delta)}$ is bounded since z_n is weakly convergent in $H^1(N'_\delta)$. It follows that if the maximum element size, which is of order ϵ_n, goes to 0, then we obtain (3.56). Inserting (3.55) and (3.56) in (3.54) yields (3.50), which in turn implies (3.46).

□

Our second task is to prove the atomistic version of Lemma 3.9 over A_1.

Lemma 3.10. *Let $\bar w_n^{\rm a}$ and $\bar w_0^{\rm a}$ be as defined in Lemma 3.4. Then*

$$\|\nabla\left(I_n \bar w_n^{\rm a} - \bar w_0^{\rm a}\right)\|_{L^2(A_1)} \to 0. \tag{3.57}$$

Proof. Consider again a sequence $\hat{w}_n^{\rm a} := I_n \bar{w}_0^{\rm a}$, which converges to $\bar{w}_0^{\rm a}$ in $H^1_{\rm loc}(\tilde{\Omega}_{\rm a})$. In particular, the sequence converges strongly on A_1. Take η to be a bump function adapted to A_1, and recall that each $\bar{w}_n^{\rm a}$ solves a problem

$$0 = \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n} \bar{w}_n^{\rm a}(\xi) : D_{\epsilon_n} v^{\rm a}(\xi) \quad \forall v^{\rm a} \in \tilde{\boldsymbol{\mathcal{U}}}^{\rm a}_{0,n}. \tag{3.58}$$

As before, to prove (3.57) we will show that

$$\|\nabla I_n \left(\hat{w}_n^{\rm a} - \bar{w}_n^{\rm a}\right)\|_{L^2(A_1)} \to 0. \tag{3.59}$$

We recall that the product rule for difference quotients involves a shift operator which we denote by T_r:

$$\begin{aligned} T_{\epsilon_n\rho} v(\xi) &= v(\xi + \epsilon_n \rho), \\ D_{\epsilon_n\rho}(uv)(\xi) &= (D_{\epsilon_n\rho} u) v + (T_{\epsilon_n\rho} u) D_{\epsilon_n\rho} v, \\ T_{\epsilon_n} u D_{\epsilon_n} v &= \left(T_{\epsilon_n\rho} u D_{\epsilon_n\rho} v\right)_{\rho\in\mathcal{R}}. \end{aligned} \tag{3.60}$$

Now set $y_n := \hat{w}_n^{\rm a} - \bar{w}_n^{\rm a}$ and note since $\eta^2 y_n \in \boldsymbol{\mathcal{U}}^{\rm a}_{0,n}$, the product rule in (3.60) gives

$$\begin{aligned} 0 &= \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n} \bar{w}_n^{\rm a}(\xi) : D_{\epsilon_n} \left(\eta^2 (y_n)\right)(\xi) \\ &= \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n} \bar{w}_n^{\rm a}(\xi) : D_{\epsilon_n} (\eta y_n) T_{\epsilon_n} \eta(\xi) \\ &\qquad + \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n} \bar{w}_n^{\rm a}(\xi) : \eta y_n D_{\epsilon_n} \eta(\xi). \end{aligned} \tag{3.61}$$

Thus

$$\begin{aligned} \int_{A_1} |\nabla I_n y_n|^2 \, dx &\lesssim \int_{\tilde{\Omega}_{\rm a}} |\nabla I_n (\eta y_n)|^2 \, dx \lesssim \langle \delta^2 \tilde{\mathcal{E}}^{\rm a}(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}) D_{\epsilon_n}(\eta y_n), D_{\epsilon_n}(\eta y_n)\rangle \\ &= \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n}(\eta y_n) : D_{\epsilon_n}(\eta y_n) \\ &= \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : T_{\epsilon_n} \eta D_{\epsilon_n}(y_n) : D_{\epsilon_n}(\eta y_n) + \sum_{\xi \in \tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V_\xi''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : y_n D_{\epsilon_n}(\eta) : D_{\epsilon_n}(\eta y_n) \end{aligned} \tag{3.62}$$

Next, simply substitute the definition, $y_n = \hat{w}_n^{\rm a} - \bar{w}_n^{\rm a}$, into the first summand above to obtain

$$
\begin{aligned}
\int_{A_1} |\nabla I_n y_n|^2 \, dx \;\lesssim\; & \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : T_{\epsilon_n}\eta D_{\epsilon_n}(\hat{w}_n^{\rm a}) : D_{\epsilon_n}(\eta y_n) \\
& - \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : T_{\epsilon_n}\eta D_{\epsilon_n}(\bar{w}_n^{\rm a}) : D_{\epsilon_n}(\eta y_n) \\
& + \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : y_n D_{\epsilon_n}(\eta) : D_{\epsilon_n}(\eta y_n) \\
= & \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : T_{\epsilon_n}\eta D_{\epsilon_n}(\hat{w}_n^{\rm a}) : D_{\epsilon_n}(\eta y_n) \\
& - \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n}\bar{w}_n^{\rm a}(\xi) : \eta y_n D_{\epsilon_n}\eta(\xi) \quad \text{using (3.61)} \\
& + \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : y_n D_{\epsilon_n}(\eta) : D_{\epsilon_n}(\eta y_n) \\
\lesssim & \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n}\hat{w}_n^{\rm a}(\xi) : D_{\epsilon_n}(\eta y_n) T_{\epsilon_n}\eta(\xi) \\
& + \|\eta y_n D_{\epsilon_n}\eta\|_{\ell^2_{\epsilon_n}(\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n})} + \|y_n D_{\epsilon_n}(\eta)\|_{\ell^2_{\epsilon_n}(\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n})} \\
\lesssim & \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n}\hat{w}_n^{\rm a}(\xi) : D_{\epsilon_n}(\eta y_n) T_{\epsilon_n}\eta(\xi) + \|y_n\|_{\ell^2_{\epsilon_n}({\rm supp}(\bar{I}_n D_{\epsilon_n}\eta))} \\
\lesssim & \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''_\xi(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n}\hat{w}_n^{\rm a}(\xi) : D_{\epsilon_n}(\eta y_n) T_{\epsilon_n}\eta(\xi) + \|I_n y_n\|_{L^2({\rm supp}(\bar{I}_n D_{\epsilon_n}\eta))},
\end{aligned}
\tag{3.63}
$$

Since $I_n y_n \to 0$ on compact subsets of $\tilde{\Omega}_{\rm a}$ and because a compact subset of $\tilde{\Omega}_{\rm a}$—say X—can be chosen so that ${\rm supp}(\bar{I}_n D_{\epsilon_n}\eta) \subset X$ for large enough n, the last term tends to 0. To show that the first term also goes to 0, we use the integral formulation (3.8):

$$
\begin{aligned}
& \sum_{\xi\in\tilde{\mathcal{L}}^{\circ\circ}_{{\rm a},n}} V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : D_{\epsilon_n}\hat{w}_n^{\rm a}(\xi) : D_{\epsilon_n}(\eta y_n) T_{\epsilon_n}\eta(\xi) \\
& = \int_{\tilde{\Omega}_{\rm a}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : \bar{I}_n D_{\epsilon_n}\hat{w}_n^{\rm a} : \bar{I}_n(D_{\epsilon_n}(\eta(y_n))\, T_{\epsilon_n}\eta)\, dx \\
& = \int_{\tilde{\Omega}_{\rm a}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : \bar{I}_n D_{\epsilon_n}\hat{w}_n^{\rm a} : \bar{I}_n(D_{\epsilon_n}(y_n) T_{\epsilon_n}\eta T_{\epsilon_n}\eta)\, dx \\
& \quad + \int_{\tilde{\Omega}_{\rm a}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : \bar{I}_n D_{\epsilon_n}\hat{w}_n^{\rm a} : \bar{I}_n(y_n D_{\epsilon_n}(\eta) T_{\epsilon_n}\eta)\, dx \\
& \lesssim \int_{\tilde{\Omega}_{\rm a}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : \bar{I}_n D_{\epsilon_n}\hat{w}_n^{\rm a} : \bar{I}_n(D_{\epsilon_n}(y_n) T_{\epsilon_n}\eta T_{\epsilon_n}\eta)\, dx + \|\bar{I}_n y_n\|_{L^2({\rm supp}(\bar{I}_n D_{\epsilon_n}\eta))} \\
& \lesssim \int_{\tilde{\Omega}_{\rm a}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n}\tilde{\boldsymbol{u}}^\infty_{{\rm a},n}(\xi)) : \bar{I}_n(D_{\epsilon_n}\hat{w}_n^{\rm a} T_{\epsilon_n}\eta T_{\epsilon_n}\eta) : \bar{I}_n(D_{\epsilon_n}(y_n))\, dx + \|I_n y_n\|_{L^2({\rm supp}(\bar{I}_n D_{\epsilon_n}\eta))}
\end{aligned}
\tag{3.64}
$$

The last term again goes to zero since $I_n y_n \to 0$ in L^2 on compact subsets of $\tilde{\Omega}_{\rm a}$, and ${\rm supp}(\bar{I}_n D_{\epsilon_n}\eta)$ lies in such a subset for large enough n. To show that the remaining integral also tends to 0 we use that

$\bar{I}_n D_{\epsilon_n}(\hat{w}_n^{\mathrm{a}} - \bar{w}_n^{\mathrm{a}}) = \bar{I}_n D_{\epsilon_n} y_n$ converges weakly to 0 on $\mathrm{supp}(T\eta)$ by Lemma 3.7, and that

$$\bar{I}_n V''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}_{\mathrm{a},n}^{\infty}(\xi)),$$

converges uniformly to $W''(0)$ on $\mathrm{supp}(T_{\epsilon_n}\eta)$, according to Lemma 3.6. Meanwhile, $T_\epsilon \eta$ converges uniformly to η, and by replacing weak convergence with strong convergence in Lemma 3.7 and modifying the proof accordingly, we see that $\bar{I}_n D_{\epsilon_n} \hat{w}_n^{\mathrm{a}}$ converges strongly to $\nabla \bar{w}_0^{\mathrm{a}}$ on $\mathrm{supp}(T_\eta)$. The integral remaining in (3.64) is then a duality pairing of a strongly convergent and a weakly convergent sequence, which converges to the pairing of the limits. That is,

$$\int_{\tilde{\Omega}_{\mathrm{a}}} \bar{I}_n V''(\epsilon_n D_{\epsilon_n} \tilde{\boldsymbol{u}}_{\mathrm{a},n}^{\infty}(\xi)) : \bar{I}_n(D_{\epsilon_n} \hat{w}_n^{\mathrm{a}} T_{\epsilon_n}\eta T_{\epsilon_n}\eta) : \bar{I}_n(D_{\epsilon_n}(y_n))\, dx \to \int_{\tilde{\Omega}_{\mathrm{a}}} \mathbb{C} : \eta^2 \nabla \bar{w}_0^{\mathrm{a}} : 0\, dx = 0. \tag{3.65}$$

□

Step 4:

Proof of Theorem 3.2. We assume the existence of a sequence satisfying (3.15), which yields sequences of normalized functions $\bar{w}_n^{\mathrm{a}}$ and $\bar{w}_n^{\mathrm{c}}$ possessing the properties of Lemma 3.4. Combining (3.45) with (3.17) shows

$$(\nabla \bar{w}_0^{\mathrm{a}}, \nabla \bar{w}_0^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})} = 1. \tag{3.66}$$

Since $\bar{w}_0^{\mathrm{a}}$ and $\bar{w}_0^{\mathrm{c}}$ have seminorm equal to 1 over $\tilde{\Omega}_o$, we see that

$$(\nabla \bar{w}_0^{\mathrm{a}}, \nabla \bar{w}_0^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})} = \|\nabla \bar{w}_0^{\mathrm{a}}\|_{L^2(\tilde{\Omega}_{\mathrm{o}})} \|\nabla \bar{w}_0^{\mathrm{c}}\|_{L^2(\tilde{\Omega}_{\mathrm{o}})}$$

Hence $\nabla \bar{w}_0^{\mathrm{a}} = \alpha \nabla \bar{w}_0^{\mathrm{c}}$ on $\tilde{\Omega}_{\mathrm{o}}$ for some real number α implying

$$1 = (\alpha \nabla \bar{w}_0^{\mathrm{c}}, \nabla \bar{w}_0^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})} = \alpha \|\nabla \bar{w}_0^{\mathrm{c}}\|^2_{L^2(\tilde{\Omega}_{\mathrm{o}})} = \alpha.$$

Thus $\nabla \bar{w}_0^{\mathrm{a}}$ and $\nabla \bar{w}_0^{\mathrm{c}}$ are equal on $\tilde{\Omega}_o$. We can therefore define an H^1 function by

$$\bar{w}_0 = \begin{cases} \bar{w}_0^{\mathrm{a}} & \text{on} \quad \tilde{\Omega}_{\mathrm{a}} \\ \bar{w}_0^{\mathrm{c}} & \text{on} \quad \tilde{\Omega}_{\mathrm{c}} \end{cases},$$

which is a global solution to the linear homogeneous Cauchy-Born equation so that $\nabla \bar{w}_0 = 0$. We conclude that $(\nabla \bar{w}_0^{\mathrm{a}}, \nabla \bar{w}_0^{\mathrm{c}})_{L^2(\tilde{\Omega}_{\mathrm{o}})} = 0$, which contradicts (3.66). □

4. Conclusion

Appendix A. Extension Theorems

In this appendix, we recall Stein's extension theorem [39] for domains with minimally smooth boundary and a modified extension operator that preserves the H^1 seminorm due to Burenkov [5].

Theorem A.1 (Stein's Extension Theorem)**.** *Let U be a connected, open set for which there exists an $\epsilon > 0$, integers $N, M > 0$, and a sequence of open sets $U_1, U_2, \ldots$ satisfying*

1. *For each $x \in \partial U$, $B_\epsilon(x) \subset U_i$ for some i,*
2. *The intersection of more than N of the sets U_i is empty,*

(3) *For each U_i, there exists a Lipschitz continuous function φ_i and domains*

$$D_i = \left\{(x', y) \in \mathbb{R}^{n+1} : y > \varphi_i(x'), |\varphi_i(x_1') - \varphi_i(x_2')| \le M\,|x_1' - x_2'|\right\}$$

such that

$$U_i \cap U = U_i \cap D_i.$$

Then there exists a bounded linear extension operator $E : H^1(U) \to H^1(\mathbb{R}^d)$. The bound of the extension depends upon the domain U through N, M, and ϵ.

Theorem A.1 can be used to prove an extension theorem with preservation of seminorm due to Burenkov [5]:

Theorem A.2 (Extension with preservation of seminorm)**.** *Let U be a connected, bounded open set for which there exists a bounded linear extension operator $E : H^1(U) \to H^1(\mathbb{R}^n)$ and a bounded projection operator P from $H^1(U)$ onto the constants with the property that for all $f \in H^1(U)$,*

$$\|f - Pf\|_{L^2(U)} \lesssim c(U)\|f\|_{H^1(U)}.$$

Then the operator defined by

$$R = P + E(Id - P)$$

is a linear extension operator with the property that

$$\|\nabla Rf\|_{L^2(U)} \le \|E\|\,(c(U) + 1)\,\|\nabla f\|_{L^2(U)}.$$

Remark A.3. *We can set E to be Stein's extension operator [39] and choose*

$$Pu = \frac{1}{m(U)} \int\limits_U u(x)\,dx.$$

In this case $c(U)$ is the Poincare constant for the domain U.

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