ANALYSIS OF BLENDED ATOMISTIC/CONTINUUM HYBRID METHODS

XINGJIE HELEN LI, CHRISTOPH ORTNER,
ALEXANDER V. SHAPEEV, AND BRIAN VAN KOTEN

Abstract. We present a comprehensive error analysis of two prototypical atomistic-to-continuum coupling methods of blending type: the energy-based and the force-based quasicontinuum methods.

Our results are valid in two and three dimensions, for finite range many-body interactions (e.g., EAM type), and in the presence of lattice defects (we consider point defects and dislocations). The two key ingredients in the analysis are (i) new force and energy consistency error estimates; and (ii) a new technique for proving energy norm stability of a/c couplings that requires only the assumption that the exact atomistic solution is a stable equilibrium.

1. Introduction

Atomistic-to-continuum coupling methods (a/c methods) are a class of concurrent multiscale schemes coupling molecular mechanics models of atomistic processes with continuum mechanics models of long-ranged elastic fields. A recent extensive overview and benchmark of a/c schemes for material defect simulation is presented in [28]. These schemes can, broadly, be categorised into sharp-interface couplings and blending methods. Each of these categories can further be divided into energy-based (conservative) and force-based (non-conservative) a/c couplings. In the present paper we develop a comprehensive error analysis of both energy-based and force-based a/c couplings of blending type, which forms the theoretical background for the optimised formulations in [26, 21].

Precisely, we will consider (i) the B-QCE scheme formulated in [38, 26], which is closely related to methods proposed in [41, 2, 1]; and (ii) the B-QCF scheme formulated in [24, 20, 21], which is closely related to methods proposed in [1, 2, 3, 14, 22, 35, 37, 41]. While our results are not be immediately applicable to these related schemes [41, 2, 1, 3, 14, 22, 35, 37], we expect that many of the techniques we develop can be employed to develop such extensions.

In recent years a comprehensive numerical analysis theory of a/c methods has begun to emerge, which is summarized in the review article [25]. In one dimension, the foundations of this theory are largely completed [25]. In two and three dimensions only partial results exist to date: in [32] sharp error bounds for an energy-based coupling scheme are proven, in the presence of point defects. However, the scheme itself is restricted to two dimensions and pair interactions, and moreover, the analysis makes an assumptions on the magnitude of the atomistic solution in order to establish stability of the a/c scheme. In [24] a sharp error estimate is established, which is valid in two and three dimensions and for general

Date: April 19, 2014.

2000 *Mathematics Subject Classification.* 65N12, 65N15, 70C20.

Key words and phrases. atomistic models, coarse graining, atomistic-to-continuum coupling, quasicontinuum method, blending.

XHL was supported by an AMS-Simons Travel Grant. CO's work was supported by EPSRC grant EP/H003096, ERC Starting Grant 335120 and by the Leverhulme Trust through a Philip Leverhulme Prize. AVS was supported by the AFOSR Award FA9550–12–1–0187.

interatomic potentials; however, to establish stability of the scheme it is assumed that the atomistic solution is globally smooth, which therefore excludes the presence of lattice defects.

Our starting assumption is that the error analysis ought to be performed in the energy-norm as this provides, to the best of our knowledge, the only route at present to include crystal defects in the analysis following [32, 12, 25].

Thus, there are two key difficulties in extending the one-dimensional analysis in [25] (and references therein) to two and three dimensions:

(1) *Energy-norm consistency:* While consistency error estimates in L^p-type norms are readily obtained from elementary Taylor expansions, consistency error estimates in the negative energy norm are more difficult to obtain, since they require an analytically convenient "weak form" of the forces. The different interaction ranges of the continuum and atomistic models make this non-trivial as can, for example, be seen from the analysis in [30], which develops such a "weak form" for energy-based sharp interface a/c couplings. In the present paper we draw from ideas in [34] to establish sharp consistency error estimates; see § 4.3 and § 4.4.
(2) *Stability:* A key observation in [24] was that force-based blending (the B-QCF scheme) with a macroscopic blending width yields a "universally stable" a/c coupling in the terminology of [33]. However, stability is proven under conditions which, to our understanding, make it impossible to extend the analysis to situations with crystal defects, and the required blending width makes the scheme prohibitively expensive. In [20] it was then shown that the B-QCF scheme is also stable in a natural energy-norm, and that only a moderate blending width is required. However, this result required the assumption that a related B-QCE scheme is stable, which was still unknown.

   In the present work, we develop a new technique that allows us to prove stability of the B-QCE scheme; see § 4.5. After extending results from [20] and employing regularity estimates for the elastic fields generated by crystal defects [12], we are able to also conclude stability of the B-QCF scheme; see § 4.6. Aside from technical conditions, our stability results only require the assumption that the atomistic equilibrium we are aiming to approximate is itself stable, but no assumptions on the magnitude or smoothness of the solution as in [32] or [24] are required.

The paper is structured as follows: In § 2 we introduce a number of concepts that we require in order to formulate the B-QCE and B-QCF schemes (§ 3.1.2 and § 3.1.3), and to state the main results in § 3.2. Our concluding remarks are also contained in that section, in § 3.3. In § 4 we present the key ideas and intermediate results that are required to prove the main results. Finally, in § 5–§ 7 we present the technical details of the proofs.

2. Prerequisites

2.1. **Generic notation.** Functions are normally maps from $\mathbb{R}^d \to \mathbb{R}^m$ or $\mathbb{Z}^d \to \mathbb{R}^m$ for some $d, m \in \{1, 2, 3\}$. Vectors in $\mathbb{R}^d, \mathbb{R}^m$ or vectorial functions are normally denoted by the symbols y, z, u, v, w, f. Lattice sites, i.e. elements of $\mathbb{Z}^d$ are normally denoted by ξ, η, while points in the continuous reference configuration are denoted by $x \in \mathbb{R}^d$. We also identify x with the identity map.

Matrices or matrix-valued functions are normally denoted by $\mathsf{A}, \mathsf{B}, \mathsf{S}, \mathsf{R}$ and so forth. Tensors of fourth or higher rank are normally denoted by $\mathbb{A}, \mathbb{B}, \mathbb{C}$, and so forth.

If a function $f : \mathbb{R}^d \to \mathbb{R}^m$ is (weakly) differentiable, then we denote its jacobi matrix at x by $\nabla f(x)$. If f is scalar-valued, then $\nabla^2 f(x)$ denotes the hessian matrix. In general, $\nabla^j f(x)$

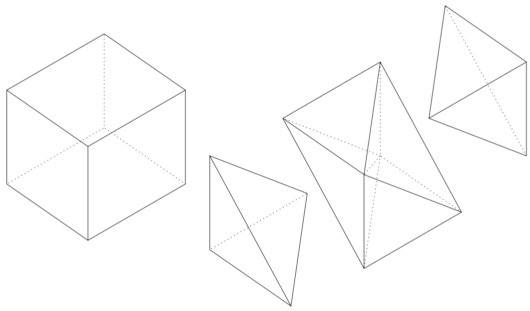

FIGURE 1. Subdivision of the cube $[0,1]^3$ into 6 tetrahedra $\hat{T}_1, \dots, \hat{T}_6$, so that the resulting partition $\mathscr{T}$ is invariant under reflection about any lattice point $\xi \in \mathbb{Z}^3$.

denotes a tensor of order $m \times d \times \cdots \times d$. Partial derivatives with respect to some variable s are denoted by $\frac{\partial}{\partial s}$ or ∂_s. If $\alpha = (\alpha_1, \dots, \alpha_d)$ is a multi-index, then $\partial_\alpha = \partial_{x_{\alpha_1}} \cdots \partial_{x_{\alpha_d}}$.

Directional derivatives are denoted by $\nabla_\rho f := \nabla f \rho$, $\rho \in \mathbb{R}^d$. If $\mathcal{R} \subset \mathbb{R}^d$ then we define a collection of directional derivatives $\nabla_{\mathcal{R}} f(x) := (\nabla_\rho f(x))_{\rho \in \mathcal{R}}$.

Our use of tensor notation is intuitive and not crucial to follow the main ideas. Nevertheless, for the sake of completeness we formally define our notation. The symbol $\otimes$ denotes the usual tensor product: if $\mathbb{A} = (A_{i_1,\dots,i_r}) \in \mathbb{R}^{n_1 \times \cdots \times n_r}$ and $\mathbb{B} = (B_{k_1,\dots,k_s}) \in \mathbb{R}^{m_1 \times \cdots \times m_s}$, then $\mathbb{A} \otimes \mathbb{B} = (A_{i_1,\dots,i_r} B_{k_1,\dots k_s}) \in \mathbb{R}^{n_1 \times \cdots \times n_r \times m_1 \times \cdots \times m_s}$. If $\mathbb{A} = (A_{i_1,\dots,i_{s+r}}) \in \mathbb{R}^{m_1 \times \cdots \times m_s \times n_1 \times \cdots \times n_r}, \mathbb{B} = (B_{j_1,\dots,j_r}) \in \mathbb{R}^{n_1 \times \cdots \times n_r}$, then the contraction operator is denoted by $(\mathbb{A} : \mathbb{C})_{j_1,\dots,j_s} = \sum_{i_1}^{n_1} \cdots \sum_{i_r}^{n_r} A_{j_1,\dots,j_s,i_1,\dots,i_r} B_{i_1,\dots,i_r}$. In particular, if $\mathbb{A}, \mathbb{B}$ have the same rank, then $\mathbb{A} : \mathbb{B} \in \mathbb{R}$ denotes the euclidean inner product.

The symbol $\langle \cdot, \cdot \rangle$ denotes an abstract duality pairing. If X, Y are normed linear spaces and $\mathscr{F} : X \to Y$ has well-defined directional derivatives at a point $u \in X$, then we denote the first of second derivatives, respectively, by

$$\langle \delta \mathscr{F}(u), v \rangle := \lim_{t \to 0} t^{-1} \big(\mathscr{F}(u + tv) - \mathscr{F}(u) \big) \quad \text{and}$$
$$\langle \delta^2 \mathscr{F}(u) v, w \rangle := \lim_{t \to 0} t^{-1} \big\langle \delta \mathscr{F}(u + tw) - \delta \mathscr{F}(u), v \big\rangle.$$

Higher variations are defined recursively, e.g., $\langle \delta^3 \mathscr{F}(u) v_1, v_2, v_3 \rangle = \lim_{t \to 0} t^{-1} \langle (\delta^2 \mathscr{F}(u + tv_3) - \delta^2 \mathscr{F}(u)) v_1, v_2 \rangle$, whenever the limit exists.

We use the standard definitions and notation $L^p, W^{k,p}, H^k$ for Lebesgue and Sobolev spaces, and ℓ^p for sequence spaces on $\mathbb{Z}^d$ or subsets thereof.

The closed ball with radius r and center x is denoted by $B_r(x)$. Further, we set $B_r := B_r(0)$.

2.2. **Lattice functions and function spaces.** For $d \in \{2,3\}, m \in \{1,2,3\}$, we denote the set of vector-valued lattice functions by

$$\mathscr{U} := \mathscr{U}(\mathbb{Z}^d)^m := \big\{ v : \mathbb{Z}^d \to \mathbb{R}^m \big\}.$$

We interpret the lattice $\mathbb{Z}^d$ as the vertex set of a simplicial grid $\mathscr{T}$, as follows:

- in 2D, $\mathscr{T} = \{\xi + \hat{T}, \xi - \hat{T} \,|\, \xi \in \mathbb{Z}^2\}$ where $\hat{T} = \mathrm{conv}\{0, e_1, e_2\}$;
- in 3D, $\mathscr{T} = \{\xi + \hat{T}_j \,|\, \xi \in \mathbb{Z}^3, j = 1, \dots, 6\}$, where $\hat{T}_1, \dots, \hat{T}_6$ subdivide the cube $[0,1]^3$ as displayed in Figure 1.

Let $\bar{\zeta} \in W^{1,\infty}(\mathbb{R}^d; \mathbb{R})$ be the P1 nodal basis function associated with the origin; that is $\bar{\zeta}$ is continuous and piecewise affine with respect to $\mathscr{T}$, $\bar{\zeta}(0) = 1$ and $\bar{\zeta}(\xi) = 0$ otherwise. We can then write the nodal interpolant as

$$\bar{v}(x) := \sum_{\xi\in\mathbb{Z}^d} v(\xi)\bar{\zeta}(x-\xi), \qquad \text{for } v \in \mathscr{U}. \tag{2.1}$$

Clearly, $\bar{v} \in W^{1,\infty}_{\rm loc}(\mathbb{R}^d)$ and $\bar{v}(\xi) = v(\xi)$ for all $\xi \in \mathbb{Z}^d$.

Using the previous definition, we introduce the discrete homogeneous Sobolev spaces

$$\mathscr{U}^{1,p} := \big\{ u \in \mathscr{U} \,\big|\, \nabla\bar{u} \in L^p \big\}, \qquad \text{for } p \in [1,\infty],$$

and the associated semi-norms $|u|_{\mathscr{U}^{1,p}} := \|\nabla\bar{u}\|_{L^p}$. This semi-norm fails to be a norm since it does not penalize translations, but this issue will not enter our analysis. For $p \in [1,\infty)$, the space of compact displacements,

$$\mathscr{U}^{\rm c} := \{ u \in \mathscr{U} \,|\, \text{supp}(u) \text{ is compact} \}$$

is dense in $\mathscr{U}^{1,p}$ in the sense that, for each $u \in \mathscr{U}^{1,p}$ there exists $u_n \in \mathscr{U}^{\rm c}$ such that $\nabla\bar{u}_n \to \nabla\bar{u}$ strongly in L^p. [31, Prop. 9].

2.2.1. *Smooth interpolant.* Since we will be primarily interested in approximation results, we require some information about the *regularity* of lattice functions. Higher-order finite differences, a natural measure of local smoothness of lattice functions, are cumbersome for our analysis, hence we introduce a $C^{2,1}$-conforming multi-quintic interpolant whose derivatives will provide equivalent information. To construct it we define the second-order nearest-neighbour finite differences

$$\begin{aligned} D^{\rm nn,0}_i u(\xi) &:= u(\xi), \\ D^{\rm nn,1}_i u(\xi) &:= \tfrac12\big(u(\xi+e_i) - u(\xi-e_i)\big), \\ D^{\rm nn,2}_i u(\xi) &:= u(\xi+e_i) - 2u(\xi) + u(\xi-e_i), \end{aligned}$$

for $\xi \in \mathbb{Z}^d, i \in \{1,\dots,d\}$. For a multi-index $\alpha \in \mathbb{Z}^d$, $|\alpha|_\infty \le 2, \alpha_i \ge 0$, we define

$$D^{\rm nn}_\alpha u(\xi) := D^{{\rm nn},\alpha_1}_1 \cdots D^{{\rm nn},\alpha_d}_d u(\xi),$$

The smooth interpolants are now defined through the following lemma. Closely related and in some respects stronger results can be found in [7, 36], but not of the specificity that we require (in particular not for $d = 3$).

Lemma 2.1. *(a) For each $u \in \mathscr{U}$ there exists a unique $\tilde{u} \in C^{2,1}(\mathbb{R}^d;\mathbb{R}^m)$ such that $\tilde{u} \in Q_5(\xi + (0,1)^d)$ for all $\xi \in \mathbb{Z}^d$ and $\partial_\alpha\tilde{u}(\xi) = D^{\rm nn}_\alpha u(\xi)$ for $\alpha \in \mathbb{Z}^d_+$, $|\alpha|_\infty \le 2$, $\xi \in \mathbb{Z}^d$.*

(b) Moreover, there exists a universal constant C such that, for $p \in [1,\infty]$, $0 \le j \le 3$,

$$\|\nabla^j \tilde{u}\|_{L^p(\xi+(0,1)^d)} \le C\|D^j u\|_{\ell^p(\xi+\{-1,0,1,2\}^d)}. \tag{2.2}$$

In particular, it follows that $\|\nabla\tilde{u}\|_{L^p} \lesssim \|\nabla\bar{u}\|_{L^p}$, where D is the collection of first-order finite differences defined in (2.4).

Proof. The proof is given in § 5.2. ☐

2.3. **The atomistic model.** We review an atomistic model from [12] for a defect in a homogeneous crystalline environment, which will form the "exact problem" that we will subsequently aim to approximate using atomistic/continuum blending schemes.

We will consider atomistic models for two classes of crystallographic defects: point defects and screw dislocations.

2.3.1. *Far-field boundary condition.* We fix domain and range dimensions $d \in \{2,3\}, m \in \{1,2,3\}$. We call $\mathbb{Z}^d$ the *reference configuration* and, with some abuse of terminology, a map $y \in \mathscr{U}$ a *deformed configuration* or *deformation.* For example, if $d = m = 3$, then $y(\xi)$ is the position of atom ξ.

We shall impose a *far-field boundary condition* $y(\xi) \sim y_0(\xi)$ as $|\xi| \to \infty$, by specifying a *reference deformation* $y_0 : \mathbb{R}^d \to \mathbb{R}^m$ and admitting only deformations from the space

$$\mathscr{Y} := \big\{ y \in \mathscr{U} \,\big|\, y = y_0 + u \text{ for some } u \in \mathscr{U}^{1,2} \big\}.$$

We explain how to choose y_0 to model various types of defects in § 2.3.3 and § 2.3.4 below. It will later become important that y_0 is defined on all of $\mathbb{R}^d$.

For future reference, we extend the definition of the two lattice interpolants as follows:

$$\bar{y} := y_0 + \bar{u} \quad \text{and} \quad \tilde{y} := y_0 + \tilde{u}. \tag{2.3}$$

(Strictly speaking, this represents a clash of notation. However, henceforth we will always apply the smooth interpolant to elements of $\mathscr{Y}$ or $\mathscr{U}^{1,2}$ and therefore adopt the latest definition (2.3).)

Remark 1. To justify how we impose the far-field boundary condition we note that, in all our model problems we will have that $y_0(\xi)$ scales linearly as $|\xi| \to \infty$, while $u \in \mathscr{U}^{1,2}$ implies that $|u(\xi)| = o(|\xi|)$ [31, Prop. 12]. Thus, we have that $y(\xi) \sim y_0(\xi) + o(|y_0(\xi)|)$ as $|\xi| \to \infty$.

The choice of the $\mathscr{U}^{1,2}$ space for the relative displacements u is due to the fact that these are precisely the "finite-energy displacements". □

2.3.2. *Energy difference functional.* We now define an energy (difference) functional on the space of deformations. First, we choose a finite *interaction range* $\mathcal{R} \subset B_{r_{\rm cut}} \cap \mathbb{Z}^d \setminus \{0\}$, where $r_{\rm cut} > 0$ is a *cut-off radius*, and we define the finite difference operator and finite difference stencil

$$\begin{aligned} D_\rho v(\xi) &:= v(\xi + \rho) - v(\xi), \qquad \text{for } v \in \mathscr{U}, \quad \xi, \rho \in \mathbb{Z}^d, \quad \text{and} \\ Dv(\xi) &:= \big(D_\rho v(\xi)\big)_{\rho \in \mathcal{R}}, \qquad \text{for } \xi \in \mathbb{Z}^d. \end{aligned} \tag{2.4}$$

We additionally make the technical assumption, without restriction of generality, that $e_i \in \mathcal{R}$ for $i = 1, \dots, d$. Then, for $y \in \mathscr{Y}$, we define an *atomistic energy difference functional* of the form

$$\mathscr{E}^{\rm a}(y) := \sum_{\xi \in \mathbb{Z}^d} V(Dy(\xi)) - V(Dy_0(\xi)), \tag{2.5}$$

where $V \in C^4((\mathbb{R}^m)^{\mathcal{R}})$ is a *site potential.* If $y - y_0 \in \mathscr{U}^{\rm c}$, then $\mathscr{E}^{\rm a}(y)$ is well-defined, and we will show in Lemma 2.2 (see also §2.3.3 and §2.3.4) that, under natural conditions on y_0, $\mathscr{E}$ can be extended to $y \in \mathscr{Y}$.

We denote the partial derivatives of V at a stencil $\mathbf{g} \in (\mathbb{R}^m)^{\mathcal{R}}$ by

$$V_{,\rho}(\mathbf{g}) := \frac{\partial V(\mathbf{g})}{\partial g_\rho} \in \mathbb{R}^m, \qquad V_{,\rho\varsigma}(\mathbf{g}) := \frac{\partial^2 V(\mathbf{g})}{\partial g_\rho \partial g_\varsigma} \in \mathbb{R}^{m \times m},$$

and so forth. For $\boldsymbol{\rho} \in \mathcal{R}^j$ we also write $V_{,\rho_1\cdots\rho_j} = V_{,\boldsymbol{\rho}} \in \mathbb{R}^{m\times\cdots\times m}$. The first and second variations of $\mathscr{E}$, for test functions $v, w \in \mathscr{U}^{\rm c}$, and writing $V_{\xi,\boldsymbol{\rho}} \equiv V_{,\boldsymbol{\rho}}(Dy(\xi))$, are given by

$$\langle \delta\mathscr{E}^{\rm a}(y), v\rangle = \sum_{\xi\in\mathbb{Z}^d} \langle \delta V(Dy(\xi)), Dv(\xi)\rangle = \sum_{\xi\in\mathbb{Z}^d}\sum_{\rho\in\mathcal{R}} V_{\xi,\rho}\cdot D_\rho v(\xi), \quad \text{and}$$

$$\langle \delta^2\mathscr{E}^{\rm a}(y)v, w\rangle = \sum_{\xi\in\mathbb{Z}^d} \big\langle \delta^2 V(Dy(\xi))Dv(\xi), Dw(\xi)\big\rangle = \sum_{\xi\in\mathbb{Z}^d}\sum_{\rho,\varsigma\in\mathcal{R}} D_\rho v(\xi)\cdot\big(V_{\xi,\rho\varsigma}D_\varsigma w(\xi)\big).$$

We require throughout that $\mathcal{R}$ and V are *point-symmetric*: $-\mathcal{R} = \mathcal{R}$, and if $\mathbf{g} \in (\mathbb{R}^m)^{\mathcal{R}}$ and $\mathbf{h} = (-g_{-\rho})_{\rho\in\mathcal{R}}$, then $V(\mathbf{g}) = V(\mathbf{h})$. In particular, this requirement implies that

$$V_{,-\boldsymbol{\rho}}(\mathsf{F}\mathcal{R}) = (-1)^j V_{,\boldsymbol{\rho}}(\mathsf{F}\mathcal{R}) \quad \text{for } \boldsymbol{\rho}\in\mathcal{R}^j, j\geq 1, \quad \mathsf{F}\in\mathbb{R}^{m\times d}. \tag{2.6}$$

Lemma 2.2. *Suppose that* $Dy_0 \in \ell^\infty(\mathbb{Z}^d; (\mathbb{R}^m)^{\mathcal{R}})$ *and* $\delta\mathscr{E}^{\rm a}(y_0) \in (\mathscr{U}^{1,2})^*$*, that is,* $\langle\delta\mathscr{E}^{\rm a}(y_0), v\rangle \leq c\|\nabla\bar{v}\|_{L^2}$ *for all* $v \in \mathscr{U}^{\rm c}$*, then there exists a unique continuous and translation invariant extension of* $u \mapsto \mathscr{E}^{\rm a}(y_0 + u), u \in \mathscr{U}^{\rm c}$ *to* $u \in \mathscr{U}^{1,2}$*. The extended functional is four times continuously Fréchet differentiable in* $\mathscr{U}^{1,2}$*.*

Proof. This result is a simplified variant of [13, Thm. 2.3] or [34, Thm. 2.8]. □

We now specify further details of the atomistic model for two interesting situations: point defects and screw dislocations.

2.3.3. *Model for point defects.* Strictly speaking, point defects occur only in 3D models, however we also admit 2D toy models. Moreover, some combinations of topological defects such as infinite vacancy-type dislocation loops or dislocation dipoles with small separation distance may occasionally also be treated as point defects, at least from an analytical perspective.

Thus, we admit $d \in \{2,3\}, m \in \{1,2,3\}$. We choose a *macroscopic strain* $\mathsf{A} \in \mathbb{R}^{m\times d}$, non-singular, and the far-field boundary condition $y_0(x) := \mathsf{A}x$. (The matrix A encodes the lattice structure, say $\mathsf{B}\mathbb{Z}^d$, as well as an applied macroscopic deformation $x \mapsto \mathsf{F}x$; in this case $\mathsf{A} = \mathsf{FB}$.)

Some point defects, such as Frenkel pairs, dislocation dipoles, can be modeled as local (but not global) minimisers of $\mathscr{E}$. Other types of point defects, such as vacancies, interstitials and impurities, can be modeled (to some extent) by adding an external *defect potential* $\mathscr{P} \in C^4(\mathscr{Y})$ to the total energy (see [13]). We shall assume throughout that

(A.P1) $\mathscr{P}$ is localised: there exists $R_{\mathscr{P}} > 0$ so that $\mathscr{P}$ depends only on $(y(\xi); |\xi| \leq R_{\mathscr{P}})$.
(A.P2) $\mathscr{P}$ is translation invariant: $\mathscr{P}(y) = \mathscr{P}(y + c)$, where $c(\xi) = c \in \mathbb{R}$.

The total energy for point defects is then given by

$$y \mapsto \mathscr{E}^{\rm a}(y) + \mathscr{P}(y).$$

Remark 2. For slightly more complex defect geometries, such as multiple interstitials, it is convenient to augment the reference configuration, $\mathbb{Z}^d$, by a finite number of points. Conceptually, our analysis is easy to extend to such cases, but we keep our simplifying assumptions for the sake of a convenient notation. We refer to [13] for details of the ideas required to carry out this extension. □

2.3.4. *Model for screw dislocations.* Consider a straight screw dislocation in a Bravais lattice $\mathsf{B}\mathbb{Z}^3$, with Burgers vector $b \in \mathsf{B}\mathbb{Z}^3$. By rotating and dilating $\mathsf{B}\mathbb{Z}^3$, we may assume without loss of generality that $b = |b|e_3$ and that e_3 is the shortest vector belonging to $\mathsf{B}\mathbb{Z}^3$ which is parallel to b. We assume, without loss of generality, that $|b| = 1$, i.e., $b = e_3$. In [19, 13] it is shown that a straight screw dislocation can be modeled by an energy of the form (2.5) with $m = 3$ and $d = 2$ and a reference deformation y_0 given by a linearised elasticity model. We briefly summarize the construction:

We seek a reference deformation of the form $y_0(x) = \mathsf{A}x + u^{\rm lin}(x)$, where $\mathsf{A} \in \mathbb{R}^{3\times 2}$, full rank. The matrix A incorporates the underlying lattice structure and any applied macroscopic in- and anti-plane deformation, while $u^{\rm lin}$ is the displacement map according to linearised Cauchy–Born elasticity: Let $W : \mathbb{R}^{3\times 2} \to \mathbb{R}\cup\{\infty\}$ be the *Cauchy–Born strain energy density* defined by $W(\mathsf{F}) = V(\mathsf{F}\mathcal{R})$ (see § 2.4 for more details), and let $\mathbb{C} := \partial^2 W(\mathsf{A}) \in \mathbb{R}^{3\times 2\times 3\times 2}$ be the corresponding linearised elasticity tensor. Then we require that $u^{\rm lin} \in C^\infty(\mathbb{R}^2 \setminus \Gamma; \mathbb{R}^3)$, where $\Gamma := \{(x_1, 0) \,|\, x_1 \geq 0\}$ is the "glide plane", and solves

$$\sum_{j=1}^{3} \sum_{\alpha,\beta=1}^{2} \mathbb{C}_{i\alpha}^{j\beta} \partial_{x_\alpha} \partial_{x_\beta} u_j^{\rm lin}(x) = 0 \qquad \text{for all } x \in \mathbb{R}^2 \setminus \Gamma. \tag{2.7}$$

In addition $u^{\rm lin}$ must have Burgers vector b; that is, we require

$$y_0(x_1, 0-) - y_0(x_1, 0+) = u^{\rm lin}(x_1, 0-) - u^{\rm lin}(x_1, 0+) = b \qquad \text{for all } x_1 > 0, \tag{2.8}$$

or in other words, $\int_C \nabla u^{\rm lin} \cdot \mathrm{d}x = b$ for any closed path C winding once around 0 in $\mathbb{R}^2$.

In [17, Sec. 12-3] and in [13, Sec. 2.4] it is shown that, if the deformation $\mathsf{A}x$ is strongly stable, i.e., there exists $c_0 > 0$ such that

$$\langle \delta^2 \mathscr{E}^{\rm a}(\mathsf{A}x) v, v\rangle \geq c_0 \|\nabla \bar{v}\|_{L^2}^2 \qquad \forall v \in \mathscr{U}^{\rm c}, \tag{2.9}$$

then a solution $u^{\rm lin} \in C^\infty(\mathbb{R}^2 \setminus \{0\}; \mathbb{R}^3)$ satisfying (2.7) and (2.8) exists, and moreover, that $\nabla u^{\rm lin} \in C^\infty(\mathbb{R}^2 \setminus \{0\}; \mathbb{R}^{3\times 2})$ with

$$|\nabla^j u^{\rm lin}(x)| \leq C_j |x|^{-j} \qquad \text{for } j \geq 1. \tag{2.10}$$

In addition to the assumptions on V made in § 2.2 we require invariance under lattice slip by a Burgers vector:

(A.Vper) V is periodic in the direction of b; that is, if $\mathbf{g}, \mathbf{h} \in (\mathbb{R}^3)^{\mathcal{R}}$ and $g_\rho - h_\rho \in b\mathbb{Z}$ for all $\rho \in \mathcal{R}$, then $V(\mathbf{g}) = V(\mathbf{h})$.

Remark 3. 1. Our assumptions on y_0 and V are compatible with projecting a full 3D model; see [13, Sec. 2.4] for the details.

2. One may also formulate an anti-plane model. In this case, we set $m = 1$, $W : \mathbb{R}^d \to \mathbb{R}$ and $u^{\rm lin}$ now solves a scaler elliptic equation; again see [13] for the details. □

2.3.5. *The atomistic variational problem.* Throughout the remainder of the paper we assume that all assumptions stated in § 2.2 hold. Moreover, we make one of the following two sets of standing assumptions:

(pPt) *Point defect problem:* $y_0 = \mathsf{A}x$ for some A such that lattice stability (2.9) holds, and assumptions (A.P1), (A.P2) are satisfied.

(pDs) *Screw dislocation problem:* y_0 is given by (2.7), (2.8) where A is such that lattice stability (2.9) holds, and in addition assumption (A.Vper) is satisfied. We set $\mathscr{P} \equiv 0$.

Unless an argument applies equally to both cases (usually this is the case), or it is clear from the context which of the two problems we are considering, then we will always specify which set of assumptions are are employing.

In either case, we seek to compute

$$y^{\rm a} \in \arg\min \big\{ \mathscr{E}^{\rm a}(y) + \mathscr{P}(y) \,\big|\, y \in \mathscr{Y} \big\}, \tag{2.11}$$

in the sense of local minimality with respect to the metric $\mathrm{dist}(y,z) = \|\nabla\bar{y} - \nabla\bar{z}\|_{L^2}$.

As usual, we shall require stronger assumptions on the solution than mere local minimality. Namely, we assume that $y^{\rm a}$ is a *strongly stable equilibrium*, by which we mean that there exists $\gamma^{\rm a} > 0$ such that

$$\begin{aligned} \big\langle \delta\mathscr{E}^{\rm a}(y^{\rm a}) + \delta\mathscr{P}(y^{\rm a}), v \big\rangle &= 0 \qquad \forall v \in \mathscr{U}^{\rm c}, \qquad \text{and} \\ \big\langle [\delta^2\mathscr{E}^{\rm a}(y^{\rm a}) + \delta^2\mathscr{P}(y^{\rm a})]v, v \big\rangle &\geq \gamma^{\rm a}\|\nabla\bar{v}\|_{L^2}^2 \qquad \forall v \in \mathscr{U}^{\rm c}. \end{aligned} \tag{2.12}$$

The existence of a strongly stable equilibrium is a property of the lattice and the interatomic potential (possibly even of the physical material). Except in some special circumstances (e.g., when the perturbation $\mathscr{P}$ is "small") it is difficult to establish under the generic assumptions we are making.

However, given the existence of a strongly stable equilibrium, we can estimate its *regularity* away from the defect core.

Lemma 2.3. *Let either (pPt) or (pDs) be satisfied and let $y^{\rm a} = y_0 + u^{\rm a}$, $u^{\rm a} \in \mathscr{U}^{1,2}$, be a strongly stable equilibrium. Then, there exists $c > 0$ such that, for $j = 1, 2, 3$, and for a.e. x, $|x| \geq 2$,*

$$\big|\nabla^j \tilde{u}^{\rm a}(x)\big| \leq \begin{cases} c|x|^{1-d-j}, & \textit{case (pPt)}, \\ c|x|^{-j-1}\log|x|, & \textit{case (pDs)}, \ d = 2. \end{cases} \tag{2.13}$$

Proof. The proof is a straightforward corollary of [13, Thm. 3.1]. ☐

2.4. **The Cauchy–Born model.** The final concept we need to introduce before formulating a/c coupling schemes is the Cauchy–Born model. The idea, briefly, is that if y varies slowly then $D_\rho y(\ell) \approx \nabla_\rho \tilde{y}(\ell)$ and hence $V(Dy(\ell)) \approx W(\nabla\tilde{y}(\ell))$, where the map $W : \mathbb{R}^{m\times d} \to \mathbb{R} \cup \{+\infty\}$, $W(\mathsf{F}) := V(\mathsf{F}\mathcal{R})$, is called the *Cauchy–Born strain energy function.* In the absence of defects, it is therefore reasonable to approximate the sum of site energies with an integral over the energy density,

$$y \mapsto \int_{\mathbb{R}^d} \Big(W(\nabla y) - W(\nabla y_0) \Big)\,\mathrm{d}x. \tag{2.14}$$

This model has been analyzed in considerable detail, e.g., in [4, 11, 27, 34]. Subject to suitable technical conditions the results in these references demonstrate that, if $y^{\rm a}$ is a "sufficiently smooth" stable equilibrium of $\mathscr{E}^{\rm a}$, then there exists a stable equilibrium $y^{\rm c}$ of (2.14) such that

$$\|\nabla y^{\rm c} - \nabla\bar{y}^{\rm a}\|_{L^2} \lesssim \|\nabla^3\tilde{y}^{\rm a}\|_{L^2} + \|\nabla^2\tilde{y}^{\rm a}\|_{L^4}^2.$$

That is, the Cauchy–Born model is *second-order accurate.*

3. Main Results

3.1. **Formulation of the B-QCE and B-QCF methods.** We wish to approximate the atomistic model using a hybrid atomistic/continuum description. The approximation is achieved in three steps: 1. We replace the infinite domain with the finite computational domain Ω_h. 2. In those parts of Ω_h where the Cauchy–Born approximation has sufficient accuracy we replace the atomistic model with the Cauchy–Born model. 3. We restrict deformations to a coarse-grained finite element space.

The key ingredient in this process is the coupling between the atomistic and continuum models, which we achieve using a blending formulation.

3.1.1. *Coarse-grained function spaces.* Let Ω_h be a polygonal (if $d = 2$) or polyhedral (if $d = 3$) domain in $\mathbb{R}^d$. Let $R^{\rm i} > 0$ be maximal and $R^{\rm o} > 0$ be minimal such that $B_{R^{\rm i}} \subset \Omega_h \subset B_{R^{\rm o}}$.

Let $\mathscr{T}_h$ be a regular partition of Ω_h into closed triangles or tetrahedra. For $T \in \mathscr{T}_h$, let $h_T := \operatorname{diam}(T)$ and r_T the diameter of the largest ball contained in T. For $x \in \Omega_h$, let $h(x) := \max_{T\in\mathscr{T}_h, x\in T} h_T$. The associated space of P1 finite element functions is denoted by $\mathrm{P1}(\mathscr{T}_h)$. If $\mathscr{N}_h$ denotes the set of finite element nodes, then the nodal interpolant of a function $v : \mathscr{N}_h \to \mathbb{R}^k$ is the unique function $I_h v \in \mathrm{P1}(\mathscr{T}_h)$ such that $I_h v = v$ on $\mathscr{N}_h$.

For a function $v : \bigcup_{T\in\mathscr{T}_h} \operatorname{int}(T) \to \mathbb{R}^k, k \in \mathbb{N}$ let $Q_h v \in \mathrm{P0}(\mathscr{T}_h)$ denote the piecewise constant mid-point interpolant, $Q_h v(x) := v(x_T)$ for $x \in T \in \mathscr{T}_h$, where $x_T := \fint_T x \,\mathrm{d}x$.

Exploiting the structure $y = y_0 + u, u \in \mathscr{U}^{1,2}$ of admissible deformations, we define the coarse-grained displacement and deformation spaces, respectively, by

$$\mathscr{U}_h := \big\{u_h \in C(\mathbb{R}^d;\mathbb{R}^m) \,\big|\, u_h|_{\Omega_h} \in \mathrm{P1}(\mathcal{T}_h), u_h|_{\mathbb{R}^d\setminus\Omega_h} = 0\big\} \quad \text{and}$$
$$\mathscr{Y}_h := \big\{y_h = y_0 + u_h \,\big|\, u_h \in \mathscr{U}_h\big\}.$$

3.1.2. *The B-QCE method.* Let $\beta \in C^{2,1}(\mathbb{R}^d)$ be a *blending function* then the B-QCE energy difference functional is defined by

$$\begin{aligned}\mathscr{E}_h^\beta(y_h) := \sum_{\xi\in\mathbb{Z}^d} \big(1 - \beta(\xi)\big)\Big(V\big(Dy_h(\xi)\big) - V\big(Dy_0(\xi)\big)\Big)& \\ + \int_{\Omega_h} Q_h\Big[\beta \cdot \big(W(\nabla y_h) - W(\nabla y_0)\big)\Big]\,\mathrm{d}x,& \qquad \text{for } y_h \in \mathscr{Y}_h.\end{aligned} \tag{3.1}$$

We assume that $1-\beta$ has compact support, hence the lattice sum is finite, while the integral is taken over a finite domain; thus $\mathscr{E}_h^\beta$ is well-defined. The application of the mid-point quadrature rule to evaluate the integral makes (3.1) fully computable.

In the B-QCE method we approximate the atomistic variational problem (2.11) with

$$y_h^{\rm bqce} \in \arg\min\big\{\mathscr{E}_h^\beta(y_h) + \mathscr{P}(y_h) \,\big|\, y_h \in \mathscr{Y}_h\big\}. \tag{3.2}$$

The B-QCE method, as we formulated it, was introduced for one-dimensional lattices in [38], and was later extended to two and three-dimensions in [26] in a formulation which differs only marginally from the one given in (3.1): in [26] the operator Q_h defined a trapezoidal rule instead of a midpoint rule. As a matter of fact, all of our results can be adapted to this case.

B-QCE shares many features with the bridging domain method [41], the Arlequin method [2], and the AtC coupling [1]. The bridging domain method and the Arlequin method differ from B-QCE primarily in that they couple the atomistic and continuum degrees of freedom weakly using Lagrange multipliers. The AtC coupling is a very general formulation which includes B-QCE and many other methods as special cases.

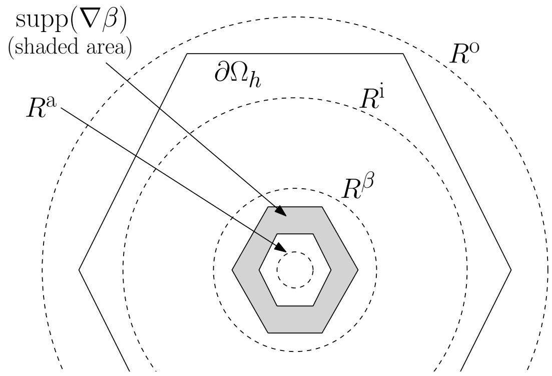

FIGURE 2. Visualisation of the definitions and assumptions made in § 3.2.

3.1.3. *The B-QCF method.* While the B-QCE method blends atomistic and continuum energies the B-QCF method blends atomistic and continuum forces. We first define the Cauchy–Born finite element functional

$$\mathscr{E}_h^{\rm c}(y_h) := \int_{\Omega_h} Q_h\big[W(\nabla y_h) - W(\nabla y_0)\big]\,{\rm d}x, \qquad \text{for } y_h \in \mathscr{Y}_h. \tag{3.3}$$

Assume again that $\beta \in C^{2,1}(\mathbb{R}^2)$ is a blending function, then the B-QCF operator is the nonlinear map $\mathscr{F}_h^\beta : \mathscr{Y}_h \to \mathscr{U}_h^*$, defined by

$$\big\langle \mathscr{F}_h^\beta(y_h), v_h \big\rangle := \big\langle \delta\mathscr{E}^{\rm a}(y_h), (1-\beta)v_h \big\rangle + \big\langle \delta\mathscr{E}_h^{\rm c}(y_h), I_h[\beta v_h] \big\rangle, \tag{3.4}$$

where $(1-\beta)v_h$ and βv_h are defined in terms of pointwise multiplication. $\mathscr{F}_h^\beta$ is well-defined since y_h and v_h are defined as functions on all of $\mathbb{R}^d$ and v_h has compact support.

In the B-QCF method we approximate the atomistic variational problem (2.11) with the variational nonlinear system

$$\big\langle \mathscr{F}_h^\beta\big(y_h^{\rm bqcf}\big) + \delta\mathscr{P}\big(y_h^{\rm bqcf}\big), v_h \big\rangle = 0 \qquad \forall v_h \in \mathscr{U}_h. \tag{3.5}$$

Remark 4. Suppose we define a blended a/c force via

$$F_\nu(y_h) := (1-\beta(\nu))\frac{\partial\mathscr{E}^{\rm a}(y_h)}{\partial y_h(\nu)} + \beta(\nu)\frac{\partial\mathscr{E}_h^{\rm c}(y_h)}{\partial y_h(\nu)} \qquad \text{for } \nu \in \mathscr{N}_h \setminus \partial\Omega_h, \quad y_h \in \mathscr{Y}_h,$$

then $-\sum_{\nu\in\mathscr{N}_h\setminus\partial\Omega_h} F_\nu(y_h)v_h(\nu) = \langle \mathscr{F}_h^\beta(y_h), v_h\rangle$. Thus, the nonlinear system $F_\nu(y_h^{\rm bqcf}) + \partial_{y_h(\nu)}\mathscr{P}(y_h^{\rm bqcf}) = 0$, $\nu \in \mathscr{N}_h \setminus \partial\Omega_h$, is equivalent to the variational form (3.5). □

The B-QCF method (3.5) is essentially the same method as those proposed in [24, 21]. It also has many parallels with methods formulated in [1, 2, 3, 14, 22, 35, 37, 41].

Both in [24] and [21] the main motivation of force-blending was that stability of the scheme can be proben, while the stability of sharp-interface force-based a/c couplings is entirely open at this point [8, 9, 10, 23]

3.2. **Approximation Error Estimates.** To formulate our approximation results, and for the subsequent analysis, we require additional assumptions on the computational domain and the mesh. See Figure 2 for a visualisation of the following definitions.

In addition to the radii $R_{\mathscr{P}}, R^{\rm i}, R^{\rm o}$ defined in § 2.3.3 and in § 3.1.1, we define $R^{\rm a}$ to be the largest and R^β to be the smallest numbers satisfying

$$\mathrm{supp}(\beta) \supset B_{R^{\rm a}+2r_{\rm cut}+\sqrt{d}} \qquad \text{and} \qquad \mathrm{supp}(1-\beta) \subset B_{R^\beta-2r_{\rm cut}-\sqrt{d}}.$$

We specify *atomistic, blending, continuum and exterior regions*

$$\begin{aligned}
\Omega^{\rm a} &:= \mathrm{supp}(1-\beta) + B_{2r_{\rm cut}+\sqrt{d}} \subset B_{R^\beta}, \\
\Omega^\beta &:= \mathrm{supp}(\nabla\beta) + B_{2r_{\rm cut}+\sqrt{d}} \subset B_{R^\beta} \setminus B_{R^{\rm a}}, \\
\Omega^{\rm c} &:= \mathrm{supp}(\beta) \cap \Omega_h + B_{2r_{\rm cut}+\sqrt{d}} \subset B_{R^{\rm o}} \setminus B_{R^{\rm a}}, \quad \text{and} \\
\Omega^{\rm ext} &:= \mathbb{R}^2 \setminus B_{R^{\rm i}/2}.
\end{aligned}$$

Further, we define *discrete atomistic and blending regions*

$$\Lambda^{\rm a} := \mathbb{Z}^d \cap (\mathrm{supp}(1-\beta) + \mathcal{R}) \quad \text{and} \quad \Lambda^\beta := \{\xi \in \mathbb{Z}^d : D\beta(\xi) \neq 0\}.$$

The fact that the various regions overlap is simply for the sake of convenience of the analysis and notation.

We assume throughout that there exist fixed constants $C_{\mathcal{T}_h}, C_1^\beta, C_2^\beta$ such that the following conditions are satisfied:

$$R_{\mathscr{P}} \leq R^{\rm a} \leq R^\beta \qquad \text{and} \qquad R^\beta \leq C_1^\beta R^{\rm a}; \tag{3.6}$$

$$\beta \in C^{2,1}, \qquad 0 \leq \beta \leq 1 \qquad \text{and} \qquad \|\nabla^j \beta\|_{L^\infty} \leq C_2^\beta (R^{\rm a})^{-j}, j = 1, 2, 3; \tag{3.7}$$

$$\mathscr{T}_h \text{ is fully refined in } \Omega^{\rm a} \qquad \text{and} \qquad \max_{T \in \mathscr{T}_h} h_T / r_T \leq C_{\mathcal{T}_h}. \tag{3.8}$$

By (3.8) we mean that, if $T \in \mathcal{T}_h$ with $T \cap \Omega^{\rm a} \neq \emptyset$, then $T \in \mathscr{T}$; as well as vice-versa.

In addition, only for $d = 2$ and only for the B-QCF method, we assume that there are constants $C_\Omega, m_\Omega \geq 1$ such that

$$R^{\rm o} \leq C_\Omega (R^{\rm a})^{m_\Omega}. \tag{3.9}$$

The two main approximation parameters to define both the B-QCE and B-QCF methods are the blending function β and the finite element mesh $\mathcal{T}_h$ (and through it, the computational domain Ω_h). The regions $\Omega^{\rm a}, \Omega^\beta, \Omega^{\rm c}, \Omega^{\rm ext}, \Lambda^{\rm a}, \Lambda^\beta$ and the radii, $R^{\rm a}, R^\beta, R^{\rm i}, R^{\rm o}$ are derivative parameters. The constants $C_{\mathcal{T}_h}, C_j^\beta, C_\Omega, m_\Omega$ in assumptions (3.6), (3.7), (3.9) and (3.8) are understood to be uniform in *all choices* of $(\beta, \mathcal{T}_h)$ that may occur in our analysis.

Throughout the remainder of the paper, we will write "$A = O(B)$" or "$|A| \lesssim B$" if there exists a constant C such that $|A| \leq CB$, where C is independent of the approximation parameters $(\beta, \mathscr{T}_h)$, but may depend on the constants $C_{\mathcal{T}_h}, C_j^\beta, C_\Omega, m_\Omega$, or on any specified functions involved in the estimate. (In particular, C may depend on a solution $y^{\rm a}$ and on derivatives $V_{,\boldsymbol{\rho}}(\mathbf{g})$ for $\mathbf{g}$ in some specified range, cf. § 4.2.2, but never on a test function.)

3.2.1. *Error estimates in terms of solution regularity.* For $y = y_0 + u \in \mathscr{Y}$ we define the

$$\begin{aligned}
\text{best-approximation error} \quad \mathbf{E}^{\rm apx}(y) &:= \|\nabla \bar{u}\|_{L^2(\Omega^{\rm ext})} + \|h\nabla^2 \tilde{u}\|_{L^2(\Omega^{\rm c})} + \|h^2 \nabla^3 \tilde{u}\|_{L^2(\Omega^{\rm c})} \\
&\quad + \|h^2 \nabla^3 y_0\|_{L^2(\Omega^{\rm c})} + \|h(\nabla y_0 - \mathsf{A}) \otimes \nabla^2 y_0\|_{L^2(\Omega^{\rm c})}, \\
\text{Cauchy–Born model error} \quad \mathbf{E}^{\rm cb}(y) &:= \|\nabla^3 \tilde{y}\|_{L^2(\Omega^{\rm c})} + \|\nabla^2 \tilde{y}\|_{L^4(\Omega^{\rm c})}^2, \qquad (3.10) \\
\text{and coupling error} \quad \mathbf{E}^{\rm int}(y) &:= \|\nabla^2 \beta\|_{L^2} + \|\nabla \beta\|_{L^\infty} \|\nabla^2 \tilde{y}\|_{L^2(\Omega^\beta)}.
\end{aligned}$$

The first term in $\mathbf{E}^{\rm apx}$ measures the finite element coarsening error (including the quadrature error), while the second term in $\mathbf{E}^{\rm apx}$ measures the error induced by reducing the problem to a bounded domain.

Theorem 3.1. *Let $y^{\rm a} = y_0 + u^{\rm a} \in \mathscr{Y}$ be a strongly stable solution to* (2.11)*. Then, there exist constants $\epsilon, R_0^{\rm a}, C > 0$, which are independent of $\mathscr{T}_h$ and β, such that, if $R^{\rm a} \geq R_0^{\rm a}$, then there exist strongly stable solutions $y_h^{\rm bqce}$ to* (3.2) *and $y_h^{\rm bqcf}$ to* (3.5) *satisfying*

$$\|\nabla \bar{y}^{\rm a} - \nabla y_h^{\rm bqce}\|_{L^2} \leq C\big(\mathbf{E}^{\rm apx}(y^{\rm a}) + \mathbf{E}^{\rm cb}(y^{\rm a}) + \mathbf{E}^{\rm int}(y^{\rm a})\big), \qquad \textit{and} \tag{3.11}$$

$$\|\nabla \bar{y}^{\rm a} - \nabla y_h^{\rm bqcf}\|_{L^2} \leq C\gamma_{\rm tr}\big(\mathbf{E}^{\rm apx}(y^{\rm a}) + \mathbf{E}^{\rm cb}(y^{\rm a})\big), \tag{3.12}$$

where $\gamma_{\rm tr} = \sqrt{1 + \log(R^{\rm a})}$ if $d = 2$ and $\gamma_{\rm tr} = 1$ if $d = 3$.

Proposition 3.2. *Under the conditions of Theorem 3.1, we have*

$$\begin{aligned}\big|\mathscr{E}^{\rm a}(y^{\rm a}) - \mathscr{E}_h^{\beta}(y_h^{\rm bqce})\big| \leq C\Big\{&\mathbf{E}^{\rm apx}(y^{\rm a})^2 + \mathbf{E}^{\rm cb}(y^{\rm a})^2 + \mathbf{E}^{\rm int}(y^{\rm a})^2 \\ &+ \|\nabla^2\beta\|_{L^2}\|\nabla\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})} + \|\nabla\beta\|_{L^2}\|\nabla^2\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})} \\ &+ \mathbf{E}^{\rm apx}(y^{\rm a})\big(\|\nabla\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})} + \|\nabla u^{\rm lin}\|_{L^4(\Omega^{\rm c})}^2\big) + H^{\rm ots}\Big\},\end{aligned} \tag{3.13}$$

where C is independent of $\mathscr{T}_h$ and β and $H^{\rm ots}$ are "higher order terms" (cf. § 3.2.2),

$$\begin{aligned}H^{\rm ots} := {}&\|\nabla^3\tilde{u}^{\rm a}\|_{L^1(\Omega^{\rm c})} + \|\nabla^2\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})}^2 \\ &+ \Big(\|h^2\nabla^3 y_0\|_{L^2(\Omega^{\rm c})} + \|h\nabla^2 y_0\|_{L^4(\Omega^{\rm c})}^2\Big)\Big(\mathbf{E}^{\rm apx}(y^{\rm a}) + \|\nabla\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})}\Big) \\ &+ \|\nabla^2\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})}\|\nabla^2 y_0\|_{L^2(\Omega^{\rm c})} + \|\nabla\beta\|_{L^\infty}\|\nabla\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})}\|\nabla^2 y_0\|_{L^2(\Omega^{\rm c})}.\end{aligned}$$

Remark 5. The B-QCF error estimate seemingly has no β-dependence, but this is only due to the strong assumptions we made on β in (3.7). Only under these assumptions are we able to state Theorem 3.1. However, it can be expected, that the result is also valid under more specialized, but otherwise much milder assumptions on β. In such a case, our intermediate results in § 4 and § 6.4 can be employed to understand the precise β-dependence of the error. □

3.2.2. *Error estimates in terms of computational cost.* Following [32] we now convert the error estimates (3.11), (3.12) and (3.13) into convergence rates in terms of the number of degrees of freedom

$$\mathrm{DOF} := \#\mathscr{T}_h.$$

The quantity DOF is directly related (but not necessarily proportional) to the computational cost of solving the associated problems (3.2) and (3.5). The estimates in terms of DOF form the basis for the optimised implementations of the B-QCE and B-QCF methods presented, respectively, in [26, 21].

We introduce additional restrictions on $\mathscr{T}_h$ and Ω_h,

$$\begin{aligned}|h(x)| \lesssim \max\big\{1, \tfrac{|x|}{R^\beta}\big\}, \quad R^{\rm o} \lesssim R^{\rm i}, \quad \text{and} \quad \mathrm{DOF} &\lesssim (R^\beta)^d \log\big(\tfrac{R^{\rm o}}{R^\beta}\big) \\ &\lesssim (R^{\rm a})^d \log R^{\rm a}.\end{aligned} \tag{3.14}$$

The second bound in (3.14) is a mild assumption on the shape regularity of Ω_h, while the last bound in (3.14) is a corollary of the first one, upon additionally requiring that (3.9) holds for both B-QCE and B-QCF.

Then, using the regularity estimates (2.13) and (2.10) it is straightforward to prove that

$$\begin{aligned}
\text{Case (pPt):} \quad & \mathbf{E}^{\rm cb}(y^{\rm a}) &&\lesssim (R^{\rm a})^{-d/2-2}, \\
& \mathbf{E}^{\rm int}(y^{\rm a}) &&\lesssim (R^{\rm a})^{d/2-2}, \\
& \mathbf{E}^{\rm apx}(y^{\rm a}) &&\lesssim (R^{\rm a})^{-d/2-1} + (R^{\rm i})^{-d/2}, \\
\text{Case (pDis):} \quad & \mathbf{E}^{\rm cb}(y^{\rm a}) &&\lesssim (R^{\rm a})^{-2}, \\
& \mathbf{E}^{\rm int}(y^{\rm a}) &&\lesssim (R^{\rm a})^{-1}, \\
& \mathbf{E}^{\rm apx}(y^{\rm a}) &&\lesssim (R^{\rm a})^{-2}\log(R^{\rm a}) + (R^{\rm i})^{-1}.
\end{aligned}$$

(Here we used the estimate $\int_R^\infty r^t \log^s r \,{\rm d}r \leq R^{t+1}\log^s(R)$ for $t < -1, s \in \mathbb{N}, R \geq 2$.) We note that the dominant term, $\mathbf{E}^{\rm int}(y^{\rm a}) \lesssim (R^{\rm a})^{d/2-2}$ originates entirely from the "blended ghost force error" term $\|\nabla^2\beta\|_{L^2}$.

Next, we note that in the B-QCE case any choice $R^{\rm i} \gg R^{\rm a}$ balances the far-field contribution, $\|\nabla\bar{u}^{\rm a}\|_{L^2(\Omega^{\rm ext})} \lesssim (R^{\rm i})^{-d/2}$ with the "blended ghost force error" $\|\nabla^2\beta\|_{L^2} \lesssim (R^{\rm a})^{d/2-2}$.

For the B-QCF case we balance the far-field error $\|\nabla\bar{u}^{\rm a}\|_{L^2(\Omega^{\rm ext})} \lesssim (R^{\rm i})^{-d/2}$ with the finite element coarsening error. Ignoring log-factors, we observe that the radius $R^{\rm i}$ ought to be balanced against the interpolation error component $\|h\nabla^2\tilde{u}^{\rm a}\|_{L^2(\Omega^{\rm c})} \lesssim (R^{\rm a})^{-d/2-1}$, which yields $R^{\rm i} \approx (R^{\rm a})^{d/2+1}$ both in the (pPt) and (pDis) cases. Hence, we obtain

$$\begin{aligned}
\text{Case (pPt):} \quad & \mathbf{E}^{\rm apx}(y^{\rm a}) \lesssim (R^{\rm a})^{-d/2-1}, \\
\text{Case (pDis):} \quad & \mathbf{E}^{\rm apx}(y^{\rm a}) \lesssim (R^{\rm a})^{-2}\log(R^{\rm a}).
\end{aligned}$$

We summarise the foregoing computations in the following theorem, using also the fact that, under the conditions of the theorem, $R^{\rm a} \lesssim ({\rm DOF})^{1/d}$, $(R^{\rm a})^{-1} \lesssim ({\rm DOF})^{-1/d}(\log {\rm DOF})^{1/d}$ and $\gamma_{\rm tr} \lesssim (\log {\rm DOF})^{1/2}$. The estimate for the energy error can be immediately obtained from analogous computations.

Theorem 3.3. *In addition to the assumptions of Theorem 3.1 suppose that* (3.14) *holds and that $R^{\rm i} \geq c_\Omega (R^{\rm a})^s$ for a constant $c_\Omega > 0$ independent of $(\beta, \mathscr{T}_h)$, where $s > 1$ for the B-QCE method and $s \geq d/2+1$ for the B-QCF method. Then, there exists a constant C, independent of $(\beta, \mathscr{T}_h)$, such that*

for the B-QCE method, for both Cases (pPt) and (pDis),

$$\|\nabla\bar{y}^{\rm a} - \nabla y_h^{\rm bqce}\|_{L^2} \leq C({\rm DOF})^{d/4-1}(\log {\rm DOF})^{-d/4+1},$$

$$\big|\mathscr{E}^{\rm a}(y^{\rm a}) - \mathscr{E}_h^\beta(y_h^{\rm bqce})\big| \leq C({\rm DOF})^{d/2-2}(\log {\rm DOF})^{-d/2+2};$$

and for the B-QCF method,

$$\|\nabla\bar{y}^{\rm a} - \nabla y_h^{\rm bqcf}\|_{L^2} \leq C \begin{cases} ({\rm DOF})^{-d/4-1}(\log {\rm DOF})^2, & \textit{case (pPt)}, \\ ({\rm DOF})^{-1}(\log {\rm DOF})^{5/2}, & \textit{case (pDis)}. \end{cases}$$

Remark 6. 1. The construction of $\mathscr{T}_h$ satisfying (3.14) is standard and can be found, e.g., in [32].

2. To construct β, we could, for example, choose $R^\beta = C_1^\beta R^{\rm a}$ for a given $R^{\rm a}$ and then choose β in the form of a radial spline satisfying the conditions (3.7). For complicated a/c interface geometries one could solve a bi-Laplace equation in a precomputation step (see [26]).

3. Finally, we could allow for a stronger mesh coarseing, $h(x) \approx (|x|/R^{\beta})^{\alpha}$ and thereby drop the log factor in DOF for a suitable choice of $\alpha > 1$, which would slightly improve the estimates. In order to preserve mesh regularity (3.8), one would need to impose that $h(x) \lesssim |x|$. Note that this does not violate any of our foregoing assumptions for suitable choices of α; see [29] for further discussion. □

3.3. **Conclusion.** We have established the first error analysis of a/c coupling schemes that is "complete" in the sense that it covers general interatomic potentials, accomodates atomistic solutions containing defects, and requires no assumption on the atomistic solution beyond its stability.

While our results are restricted to two specific a/c coupling schemes, we anticipate that the techniques we have developed allow extensions to a much wider range of blending type a/c couplings. We emphasize, however, that most of our techniques are specialised for blending type schemes. In particular, the technique of Lemma 4.10, which is the main new technical ingredient to prove stability of B-QCE and B-QCF, is unlikely to generalise to sharp-interface couplings. To that end the ideas present in [23] and [33] are more promising starting points.

We remark on a seemingly immediate extension which, surprisingly, seems not straightforward: The main assumption among those formulated in § 3.2 is that the finite element mesh is fully refined in the blending region. This is highly convenient from the perspective of both analysis and implementation, but it is likely that, in practice, a coarse mesh in the blending region would yield a more efficient scheme; see, e.g., [41], where this is in fact a crucial ingredient. Most of our results do not require this restriction, but there are several steps (in particular in § 6.1) which appear to be more difficult without it.

4. Key Intermediate Results

The purpose of this section is to give a detailed overview of the main steps and ideas employed in the proof of the main results, and to state some key intermediate results that are of independent interest.

4.1. **Framework.** We adopt the analytical framework of [25], which is analogous to that of finite element methods for (regular) nonlinear PDE, employing quasi-best approximation, consistency and stability.

Briefly, let $\mathscr{G}_h = \delta\mathscr{E}_h^{\beta} + \delta\mathscr{P}$ for the B-QCE scheme or $\mathscr{G}_h = \mathscr{F}_h^{\beta} + \delta\mathscr{P}$ for the B-QCF scheme. Let $\Pi_h : \mathscr{U} \to \mathscr{U}_h$ be a suitable "quasi-best approximation operator" (we define it in § 4.2.4), then we shall require that $\mathscr{G}_h$ is *consistent*,

$$\big\langle \mathscr{G}_h(\Pi_h y^{\rm a}), v_h \big\rangle \leq \eta \|\nabla v_h\|_{L^2} \qquad \forall v_h \in \mathscr{U}_h, \tag{4.1}$$

for some "small" consistency error η that depends on $y^{\rm a}$, $\mathscr{T}_h$ and β; and *stable*,

$$\big\langle \delta\mathscr{G}_h(\Pi_h y^{\rm a}) v_h, v_h \big\rangle \geq c_0 \|\nabla v_h\|_{L^2}^2 \qquad \forall v_h \in \mathscr{U}_h. \tag{4.2}$$

We then empoy the Inverse Function Theorem to prove that, if η/c_0 is sufficiently small (adding some technical assumptions), then there exists $w_h \in \mathscr{U}_h$ such that $\|\nabla w_h\|_{L^2} \leq 2\eta/c_0$ and $\mathscr{G}_h(\Pi_h y^{\rm a} + w_h) = 0$.

The condition that η/c_0 is sufficiently small corresponds to the assumption that $R^{\rm a}$ is sufficiently large in Theorem 3.1.

Thus, we have constructed a B-QC solution $y_h^{\rm bqc} := \Pi_h y^{\rm a} + w_h$ satisfying

$$\|\nabla \bar{y}^{\rm a} - \nabla y_h^{\rm bqc}\|_{L^2} \leq 2\frac{\eta}{c_0} + \|\nabla \bar{y}^{\rm a} - \nabla \Pi_h y^{\rm a}\|_{L^2}. \tag{4.3}$$

The second term on the right-hand side is the quasi-best approximation error.

In the present section we shall make this generic outline concrete. We shall present the key ideas in our analysis but postpone the technical aspects of the proofs to later sections.

4.2. **Further Preliminaries.** Here we introduce additional ingredients that we require to motivate and state the key intermediate results.

4.2.1. *Expansion of discrete strain.* Let $y \in \mathscr{Y}$ be a deformation. Much of our analysis depends on Taylor expansions of finite differences within the a neighbourhood

$$\nu_x := B_{2r_{\rm cut}+\sqrt{d}}(x) \tag{4.4}$$

of some $x \in \mathbb{R}^d$, containing all those lattice points ξ for which $\mathsf{S}^{\rm a}(y; x)$ depends on $D_\rho y(\xi), \rho \in \mathcal{R}$ ($\mathsf{S}^{\rm a}$ is the atomistic stress defined in § 4.2.3) and an additional $\sqrt{d}$ buffer, which we require in view of the "convolution trick" (4.14).

Lemma 4.1. *Let $z \in C^{2,1}(\nu_x)$ and $|x - \xi| \le r_{\rm cut} + \sqrt{d}, \rho \in \mathcal{R}$, then*

$$\big|D_\rho z(\xi) - \nabla_\rho z(x)\big| \le C\|\nabla^2 z\|_{L^\infty(\nu_x)}, \tag{4.5}$$

$$\big|D_\rho z(\xi) - \big[\nabla_\rho z(x) + \nabla_\rho \nabla_{\xi - x} z(x) + \tfrac12 \nabla_\rho^2 z(x)\big]\big| \le C\|\nabla^3 z\|_{L^\infty(\nu_x)}, \tag{4.6}$$

where C is a generic constant.

Proof. The results are obtained by straightforward Taylor expansions about x. □

Normally, we would like to perform the expansions (4.5), (4.6) with $z = \tilde{y}$, but this is only possible if $\tilde{y}$ is smooth in ν_x, which fails in the dislocation case when ν_x intersects the branch-cut. To still use these Taylor expansions, we therefore construct *equivalent local deformations* that are smooth in ν_x: for $x \in \mathbb{R}^d$, and $|x' - x| < |x|$, let

$$y^x(x') := \int_{t=0}^1 \nabla\tilde{y}\big((1-t)x + tx'\big)(x' - x)\,{\rm d}t, \tag{4.7}$$

then $y^x \in C^{2,1}$ in its domain of definition, with $\nabla^j y^x = \nabla^j \tilde{y}$, $j \ge 1$, and $y^x - \tilde{y} \in b\mathbb{Z}$. The latter property, together with (A.Vper) ensures that, for $|x| > 2r_{\rm cut} + \sqrt{d}$,

$$V_{,\boldsymbol\rho}(Dy(\xi)) = V_{,\boldsymbol\rho}(Dy^x(\xi)) \qquad \text{for all } \xi \in \mathbb{Z}^d,\ |x - \xi| \le r_{\rm cut} + \sqrt{d}. \tag{4.8}$$

We will employ (4.8) in the consistency proofs in an ad-hoc fashion whenever we need to replace a finite difference stencil $Dy(\xi)$ with a stencil $Dy^x(\xi)$ in order to then perform a Taylor expansion.

4.2.2. *Expansion of the potential.* Since our analysis is based on local arguments, we require bounds on the interatomic potential in the neighbourhood of some given discrete deformation. Let $y \in \mathscr{Y}$ be such a deformation, and let $\epsilon > 0$, then we define

$$M_\epsilon^{(\boldsymbol\rho)}(y) := \sup_{\xi \in \mathbb{Z}^d} \sup_{\substack{\mathbf{g} \in (\mathbb{R}^m)^{\mathcal{R}} \\ \max_{\rho \in \mathcal{R}} \frac{|D_\rho y(\xi) - g_\rho|}{|\rho|} \le \epsilon}} \sup_{\substack{\mathbf{h} = (h_i)_{i=1}^j \in (\mathbb{R}^m)^j \\ |h_1| = \dots = |h_j| = 1}} V_{,\boldsymbol\rho}(\mathbf{g}) : \otimes_{i=1}^j h_i \qquad \text{for } \boldsymbol\rho \in \mathcal{R}^j. \tag{4.9}$$

Our assumptions on V and y_0 ensure that $M_\epsilon^{(\boldsymbol\rho)}(y)$ is finite for all $\epsilon > 0$ and $y \in \mathscr{Y}$.

Lemma 4.2. *Let $y \in \mathscr{Y}, Dy \in \ell^\infty$, and $\epsilon > 0$ then, for $z \in \mathscr{Y}, \|\nabla\tilde{z} - \nabla\bar{y}\|_{L^\infty} \leq \epsilon$, $|x| > 2r_{\rm cut} + \sqrt{d}$ and $|x - \xi| \leq r_{\rm cut} + \sqrt{d}$,*

$$\big|V_{,\rho}(Dz(\xi)) - V_{,\rho}(\nabla_{\mathcal{R}}\tilde{z}(x))\big| \leq C_2\|\nabla^2\tilde{z}\|_{L^\infty(\nu_x)}, \qquad \textit{and} \tag{4.10}$$

$$\Big|V_{,\rho}(Dz(\xi)) - \Big[V_{,\rho}(\nabla_{\mathcal{R}}\tilde{z}(x)) + \sum_{\varsigma\in\mathcal{R}} V_{,\rho\varsigma}(\nabla_{\mathcal{R}}\tilde{z}(x))\big(\nabla_\varsigma\tilde{z}(x) - D_\varsigma z^x(\xi)\big)\Big]\Big| \tag{4.11}$$
$$\leq C_3\|\nabla^2\tilde{z}\|^2_{L^\infty(\nu_x)},$$

where the constants C_j depend on $M^{(\boldsymbol{\rho})}_\epsilon(y)$, $\boldsymbol{\rho} \in \mathcal{R}^j$.

Proof. Using the definition of z^x according to (4.7) and (4.9) the estimates follow from Taylor expansions of $V_{,\rho}$. □

4.2.3. *Atomistic stress.* To prove consistency we will employ "weak forms" of the atomistic and the B-QC formulations that are local in the test function gradient. The first step is to derive first Piola–Kirchhoff stresses for the three models and estimate their discrepancy in terms of the local regularity of the underlying deformation. This analysis is based on the atomistic stress function analyzed in [34], which is closely related to Hardy stress [16].

A canonical representation of $\delta\mathscr{E}^{\rm a}$ is

$$\big\langle\delta\mathscr{E}^{\rm a}(y), v\big\rangle = \sum_{\xi\in\mathbb{Z}^d}\sum_{\rho\in\mathcal{R}} V_{\xi,\rho}\cdot D_\rho v(\xi), \quad \text{where} \quad V_{\xi,\rho} := V_{,\rho}(Dy(\xi)). \tag{4.12}$$

To convert $\delta\mathscr{E}^{\rm a}$ into a "weak form" that is local in ∇v we replace v with

$$v^* := \bar{\zeta} * \bar{v} \tag{4.13}$$

and rewrite the finite differences $D_\rho v^*(\xi)$ as follows:

$$\begin{aligned} D_\rho v^*(\xi) &= \int_{s=0}^1 \nabla_\rho v^*(\xi + s\rho)\,{\rm d}s = \int_{\mathbb{R}^d}\int_{s=0}^1 \bar{\zeta}(\xi + s\rho - x)\nabla_\rho\bar{v}(x)\,{\rm d}s\,{\rm d}x \\ &= \int_{\mathbb{R}^d}\omega_\rho(\xi - x)\nabla_\rho\bar{v}\,{\rm d}x \qquad \text{where} \quad \omega_\rho(x) := \int_{s=0}^1\bar{\zeta}(x + s\rho)\,{\rm d}s, \end{aligned} \tag{4.14}$$

to obtain

$$\begin{aligned} \big\langle\delta\mathscr{E}^{\rm a}(y), v^*\big\rangle &= \sum_{\xi\in\mathbb{Z}^d}\sum_{\rho\in\mathcal{R}} V_{\xi,\rho}\cdot\int_{\mathbb{R}^d}\omega_\rho(\xi - x)\,\nabla_\rho\bar{v}(x)\,{\rm d}x \\ &= \int_{\mathbb{R}^d}\bigg\{\sum_{\xi\in\mathbb{Z}^d}\sum_{\rho\in\mathcal{R}}\big[V_{\xi,\rho}\otimes\rho\big]\omega_\rho(\xi - x)\bigg\} : \nabla\bar{v}\,{\rm d}x. \end{aligned}$$

Thus, we have shown that, for $y \in \mathscr{Y}$ and $v \in \mathscr{U}^{\rm c}$,

$$\begin{aligned} \big\langle\delta\mathscr{E}^{\rm a}(y), v^*\big\rangle &= \int_{\mathbb{R}^d}\mathsf{S}^{\rm a}(y;x) : \nabla\bar{v}(x)\,{\rm d}x, \qquad \text{where} \\ \mathsf{S}^{\rm a}(y;x) &:= \sum_{\xi\in\mathbb{Z}^d}\sum_{\rho\in\mathcal{R}}\big[V_{\xi,\rho}\otimes\rho\big]\omega_\rho(\xi - x). \end{aligned} \tag{4.15}$$

(The representation (4.15) is of course equivalent to (4.12) since neither require any regularity on y. We use the term "weak form" only in analogy with the continuum theory.)

Note that (4.15) is in close analogy to the first Piola–Kirchhoff stress of the Cauchy–Born model,

$$\big\langle\delta\mathscr{E}^{\rm c}(y), v\big\rangle = \int_{\mathbb{R}^d}\mathsf{S}^{\rm c}(y) : \nabla v\,{\rm d}x, \qquad \text{where } \mathsf{S}^{\rm c}(y;x) = \partial W(\nabla y). \tag{4.16}$$

To see the connection between the atomistic and Cauchy–Born stress we replace $Dy(\xi)$ with $Dy^x(\xi)$ and expand analogously to (4.6) and $V_{,\rho}$ analogously to (4.11), to obtain

$$\mathsf{S}^{\mathrm{a}}(y;x) - \mathsf{S}^{\mathrm{c}}(y;x) \sim \mathbb{C}_2(x) : \nabla^3 y(x) + \mathbb{C}_3(x) : \big(\nabla^2 y(x) \otimes \nabla^2 y(x)\big) + \mathrm{HOTs}, \tag{4.17}$$

where $\mathbb{C}_2(x)$ is a sixth order tensor depending on $V_{,\boldsymbol{\rho}}(\nabla_{\mathcal{R}} y(x))$, $\boldsymbol{\rho} \in \mathcal{R}^2$, $\mathbb{C}_3(x)$ is an eighth order tensor depending on $V_{,\boldsymbol{\rho}}(\nabla_{\mathcal{R}} y(x)), \boldsymbol{\rho} \in \mathcal{R}^3$, and HOTs are formally higher-order terms, such as $O(|\nabla^2 y|^3)$ or $O(|\nabla^4 y|)$.

The calculation (4.17) exploits the fact that we can write $V_{\xi,\boldsymbol{\rho}} = V_{,\boldsymbol{\rho}}(Dy(\xi)) = V_{,\boldsymbol{\rho}}(Dy^x(\xi))$ for $|x-\xi| \leq r_{\mathrm{cut}} + \sqrt{d}$, which removes discontinuities from y, as well as the following two identities: [34, Lemma 4.4]

$$\sum_{\xi \in \mathbb{Z}^d} \omega_\rho(\xi - x) = 1, \qquad \text{and} \tag{4.18}$$

$$\sum_{\xi \in \mathbb{Z}^d} \omega_\rho(\xi - x)\,(\xi - x) = -\tfrac{1}{2}\rho. \tag{4.19}$$

The following lemma provides a rigorous estimate along the lines of (4.17).

Lemma 4.3. *Suppose that $y \in \mathscr{Y}$ and $\epsilon > 0$, then for $z \in \mathscr{Y}, \|\nabla \bar{z} - \nabla \bar{y}\|_{L^\infty} \leq \epsilon$,*

$$\big|\mathsf{S}^{\mathrm{a}}(z;x) - \mathsf{S}^{\mathrm{c}}(\tilde{z};x)\big| \leq C\big(\|\nabla^3 \tilde{z}\|_{L^\infty(\nu_x)} + \|\nabla^2 \tilde{z}\|^2_{L^\infty(\nu_x)}\big),$$

where ν_x is defined in (4.4) *and C depends on $M_\epsilon^{(\boldsymbol{\rho})}(y), \boldsymbol{\rho} \in \mathcal{R}^j, j = 2, 3$.*

Proof. This result is essentially contained in [34, Thm. 4.3]. The only modification required is to replace the expansion of $D_\rho \tilde{z}(\xi)$ with that of $D_\rho z^x(\xi)$ as detailed in § 4.2.1. It is also a simplified case of Lemma 6.4. ☐

4.2.4. *Best approximation operator.* We construct a quasi-best approximation operator $\Pi_h : \mathscr{Y} \to \mathscr{Y}_h$. With slight abuse of notation, we write $\Pi_h y = y_0 + \Pi_h u$, where $y = y_0 + u$, $u \in \mathscr{U}^{1,2}$, and Π_h is also understood as an operator from $\mathscr{U} \to \mathscr{U}_h$.

Given $u \in \mathscr{U}^{1,2}$ we define $\Pi_h u := I_h T_R u$, where I_h is the nodal interpolation operator defined in § 3.1.1 and T_R is a truncation operator defined as follows: we fix some arbitrary $\eta \in C^3(0,\infty)$ (e.g. a quintic spline) with $\eta(t) = 1$ in $[0, 1/2)$ and $\eta = 0$ in $[1,\infty)$, and define

$$T_R u(\xi) := \eta\big(\tfrac{|\xi|}{R^{\mathrm{i}}}\big)\big(u(\xi) - ⨍_{B_{R^{\mathrm{i}}} \setminus B_{R^{\mathrm{i}}/2}} \bar{u}\,\mathrm{d}x\big). \tag{4.20}$$

Clearly, $T_R u \in \mathscr{U}^{\mathrm{c}}$ with $\mathrm{supp}(T_R u) \subset \Omega_h$ and hence $\Pi_h u \in \mathscr{U}_h$.

Lemma 4.4. *There exists a constant C such that,*

$$\|\nabla \Pi_h y - \nabla \bar{y}\|_{L^2} \leq C \mathbf{E}^{\mathrm{apx}}(y) \qquad \text{for } y \in \mathscr{Y},$$

where $\mathbf{E}^{\mathrm{apx}}$ is defined in (3.10).

Proof. The result follows immediately upon combining [12, Lemma 4.3], Lemma 2.1, and standard interpolation error estimates. ☐

4.3. **B-QCE consistency error.** We have now assembled the prerequisites to define and estimate the B-QCE consistency error. The first variation of $\mathscr{E}_h^\beta$ is given by

$$\big\langle \delta\mathscr{E}_h^\beta(y_h), v_h\big\rangle = \sum_{\xi\in\mathbb{Z}^d}(1-\beta(\xi))\big\langle \delta V(Dy_h(\xi)), Dv_h(\xi)\big\rangle + \int_{\mathbb{R}^d} Q_h\big[\beta\partial W(\nabla y_h) : \nabla v_h\big]\,\mathrm{d}x,$$

for $y_h \in \mathscr{Y}_h, v_h \in \mathscr{U}_h$. Since v_h cannot be immediately replaced with a function v^* (to apply the convolution trick (4.14)) we shall not convert this directly to a "weak formulation". Instead, suppose that $y \in \mathscr{Y}, v \in \mathscr{U}^{\mathrm{c}}$ such that $y_h(\xi) = y(\xi)$ and $v^*(\xi) = v_h(\xi)$ for all $\xi \in \Lambda^{\mathrm{a}}$. Then, arguing analogously as in § 4.2.3 we can compute

$$\begin{aligned}\big\langle \delta\mathscr{E}^{\mathrm{a}}(y), v^*\big\rangle &= \sum_{\xi\in\mathbb{Z}^d}(1-\beta(\xi))\big\langle \delta V(Dy(\xi)), Dv^*(\xi)\big\rangle + \sum_{\xi\in\mathbb{Z}^d}\beta(\xi)\big\langle \delta V(Dy(\xi)), Dv^*(\xi)\big\rangle \\ &= \sum_{\xi\in\mathbb{Z}^d}(1-\beta(\xi))\big\langle \delta V(Dy_h(\xi)), Dv_h(\xi)\big\rangle \\ &\qquad + \int_{\mathbb{R}^d}\bigg\{\sum_{\xi\in\mathbb{Z}^d}\beta(\xi)\sum_{\rho\in\mathcal{R}}\big[V_{\xi,\rho}\otimes\rho\big]\omega_\rho(\xi-x)\bigg\} : \nabla\bar{v}\,\mathrm{d}x,\end{aligned}$$

where $V_{\xi,\rho} = V_{,\rho}(Dy(\xi))$. Thus, we obtain

$$\begin{aligned}&\big\langle \delta\mathscr{E}_h^\beta(y_h), v_h\big\rangle - \big\langle \delta\mathscr{E}^{\mathrm{a}}(y), v^*\big\rangle \\ &\quad= \int_{\mathbb{R}^d} Q_h\big[\beta\partial W(\nabla y_h) : \nabla v_h\big]\,\mathrm{d}x - \int_{\mathbb{R}^d}\bigg\{\sum_{\xi\in\mathbb{Z}^d}\beta(\xi)\sum_{\rho\in\mathcal{R}}\big[V_{\xi,\rho}\otimes\rho\big]\omega_\rho(\xi-x)\bigg\} : \nabla\bar{v}\,\mathrm{d}x,\end{aligned} \tag{4.21}$$

with obvious analogies between the two groups on the right-hand side. To complete the definition of the atomistic test function, we take $v = \Pi_h' v_h$, where $\Pi_h' : \mathscr{U}_h \to \mathscr{U}^{\mathrm{c}}$ is a dual approximation operator given by the conditions

$$\begin{aligned}(\Pi_h' v_h)^*(\xi) &= v_h(\xi), \text{ for } \xi \in \Lambda^{\mathrm{a}}, \quad \text{and} \\ \Pi_h' v_h(\xi) &= (\bar\zeta * v_h)(\xi), \quad \text{for } \xi \in \mathbb{Z}^d \setminus \Lambda^{\mathrm{a}}.\end{aligned} \tag{4.22}$$

We prove in Lemma 5.5 that Π_h' is well-defined.

In order to estimate the consistency error we must estimate (1) the quadrature error, which is standard; (2) the conformity error encoded in the usage of two different test functions, which requires a specific non-standard choice of v, cf. § 6.1; and (3) the modelling error encoded in the difference between the two "stresses".

To indicate how we estimate the latter, we consider the simplified "stress error"

$$\mathsf{R}^\beta(y;x) := \beta(x)\partial W(\nabla y(x)) - \sum_{\xi\in\mathbb{Z}^d}\beta(\xi)\sum_{\rho\in\mathcal{R}}\big[V_{\xi,\rho}\otimes\rho\big]\omega_\rho(\xi-x), \tag{4.23}$$

where y is now a smooth function and $V_{\xi,\rho} = V_{,\rho}(Dy(\xi))$. A formal Taylor expansion, similar as the one leading to (4.17), but also expanding $\beta(\xi)$ in terms of $\nabla^j\beta(x)$, yields

$$\begin{aligned}\mathsf{R}^\beta(y;x) \sim{}& \mathbb{D}_1(x) : \nabla^2\beta(x) + \mathbb{D}_2(x) : \big(\nabla\beta(x)\otimes\nabla^2 y(x)\big) \\ &+ \beta(x)\Big(\mathbb{C}_2(x) : \nabla^3 y(x) + \mathbb{C}_3(x) : \big(\nabla^2 y(x)\otimes\nabla^2 y(x)\big)\Big) + \text{HOTs},\end{aligned} \tag{4.24}$$

where $\mathbb{D}_1(x)$ is a fourth order tensor that depends on $V_{,\rho}(\nabla_{\mathcal{R}} y(x))$, $\rho\in\mathcal{R}$, $\mathbb{D}_2(x)$ is a sixth order tensor that depends on $V_{,\boldsymbol{\rho}}(\nabla_{\mathcal{R}} y(x)), \boldsymbol{\rho}\in\mathcal{R}^2$, $\mathbb{C}_2, \mathbb{C}_3$ are the same tensors as in (4.17) and HOTs are formally higher order terms.

Theorem 4.5 (Consistency of B-QCE). *Suppose that $y \in \mathscr{Y}$, then there exist $\epsilon = \epsilon(\mathbf{E}^{\rm apx}(y))$ such that, for all $v_h \in \mathscr{U}_h$,*

$$\big\langle \delta\mathscr{E}_h^{\beta}(\Pi_h y), v_h \big\rangle - \big\langle \delta\mathscr{E}^{\rm a}(y), \Pi_h' v_h \big\rangle \leq C\big(\mathbf{E}^{\rm apx}(y) + \mathbf{E}^{\rm cb}(y) + \mathbf{E}^{\rm int}(y)\big)\, \|\nabla v_h\|_{L^2},$$

where C depends on $M^{(\epsilon)}_{\boldsymbol{\rho}}(y)$, $\boldsymbol{\rho} \in \mathcal{R}^j$, $1 \leq j \leq 4$.

4.4. **B-QCF consistency error.** The consistency analysis of the B-QCF scheme faces different challenges than that of the B-QCE scheme. Consider again $y \in \mathscr{Y}, y_h \in \mathscr{Y}_h, v_h \in \mathscr{U}_h$ and a microscopic test function $v \in \mathscr{U}^{\rm c}$, then we need to estimate

$$\langle \mathscr{F}_h^{\beta}(y_h), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v\rangle = \langle \delta\mathscr{E}^{\rm a}(y_h), (1-\beta)v_h\rangle + \langle \delta\mathscr{E}_h^{\rm c}(y_h), I_h[\beta v_h]\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v\rangle.$$

Choosing $v := \Pi_h'' v_h$, where $\Pi_h'' : \mathscr{U}_h \to \mathscr{U}^{\rm c}$ is another dual approximation operator defined through

$$\Pi_h'' v_h := (1-\beta) v_h|_{\mathbb{Z}^d} + w^*, \qquad \text{where} \qquad w(\xi) = (\bar\zeta * I_h[\beta v_h])(\xi), \tag{4.25}$$

we obtain

$$\langle \mathscr{F}_h^{\beta}(y_h), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v\rangle = \langle \delta\mathscr{E}_h^{\rm c}(y_h), I_h[\beta v_h]\rangle - \langle \delta\mathscr{E}^{\rm a}(y), w^*\rangle,$$

from which we can estimate (see § 6.4.1 for the details)

$$\langle \mathscr{F}_h^{\beta}(\Pi_h y), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v\rangle \leq C\big(\mathbf{E}^{\rm apx}(y) + \mathbf{E}^{\rm cb}(y)\big)\|\nabla I_h[\beta v_h]\|_{L^2}. \tag{4.26}$$

Thus, we need to estimate $\|\nabla I_h[\beta v_h]\|_{L^2}$ in terms of $\|\nabla v_h\|_{L^2}$, which is provided in the following lemma. The key technical ingredient in its proof is a sharp trace inequality.

Lemma 4.6. *Suppose that the blending function β satisfies* (3.6)*, then there exists a generic constant C, such that*

$$\|\nabla I_h[\beta v_h]\|_{L^2} \leq C\,\gamma_{\rm tr}\|\nabla v_h\|_{L^2} \qquad \forall v_h \in \mathscr{U}_h, \tag{4.27}$$

$$\text{where } \gamma_{\rm tr} = \begin{cases} \sqrt{1+\log(R^{\rm o}/R^{\rm a})}, & d=2, \\ 1, & d=3. \end{cases} \tag{4.28}$$

Proof. The proof is given in § 6.4.2. □

Based on the previous lemma we can establish the following B-QCF consistency estimate.

Theorem 4.7 (Consistency of B-QCF). *Suppose that $y \in \mathscr{Y}$, then there exists $\epsilon = \epsilon(\mathbf{E}^{\rm apx}(y)) > 0$ such that, for all $v_h \in \mathscr{U}_h$,*

$$\big\langle \mathscr{F}_h^{\beta}(\Pi_h y), v_h \big\rangle - \big\langle \delta\mathscr{E}^{\rm a}(y), \Pi_h'' v_h \big\rangle \leq C\,\gamma_{\rm tr}\big(\mathbf{E}^{\rm apx}(y) + \mathbf{E}^{\rm cb}(y)\big)\, \|\nabla v_h\|_{L^2}$$

where C depends on $M^{(\epsilon)}_{\boldsymbol{\rho}}(y)$, $\boldsymbol{\rho} \in \mathcal{R}^j, j = 2, 3$.

Proof. The result immediately follows from (4.26), which is proven in § 6.4.1, and from Lemma 4.6. □

4.5. **Stability of B-QCE.** The aim of our stability result is to show that, if y is a stable equilibrium of the atomistic model, then choosing sufficiently large atomistic and blending regions, we ensure that $\Pi_h y$ is stable in the B-QCE model.

Theorem 4.8. *Suppose $y \in \mathscr{Y}$ is a stable atomistic configuration, i.e.,*

$$0 < \gamma^{\rm a}(y) := \inf_{v \in \mathscr{U}^{\rm c}\setminus\{0\}} \frac{\langle \delta^2 \mathscr{E}^{\rm a}(y)v + \delta^2 \mathscr{P}(y)v, v\rangle}{\|\nabla \bar{v}\|_{L^2}^2}, \tag{4.29}$$

and denote

$$\gamma_h^\beta(y_h) := \inf_{v_h \in \mathscr{U}_h\setminus\{0\}} \frac{\langle \delta^2 \mathscr{E}_h^\beta(y_h)v_h + \delta^2 \mathscr{P}(y_h)v_h, v_h\rangle}{\|\nabla v_h\|_{L^2}^2}.$$

Then there exists $\Delta\gamma(R^{\rm a}) \to 0$ as $R^{\rm a} \to \infty$ such that $\gamma_h^\beta(\Pi_h y) \geq \gamma^{\rm a}(y) - \Delta\gamma(R^{\rm a})$.

Positivity of $\gamma^{\rm a}$ is a property of the interatomic potential and of the defect that we are aiming to compute, hence we postulated this as an *assumption*.

The idea of the stability proof is to take a sequence of approximation parameters $(\beta_j, \mathscr{T}_{h,j})$ with $R_j^{\rm a} \uparrow \infty$ and of minimising test functions $v_j \in \mathscr{U}_{h,j}$ (the space is now indexed by j) such that $\|\nabla v_j\|_{L^2} = 1$ and $\big\langle\big(\delta^2\mathscr{E}_h^\beta(\Pi_{h,j}y) + \delta^2\mathscr{P}(\Pi_{h,j}y)\big)v_j, v_j\big\rangle = \gamma_h^\beta$. Due to the bound $\|\nabla v_j\|_{L^2} = 1$, we can extract a weakly convergent subsequence (still denoted by v_j). This sequence is then decomposed into three components (scales): $v_j = v_j^{\rm a} + v_j^{\rm b} + v_j^{\rm c}$, for each of which we use a different stability argument:

- $\nabla v_j^{\rm a}$ converges strongly at the atomic scale. It is concentrated near the defect core, hence for a sufficiently large atomistic region stability of the defect implies stability for this test function.
- $\nabla v_j^{\rm b}$ converges weakly to zero at the atomic scale but strongly at the "interfacial scale"; i.e., after a rescaling $w_j^{\rm b}(x) = \delta v_j^{\rm b}(x/\epsilon)$, where $\epsilon \approx (R^{\rm a})^{-1}$ and δ is chosen so that $\|\nabla w_j^{\rm b}\|_{L^2} = \|\nabla v_j^{\rm b}\|_{L^2}$. This scaling keeps the interface (i.e., $\mathrm{supp}(\nabla\beta)$) near $|x| = 1$ as $\varepsilon \to 0$. Consistency of B-QCE implies that the action of the B-QCE hessian on this test function is approximately the same as that of the Cauchy–Born hessian, hence stability of the continuum model implies stability for this component of the test function.
- $\nabla v_j^{\rm c}$ converges weakly to zero both at the atomic and "interfacial scale" (which means that it is not concentrated near a defect or interface). We can then exploit that, for a subsequence, $v_j^{\rm c} \to 0$ strongly in $L^2(B_{R^\beta})$ to reduce the action of the B-QCE hessian on this test function to the independent actions of the linearized atomistic and continuum operators which are both stable.
- All cross-terms can be neglected in the limit as $j \to \infty$ due to an approximate orthogonality between the three components.

In practice, the idea outlined above is carried out in two steps. First, we reduce the question to stability of a homogeneous deformation, by only splitting $v_j = v_j^{\rm a} + (v_j^{\rm b} + v_j^{\rm c})$.

Lemma 4.9. *Under assumptions and notation of Theorem 4.8, there exists $\Delta\gamma(R^{\rm a}) \to 0$ as $R^{\rm a} \to \infty$ such that $\gamma_h^\beta(\Pi_h y) \geq \min\big\{\gamma^{\rm a}(y), \gamma_h^\beta(\mathsf{A}x)\big\} - \Delta\gamma(R^{\rm a})$.*

Thus, we are left to establish positivity of $\gamma_h^\beta(\mathsf{A}x)$. We will use the fact that positivity of $\gamma^{\rm a}(\mathsf{A}x)$ follows from the positivity of $\gamma^{\rm a}(y)$.

Lemma 4.10. *Under assumptions and notation of Theorem 4.8, there exists $\Delta\gamma(R^{\rm a}) \to 0$ as $R^{\rm a} \to \infty$ such that $\gamma_h^\beta(\mathsf{A}x) \geq \gamma^{\rm a}(\mathsf{A}x) - \Delta\gamma(R^{\rm a})$.*

Both Lemma 4.9 and Lemma 4.10 are proven in § 7.1.

Proof of Theorem 4.8. In view of Lemmas 4.9 and 4.10 we only need to note that $\gamma^{\rm a}(\mathsf{A}x) \geq \gamma^{\rm a}(y)$ which is proved in [12]. □

We remark that our arguments to obtain convergence of the stability constants employ compactness principles and do not yield convergence rates as in 1D [25].

4.6. **Stability of B-QCF.** The B-QCF stability result is analogous to the B-QCE stability result. Unlike in the B-QCE case we state the result only for stable equilibria (rather than general deformations) since we require some regularity of the underlying deformation in the proof.

Theorem 4.11. *Suppose $y^{\rm a} \in \mathscr{Y}$ is a strongly stable solution of* (2.11)*, i.e.,* (4.29) *holds, and let*

$$\mu_h^\beta := \inf_{v_h \in \mathscr{U}_h \setminus \{0\}} \frac{\langle \delta \mathscr{F}_h^\beta(\Pi_h y^{\rm a}) v_h + \delta^2 \mathscr{P}(\Pi_h y^{\rm a}) v_h, v_h \rangle}{\|\nabla v_h\|_{L^2}^2}.$$

Then there exists $\Delta\gamma(R^{\rm a}) \to 0$ as $R^{\rm a} \to \infty$ such that $\mu_h^\beta(\Pi_h y) \geq \gamma^{\rm a}(y) - \Delta\gamma(R^{\rm a})$.

It is possible to adapt the proof of Theorem 4.8 to prove this result, however, we obtain it via an alternative route using an auxiliary result that it interesting in its own right: We modify a result from [20], which shows in a simplified case that the B-QCE hessian and B-QCF jacobian are "close". Here, we only establish that their stability constants converge to the same limit as $R^{\rm a} \to \infty$.

Lemma 4.12. *Under the assumptions and notation of Theorem 4.11, there exists a constant C such that*

$$\big|\mu_h^\beta - \gamma_h^\beta(\Pi_h y^{\rm a})\big| \leq C \begin{cases} (R^{\rm a})^{-1} (\log R^{\rm a})^{1/2}, & \text{if } d = 2, \\ (R^{\rm a})^{-1}, & \text{if } d = 3. \end{cases}$$

The proof of Lemma 4.12 is given in § 7.2.

Proof of Theorem 4.11. The result is an immediate corollary of Theorem 4.8 and Lemma 4.12. □

4.7. **Proofs of the error estimates.** We have now assembled all required auxiliary results to complete the proof of Theorem 3.1.

Proof of Theorem 3.1. Let $y^{\rm a}$ be a fixed strongly stable atomistic equilibrium. Using the notation established in § 4.1, we define $\mathscr{R}_h : \mathscr{U}_h \to \mathscr{U}_h^*$,

$$\langle \mathscr{R}_h(w_h), v_h \rangle := \langle \mathscr{G}_h(\Pi_h y^{\rm a} + w_h), v_h \rangle \quad \forall v_h \in \mathscr{U}_h.$$

1. Stability: Theorems 4.8 and 4.11 show that there exists $R_1^{\rm a}$ such that, for $R^{\rm a} \geq R_1^{\rm a}$, we have (4.2) for a constant $c_0 > 0$ that depends on $R_1^{\rm a}$, but is independent of $R^{\rm a}$. This implies that $\|\delta \mathscr{R}_h(0)^{-1}\|_{L(\mathscr{U}_h^*, \mathscr{U}_h)} \leq c_0^{-1}$.

2. Consistency: Theorems 4.5 and 4.7 imply that

$$\|\mathscr{R}_h(0)\|_{\mathscr{U}_h^*} = \|\mathscr{G}_h(\Pi_h y^{\rm a})\|_{\mathscr{U}_h^*} \to 0, \quad \text{as } R^{\rm a} \to 0,$$

uniformly in all choices of $(\beta, \mathscr{T}_h)$. In particular, for any $\epsilon > 0$ we can choose a constant $R_0^{\rm a} \geq R_1^{\rm a}$ such that $\|\mathscr{R}_h(0)\|_{\mathscr{U}_h^*} \leq \epsilon$ whenever $R^{\rm a} \geq R_0^{\rm a}$.

(In the B-QCF case, due to the logarithmic prefactor $\gamma_{\rm tr}$ in the consistency error estimates, this requires the regularity estimates (2.13).)

3. Inverse function theorem: Our assumptions on V and the fact that $\mathbf{E}^{\rm apx}(y^{\rm a}) \le \epsilon$ for $R^{\rm a} \ge R^{\rm a}_0$ implies that $\|\delta\mathscr{G}_h(y_h) - \delta\mathscr{G}_h(z_h)\|_{L(\mathscr{U}_h,\mathscr{U}_h^*)} \le L\|\nabla y_h - \nabla z_h\|_{L^2}$ for all $y_h, z_h \in \mathscr{U}_h$, or, equivalently,

$$\|\delta\mathscr{R}_h(w_h) - \delta\mathscr{R}_h(z_h)\|_{L(\mathscr{U}_h,\mathscr{U}_h^*)} \le L\|\nabla w_h - \nabla z_h\|_{L^2} \qquad \forall w_h, z_h \in \mathscr{U}_h.$$

The inverse function (see, e.g., [25]) states that, if $\|\mathscr{R}_h(0)\|_{\mathscr{U}_h^*} L c_0^{-2} < 1$, then there exists $w_h \in \mathscr{U}_h$ such that $\mathscr{R}_h(w_h) = 0$ and $\|\nabla w_h\|_{L^2} \le 2c_0^{-1}\|\mathscr{R}_h(0)\|_{\mathscr{U}_h^*}$. This can clearly achieved by setting ϵ sufficiently small. Setting $y_h^{\rm bqc} := \Pi_h y^{\rm a} + w_h$ we therefore obtain that

$$\|\nabla\Pi_h^{\rm a} y^{\rm a} - \nabla y_h^{\rm bqc}\|_{L^2} \le 2c_0^{-1}\|\mathscr{R}_h(0)\|_{\mathscr{U}_h^*}.$$

Inserting the estimates for $\|\mathscr{R}_h(0)\|_{\mathscr{U}_h^*}$ from Theorems 4.5 and 4.7, and the fact that $\|\nabla\Pi_h^{\rm a} - \nabla\bar{y}^{\rm a}\|_{L^2} \lesssim \mathbf{E}^{\rm apx}(y^{\rm a})$, we obtain the two error estimates (3.11) and (3.12). □

5. Proofs of Interpolation and Approximation Results

5.1. **Analysis of the quasi-interpolant.** Recall the definitions of $\bar{v}$ from (2.1) and of $v^* := \bar\zeta * \bar{v}$ from (4.13). To summarize results concerning v^* we first need the following lemma.

Lemma 5.1. *The partition $\mathscr{T}$ is invariant under reflections about all lattice points $\xi \in \mathbb{Z}^d$. In particular, we have $\bar\zeta(\xi - x) = \bar\zeta(\xi + x)$ for all $\xi \in \mathbb{Z}^d, x \in \mathbb{R}^d$.*

Proof. In 2D the result is geometrically evident.

In 3D, one first observes that the partition $\{\hat{T}_1, \dots, \hat{T}_6\}$ of the unit cube $[0,1]^3$, shown in Figure 1, is invariant under the map $x \mapsto (1,1,1) - x$ (which is the reflection about $(1/2,1/2,1/2)$). Moreover, since $\mathscr{T}$ is translation invariant by construction, we obtain for $\xi \in \mathbb{Z}^d$,

$$\xi - T = \big[\xi - (1,1,1)\big] + \big[(1,1,1) - T\big] \in \mathscr{T}. \qquad \square$$

Based on Lemma 5.1 the analysis in [31] allows us to deduce the following statements: Let $v \in \mathscr{U}$, then $\bar{v} \in W^{1,\infty}_{\rm loc}(\mathbb{R}^d;\mathbb{R}^m)$ and $v^* \in W^{3,\infty}_{\rm loc}(\mathbb{R}^d;\mathbb{R}^m)$ [31, Lemma 1]. Further, there exists a constant c, independent of p, such that, for all $u \in \mathscr{U}$ and $p \in [1,\infty]$, [31, Theorem 2]

$$c\|\nabla\bar{u}\|_{L^p} \le \|\nabla u^*\|_{L^p} \le \|\nabla\bar{u}\|_{L^p}. \tag{5.1}$$

5.2. **Analysis of the smooth nodal interpolant.** Let $n \in \mathbb{Z}_+$. For each multi-index $\alpha \in \mathbb{Z}^d_+$, $|\alpha|_\infty \le n$, denote by ∂_α the respective partial derivative and let D_α be a finite difference approximation to ∂_α. We assume that each D_α is exact on polynomials of degree n and is supported on

$$\mathscr{N}_n = \{\xi \in \mathbb{Z}^d : |\xi| \le \lceil \tfrac{n}{2} \rceil\}.$$

Next, for a lattice function u, introduce a d-dimensional Hermite interpolation based on derivatives ∂_α, $|\alpha|_\infty \le n$. Namely, in each cell $\xi + B_d$, where

$$B_d = \{x : 0 \le x_i < 1,\ i = 1,2,\dots,d\}$$

is the d-dimensional unit cube, define a $Q_{2n+1}(\mathbb{R}^d)$ polynomial, i.e., a polynomial in x_1, x_2, …, x_d, of degree at most $2n+1$ in each variable (and thus of degree at most $d(2n+1)$) $P_{u,\xi}(x)$ such that

$$\partial_\alpha P_{u,\xi}(x) = D_\alpha u(x) \quad \text{for all } 2^d \text{ verticies } x \text{ of the cell } \xi + B_d \tag{5.2}$$

and define

$$\tilde{u}(x) := P_{u,\xi}(x) \quad \text{if } x \in \xi + B_d. \tag{5.3}$$

Lemma 5.2. *The relation* (5.3) *uniquely defines* $\tilde{u}$ *for any lattice function* $u : \mathbb{Z}^d \to \mathbb{R}$.

Proof. For $\mu \in \mathbb{Z}^d_+$, $|\mu|_\infty \le 2n+1$, let $B_{2n+1,\mu}(x) := \prod_{i=1}^d x_i^{2n+1-\mu_i}(1-x_i)^{\mu_i}$ be the multivariate Bernstein polynomial. These polynomials form a basis of $Q_{2n+1}(\mathbb{R}^d)$ and on the other hand upper-triangularize the linear system (5.2). Hence the solution $P_{u,\xi}$ to (5.2) exists and is unique. □

Lemma 5.3 (Regularity). *For any lattice function* $u : \mathbb{Z}^d \to \mathbb{R}$, $\tilde{u} \in C^{n,1}_{\rm loc}(\mathbb{R}^d)$.

Proof. It is enough to prove that across any face shared by two cells, the function and normal derivatives up to order n are continuous.

Indeed, without loss of generality, consider two adjacent cells, B_d and $B_d - e_d$, where $e_d = (0, \dots, 0, 1) \in \mathbb{R}^d$. For $y \in \mathbb{R}^{d-1}$ denote $\bar{y} = (y_1, \dots, y_{d-1}, 0) \in \mathbb{R}^d$. Let $m \in \{0, 1, \dots, n\}$ be the order of the normal derivative and consider the polynomial $p(y) = \big(\frac{\partial}{\partial x_d}\big)^m (P_{u,0}(\bar{y}) - P_{u,-e_d}(\bar{y}))$. By construction of $P_{u,0}$ and $P_{u,-e_d}$, we have that $p \in Q_{2n+1}(\mathbb{R}^{d-1})$ and satisfies

$$\partial_\beta p(y) = 0 \quad \text{for all } \beta \in \mathbb{Z}^{d-1}_+ \text{ such that } |\beta|_\infty \le n \text{ and all vertices } y \text{ of } B_{d-1}.$$

Due to Lemma 5.2 such a polynomial is unique, hence we obtain $p(y) \equiv 0$, which implies continuity of $\tilde{u}$ and its derivatives. □

Lemma 5.4 (Stability). *For any* $u : \mathbb{Z}^d \to \mathbb{R}$ *and* $\beta \in \mathbb{Z}^d_+ : |\beta|_1 \le n+1$,

$$\|\partial_\beta \tilde{u}\|_{L^p(B_d)} \le C \|D^{{\rm cn},|\beta|_1} u\|_{\ell^p} \tag{5.4}$$

for some constant C *independent of* u, *where* $D^{{\rm cn},m}$ *is the collection of all finite differences of order* m *whose stencil lies within*

$$\bar{\mathscr{N}_n} = \{\xi \in \mathbb{Z}^d : |\xi + \tfrac{1}{2}| \le \lceil \tfrac{n}{2} \rceil + \tfrac{1}{2}\}.$$

Proof. Since both $\|\partial_\beta \tilde{u}\|_{L^p(B_d)}$ and $\|D^{|\beta|_1}_{\bar{\mathscr{N}_n}} u\|_{\ell^p}$ are seminorms on the finite dimensional space $\{u : \bar{\mathscr{N}_n} \to \mathbb{R}\}$, (5.4) may fail to hold only if there exists $u^\dagger : \bar{\mathscr{N}_n} \to \mathbb{R}$ such that $\partial_\beta \tilde{u}^\dagger \not\equiv 0$ on B_d, but $D^{|\beta|_1}_{\bar{\mathscr{N}_n}} u^\dagger = 0$. The latter may happen only if $u^\dagger$ is a polynomial of degree $|\beta|_1 - 1$. Then, since D_α are exact on such polynomials (note that $|\beta|_1 - 1 \le n$), $D_\alpha u^\dagger(\xi) = \partial_\alpha u^\dagger(\xi)$ for any vertex ξ of B_d, therefore $P_{u^\dagger,0}(x) = u^\dagger(x)$ for all $x \in \mathbb{R}^d$, and hence $\partial_\beta \tilde{u}^\dagger = \partial_\beta P_{u^\dagger,0} = 0$ on B_d. □

Proof of Lemma 2.1. Applying Lemmas 5.2 and 5.3 with $n = 2$ proves part (a). To show part (b), we apply Lemma 5.4 and note that any finite difference entering (5.4) also enters (2.2). □

5.3. **Dual interpolant for B-QCE.** Recall the definition of Π'_h from (4.22).

Lemma 5.5. *The operator* $\Pi'_h : \mathscr{U}_h \to \mathscr{U}^{\rm c}$ *is well-defined. Moreover, it satisfies the estimates*

$$\|\nabla (\Pi'_h v_h)^*\|_{L^2} \le \|\nabla \overline{\Pi'_h v_h}\|_{L^2} \le C \|\nabla v_h\|_{L^2}, \quad \textit{and} \tag{5.5}$$

$$\|v_h - \overline{\Pi'_h v_h}\|_{L^2} \le C \|\nabla v_h\|_{L^2}, \tag{5.6}$$

where C *is a generic constant.*

Proof. To see that $v := \Pi'_h v_h$ is well-defined by (4.22), we first define $w \in \mathscr{U}^{\rm c}$, $w(\xi) := (\bar\zeta * v_h)(\xi)$. From standard quasi-interpolation arguments (see, e.g., [39, 40]) we can deduce that

$$\|\bar w - v_h\|_{L^2} \leq C\|\nabla v_h\|_{L^2}.$$

Writing $v := w + z$, (4.22) becomes

$$\begin{aligned} (\bar\zeta * z)(\xi) &= g(\xi), \qquad && \xi \in \Lambda^{\rm a}, \\ z(\xi) &= 0, && \xi \in \mathbb{Z}^d \setminus \Lambda^{\rm a}, \end{aligned}$$

where $g(\xi) = v_h(\xi) - \bar\zeta * w(\xi) = v_h(\xi) - (\bar\zeta * \bar\zeta * v_h)(\xi)$. Testing the first line with a test function $\varphi \in \mathscr{U}^{\rm c}$, $\varphi = 0$ in $\mathbb{Z}^d \setminus \Lambda^{\rm a}$, and using the fact that

$$\sum_{\xi\in\mathbb{Z}^d} (\bar\zeta * z)(\xi)\varphi(\xi) = \int_{\mathbb{R}^d} \sum_{\xi\in\mathbb{Z}^d} \bar\zeta(x-\xi)\bar z(x)\varphi(\xi)\,{\rm d}x = \int_{\mathbb{R}^d} \bar z(x)\cdot\bar\varphi(x)\,{\rm d}x,$$

we obtain the variational form

$$\int_{\mathbb{R}^d} \bar z(x)\cdot\bar\varphi(x)\,{\rm d}x = \sum_{\xi\in\Lambda^{\rm a}} g(\xi)\cdot\varphi(\xi) \qquad \text{for all } \varphi\in\mathscr{U}^{\rm c}, \varphi|_{\mathbb{Z}^d\setminus\Lambda^{\rm a}} = 0,$$

from which it is now obvious that a unique solution exists.

Testing with $\varphi = z$, we obtain that

$$\|\bar z\|_{L^2} \leq C\|g\|_{\ell^2}.$$

Exploiting the assumption that $\mathscr{N}_h$ and $\Lambda^{\rm a}$ coincide in $\Omega^{\rm a}$ it is straightforward to show that

$$\|g\|_{\ell^2} \leq C\|\nabla v_h\|_{L^2},$$

and we further obtain that

$$\|\nabla(\bar v - v_h)\|_{L^2} \leq C_1\|\bar v - v_h\|_{L^2} \leq C_1\big(\|\bar z\|_{L^2} + \|\bar w - v_h\|_{L^2}\big) \leq C_2\|\nabla v_h\|.$$

In particular, $\|\nabla\bar v\|_{L^2} \leq C\|\nabla v_h\|_{L^2}$. This completes the proof of Lemma 5.5. □

5.4. **Inverse estimates.** Before we embark on the proof of the consistency estimates, we another technical tool that allows us to convert local L^∞ bounds into L^p bounds. This is motivated by the form of the estimate in Lemma 4.3.

Performing such conversions are standard norm-equivalence arguments if the functions involved are piecewise polynomial:

$$\|\nabla^j\tilde v\|_{L^\infty(T)} \lesssim \|\nabla^j\tilde v\|_{L^p(T)} \qquad \forall v\in\mathscr{U}, T\in\mathscr{T}, j = 0,\dots,3, p\in[1,\infty]. \tag{5.7}$$

In the point defect case, this also extends to $y = y_0 + u$, where $y_0 = \mathsf{A}x$.

However, we will also need to perform such estimates for $y_0 = \mathsf{A}x + u^{\rm lin}$. To that end, we now construct a piecewise polynomial interpolant of y_0 that takes into account the structure of $u^{\rm lin}$. For $y \in \mathscr{Y}$, $x\in\mathbb{R}^d$, $|x| > 2r_{\rm cut} + 2\sqrt{d}$, we define

$$\hat y^x(x') := \widetilde{y^x}(x') \qquad \text{for } x'\in\nu_x, \tag{5.8}$$

where $\widetilde{y^x}$ is the $C^{2,1}$-conforming piecewise polynomial interpolant defined through Lemma 2.1. (Since $\hat y^x$ is piecewise polynomial, it is *not* of the form $y_0 + \tilde u$ for any $u\in\mathscr{U}^{1,2}$.)

The interpolant is clearly well-defined and we obtain the following bounds from standard interpolation error estimate arguments (e.g., see [6]): for $Q = \xi + (0,1)^d \subset B_{2r_{\rm cut}+2\sqrt{d}}(x)$ and $\omega_Q = \xi + (-1,2)^d$, $q \in [1,\infty]$, we have

$$\|\nabla\tilde{y} - \nabla\hat{y}^x\|_{L^\infty(Q)} \le C_1 \|\nabla^3\tilde{y}\|_{L^q(\omega_Q)}, \tag{5.9}$$

$$\|\nabla^j\hat{y}^x\|_{L^\infty(Q)} \le C_2 \|\nabla^j\hat{y}^x\|_{L^q(Q)} \text{ for } j = 1,2,3, \quad \text{and} \tag{5.10}$$

$$\|\nabla^j\hat{y}^x\|_{L^q(Q)} \le C_3 \|\nabla^j\tilde{y}\|_{L^q(\omega_Q)} \text{ for } j = 2,3, \tag{5.11}$$

where the constants C_1, C_2, C_3 are generic. While (5.10) is obvious, the two other estimates require some comments.

Proof of (5.9). Since, for $d = 2$, $W^{3,1}$ is embedded in C, standard interpolation error arguments yield

$$\|\nabla\tilde{y} - \nabla\hat{y}^x\|_{L^\infty(Q)} = \|\nabla y^x - \nabla\widetilde{y^x}\|_{L^\infty(Q)} \lesssim \|\nabla^3 y^x\|_{L^1(\omega_Q)} = \|\nabla^3\tilde{y}\|_{L^1(\omega_Q)}.$$

For $d = 3$ the embedding fails, however, in this case $\tilde{y}$ is piecewise polynomial; that is, $\tilde{y} = \hat{y}^x$, hence the result is true in this case as well. □

Proof of (5.11). Let p be an arbitrary polynomial of degree $j-1$, then

$$\begin{aligned}\|\nabla^j\hat{y}^x\|_{L^q(Q)} &= \|\nabla^j(\hat{y}^x - p)\|_{L^q(Q)} \lesssim \|\nabla(\hat{y}^x - p)\|_{L^q(Q)} \\ &\lesssim \|\nabla(\hat{y}^x - y^x)\|_{L^q(Q)} + C\|\nabla(y^x - p)\|_{L^q(Q)}.\end{aligned}$$

From (5.9) and the Bramble-Hilbert Lemma, we obtain (5.11). □

6. Consistency Proofs

6.1. **B-QCE coarsening error.** Throughout this section and the next we assume the conditions of Theorem 4.5. Thus, let $y = y_0 + u \in \mathscr{Y}$ be fixed, let $y_h = y_0 + u_h := \Pi_h y^{\rm a}$ be its quasi-best approximation and let $v_h \in \mathscr{U}^{\rm c}$ be an arbitrary test function. We choose $v := \Pi_h' v_h \in \mathscr{U}^{\rm c}$, where Π_h' is defined in (4.22) and analysed in § 5.3, and estimate the B-QCE consistency error

$$\langle \delta\mathscr{E}_h^\beta(y_h), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y^{\rm a}), v^*\rangle.$$

Using the fact that $v^*(\xi) = v_h(\xi)$ for all $\xi \in \Lambda^{\rm a}$, and employing (4.23) we split the error as follows,

$$\begin{aligned}&\langle \delta\mathscr{E}_h^\beta(y_h), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v^*\rangle \\ &= \int_{\mathbb{R}^d} Q_h\big[\beta\big(\partial W(\nabla y_h) - \partial W(\nabla\tilde{y})\big) : \nabla v_h\big]\,{\rm d}x + \int_{\mathbb{R}^d} (Q_h - {\rm Id})\big[\beta\partial W(\nabla\tilde{y}) : \nabla v_h\big]\,{\rm d}x \\ &\quad + \int_{\mathbb{R}^d} \beta\partial W(\nabla\tilde{y}) : (\nabla v_h - \nabla\bar{v})\,{\rm d}x + \int_{\mathbb{R}^d} \mathsf{R}^\beta(\tilde{y};x) : \nabla\bar{v}\,{\rm d}x \\ &:= {\rm T}_1 + {\rm T}_2 + {\rm T}_3 + {\rm T}_4,\end{aligned}$$

where R^β is defined in (4.23). In the consistency error analysis of the B-QCF method in § 6.4 we use an analogous splitting, hence the following estimates for the terms ${\rm T}_1, {\rm T}_2, {\rm T}_3$ will be used there as well.

Lemma 6.1. *Under the conditions of Theorem 4.5, the terms* ${\rm T}_1$ *and* ${\rm T}_2$ *are bounded by*

$$\begin{aligned}{\rm T}_1 &\lesssim \Big(\|\nabla u_h - \nabla\tilde{u}\|_{L^2(\Omega^{\rm c})} + \|h^2\nabla^3\tilde{u}\|_{L^2(\Omega^{\rm c})}\Big)\|\nabla v_h\|_{L^2} \quad \textit{and} \\ {\rm T}_2 &\lesssim \Big(\big\|h^2\nabla^2\big[\beta\partial W(\nabla\tilde{y})\big]\big\|_{L^2}\Big)\|\nabla v_h\|_{L^2}.\end{aligned}$$

Proof. 1. Estimate of T_1*:* Let $T \in \mathcal{T}_h$ such that $\beta \neq 0$ on T, then

$$\begin{aligned}\int_T Q_h\big[\beta\big(\partial W(\nabla y_h) - \partial W(\nabla \tilde{y})\big) : \nabla v_h\big]\,\mathrm{d}x \\ &\le |T|^{1/2}\|\partial W(\nabla y_h) - \partial W(\nabla \tilde{y})\|_{L^\infty(T)}\|\nabla v_h\|_{L^2(T)} \\ &\lesssim |T|^{1/2}\|\nabla u_h - \nabla \tilde{u}\|_{L^\infty(T)}\|\nabla v_h\|_{L^2(T)},\end{aligned}$$

where C depends on $\partial^2 W$ in a neighbourhood of $\nabla\tilde{y}$ and hence on $M_\epsilon^{(\boldsymbol{\rho})}(y), \boldsymbol{\rho} \in \mathcal{R}^2$. Employing the embedding $H^2 \subset C$,

$$|T|^{1/2}\|\nabla u_h - \nabla \tilde{u}\|_{L^\infty(T)} \lesssim \Big(\|\nabla u_h - \nabla \tilde{u}\|_{L^2(T)} + \|h^2 \nabla^3 \tilde{u}\|_{L^2(T)}\Big),$$

where C depends only on the shape regularity of the mesh. Summing over all T, we obtain the stated result.

2. Estimate of T_2*:* For any piecewise linear (not necessarily continuous) ψ_h we have

$$\begin{aligned}\mathrm{T}_2 &= \int_{\mathbb{R}^d} (Q_h - \mathrm{Id})\big[\beta\partial W(\nabla\tilde{y}) - \psi_h\big] : \nabla v_h\,\mathrm{d}x \\ &\le \big\|(Q_h - \mathrm{Id})\big[\beta\partial W(\nabla\tilde{y}) - \psi_h\big]\big\|_{L^2}\|\nabla v_h\|_{L^2}.\end{aligned}$$

Therefore, by the Bramble-Hilbert Lemma,

$$\mathrm{T}_2 \lesssim \big\|h^2\nabla^2\big[\beta\partial W(\nabla\tilde{y})\big]\big\|_{L^2}\|\nabla v_h\|_{L^2},$$

where the constant depends again on the shape regularity of $\mathcal{T}_h$. □

Lemma 6.2. *Under the conditions of Theorem 4.5, the term* T_3 *is bounded above by*

$$\mathrm{T}_3 \lesssim \Big(\big\|\nabla^2\big[\beta\partial W(\nabla\tilde{y})\big]\big\|_{L^2} + \|h\nabla^2\tilde{u}\|_{L^2(\Omega^c)} + \|h\nabla^2 y_0 \otimes (\nabla y_0 - \mathsf{A})\|_{L^2(\Omega^c)}\Big)\|\nabla v_h\|_{L^2}.$$

Proof. Let ζ_ν be the nodal basis function associated with a node $\nu \in \mathscr{N}_h$, with support ω_ν, and let $f := -\operatorname{div}\big[\beta\partial W(\nabla\tilde{y})\big]$. We integrate the term T_3 by parts, and then use the fact that ζ_ν form a partition of unity, to obtain

$$\begin{aligned}\mathrm{T}_3 &= -\int_{\mathbb{R}^d} \operatorname{div}\big[\beta\partial W(\nabla\tilde{y})\big]\cdot(v_h - \bar{v})\,\mathrm{d}x \\ &= \sum_{\nu\in\mathscr{N}_h}\int_{\mathbb{R}^d} f(x)\cdot(v_h(\nu) - \bar{v}(x))\zeta_\nu(x)\,\mathrm{d}x.\end{aligned}$$

Case 1: If $\nu \in \Lambda^{\mathrm{a}} \cap \mathscr{N}_h$, then $\zeta_\nu(x) = \bar{\zeta}(x-\nu)$ and hence

$$\int_{\mathbb{R}^d}(v_h(\nu) - \bar{v}(x))\zeta_\nu(x)\,\mathrm{d}x = v_h(\nu) - v^*(\nu) = 0, \tag{6.1}$$

by definition of v^* and v. Therefore,

$$\int_{\mathbb{R}^d} f(x)\cdot(v_h(\nu) - \bar{v}(x))\zeta_\nu(x)\,\mathrm{d}x \lesssim \|\nabla f\|_{L^2(\omega_\nu)}\|\zeta_\nu^{1/2}(v_h(\nu) - \bar{v}(x))\|_{L^2(\omega_\nu)}$$

where $\omega_\nu = \operatorname{supp}\zeta_\nu$. Exploiting again (6.1) we can estimate

$$\begin{aligned}\|\zeta_\nu^{1/2}(v_h(\nu)-\bar v)\|_{L^2(\omega_\nu)}^2 &= \int_{\omega_\nu}(v_h(\nu)-\bar v)\cdot\big[(v_h(\nu)-\bar v)\zeta_\nu\big]\,\mathrm{d}x\\ &= \int_{\omega_\nu}\big((\bar v)_{\omega_\nu}-\bar v\big)\cdot\big[(v_h(\nu)-\bar v)\zeta_\nu\big]\,\mathrm{d}x\\ &\le \|(\bar v)_{\omega_\nu}-\bar v\|_{L^2(\omega_\nu)}\|\zeta_\nu(v_h(\nu)-\bar v)\|_{L^2(\omega_\nu)}\\ &\lesssim \|\nabla\bar v\|_{L^2(\omega_\nu)}\|\zeta_\nu^{1/2}(v_h(\nu)-\bar v)\|_{L^2(\omega_\nu)},\end{aligned}$$

and hence we arrive at

$$\int_{\mathbb{R}^d} f(x)\cdot(v_h(\nu)-\bar v(x))\zeta_\nu(x)\,\mathrm{d}x \lesssim \|\nabla f\|_{L^2(\omega_\nu)}\|\nabla v_h\|_{L^2(\omega_\nu)} \qquad \text{for } \nu\in\mathscr{N}_h\cap\Lambda^{\mathrm{a}}. \tag{6.2}$$

Case 2: Because of the way v is defined, we do not have (6.1) for $\nu\in\mathscr{N}_h\setminus\Lambda^{\mathrm{a}}$, but on the other hand $\beta\equiv 1$ in this case, which means that the second-order estimate is not crucial. In this case, using elementary interpolation error estimates, we obtain only

$$\begin{aligned}\int_{\mathbb{R}^d} f(x)\cdot(v_h(\nu)-\bar v(x))\zeta_\nu(x)\,\mathrm{d}x &\le \|hf\|_{L^2(\omega_\nu)}\big(\|h^{-1}(v_h(\nu)-v_h)\|_{L^2(\omega_\nu)}+\|h^{-1}(v_h-\bar v)\|_{L^2(\omega_\nu)}\big)\\ &\le \|hf\|_{L^2(\omega_\nu)}\big(\|\nabla v_h\|_{L^2(\omega_\nu)}+\|v_h-\bar v\|_{L^2(\omega_\nu)}\big).\end{aligned}$$

Summing the estimates over all ν and estimating the overlaps of the patches (the shape regularity of the mesh enters again here; this is a standard argument from a posteriori error analysis), we deduce that

$$\mathrm{T}_3 \lesssim \Big(\big\|\nabla\operatorname{div}(\beta\partial W(\nabla\tilde y))\big\|_{L^2}+\big\|\beta h\operatorname{div}\partial W(\nabla\tilde y)\big\|_{L^2}\Big)\big(\|\nabla v_h\|_{L^2}+\|v_h-\bar v\|_{L^2}\big).$$

and, finally, employing Lemma 5.5,

$$\mathrm{T}_3 \lesssim \Big(\big\|\nabla\operatorname{div}(\beta\partial W(\nabla\tilde y))\big\|_{L^2}+\big\|\beta h\operatorname{div}\partial W(\nabla\tilde y)\big\|_{L^2}\Big)\|\nabla v_h\|_{L^2}. \tag{6.3}$$

Note that we have inserted β in $\big\|\beta h\operatorname{div}\partial W(\nabla\tilde y)\big\|_{L^2}$ merely to indicate that it is restricted to the continuum region. Inserting the estimate

$$\begin{aligned}|\operatorname{div}\partial W(\nabla\tilde y)| &\le \big|\operatorname{div}\partial W(\nabla\tilde y)-\operatorname{div}\partial W(\nabla y_0)\big|\\ &\quad+\big|\operatorname{div}\partial W(\nabla y_0)-\operatorname{div}\partial^2 W(\mathsf{A}):(\nabla y_0-\mathsf{A})\big|\\ &\lesssim |\nabla^2\tilde u|+|\nabla^2 y_0|\,|\nabla y_0-\mathsf{A}|.\end{aligned}$$

into (6.3) yields the stated result. □

We can now combine the foregoing results to arrive at the complete coarsening error estimate.

Lemma 6.3 (B-QCE coarsening error). *Under the conditions of Theorem 4.5,*

$$\langle\delta\mathscr{E}_h^\beta(\Pi_h y_h),v_h\rangle-\langle\delta\mathscr{E}^{\mathrm{a}}(y),(\Pi_h' v_h)^*\rangle \lesssim \Big(\mathbf{E}^{\mathrm{apx}}(y)+\mathbf{E}^{\mathrm{cb}}(y)+\mathbf{E}^{\mathrm{int}}(y)+\|\mathsf{R}^\beta(\tilde y)\|_{L^2}\Big)\|\nabla v_h\|_{L^2} \quad \textit{for all } v_h\in\mathscr{U}_h. \tag{6.4}$$

Proof. Using Lemma 6.1 and Lemma 6.2, the bound

$$|\nabla^2(\beta\partial W(\nabla\tilde y))| \lesssim |\beta\nabla^3\tilde y|+|\nabla\beta\nabla^2\tilde y|+|\nabla^2\beta|,$$

and the estimate

$$\mathrm{T}_4 \le \|R^\beta\|_{L^2}\|\nabla\bar v\|_{L^2} \lesssim \|R^\beta\|_{L^2}\|\nabla v_h\|_{L^2},$$

where we employed Lemma 5.5, we obtain the result. □

6.2. **B-QCE modelling error estimate.** To complete the B-QCE consistency error analysis it remains to provide a sharp bound on the B-QCE stress error R^β, which is defined in (4.23).

Lemma 6.4. *Let $\epsilon > 0$ and $z \in C^{2,1}(\nu_x)$ with $\|\nabla z - \nabla\tilde{y}\|_{L^\infty} \le \epsilon$, then*

$$\big|\mathsf{R}^\beta(z;x)\big| \le C\big(\|\nabla^2\beta\|_{L^\infty(\nu_x)} + |\nabla\beta(x)|\,|\nabla^2 z(x)| + \|\nabla^3 z\|_{L^\infty(\nu_x)} + \|\nabla^2 z\|^2_{L^\infty(\nu_x)}\big), \tag{6.5}$$

where C depends on $M^{(\boldsymbol{\rho})}_\epsilon(y), \boldsymbol{\rho} \in \mathcal{R}^j, j = 1, \dots, 3$.

Proof. Throughout the proof we define $V_{\xi,\rho} := V_{,\rho}(Dz(\xi))$ and $\bar{V}_{,\rho} := V_{,\rho}(\nabla_{\mathcal{R}} z(x))$. Further, we define $\beta \equiv \beta(x)$ and $\nabla\beta \equiv \nabla\beta(x)$. Finally, we denote

$$\epsilon_j := \|\nabla^j z\|_{L^\infty(\nu_x)}, \quad \text{and} \quad \delta_j := \|\nabla^j \beta\|_{L^\infty(\nu_x)}.$$

We begin by noting that, since $\mathcal{R}$ and the support of ω_ρ are both bounded, the sum over ξ in the definition of R^β

$$\mathsf{R}^\beta(z;x) := \beta(x)\partial W(\nabla z(x)) - \sum_{\xi\in\mathbb{Z}^d} \beta(\xi) \sum_{\rho\in\mathcal{R}} \big[V_{\xi,\rho} \otimes \rho\big]\omega_\rho(\xi - x)$$

is only over a bounded set. Therefore, we can insert the expansion (4.11) to obtain

$$\begin{aligned}
\mathsf{R}^\beta(z;x) :=\ & \beta(x)\partial W(\nabla z(x)) \\
& - \sum_{\xi\in\mathbb{Z}^d} \beta(\xi) \sum_{\rho\in\mathcal{R}} \Big[\Big(\bar{V}_{,\rho} + \sum_{\varsigma\in\mathcal{R}} \bar{V}_{,\rho\varsigma}(D_\varsigma z - \nabla_\varsigma z) + O(\epsilon_2^2)\Big) \otimes \rho\Big]\omega_\rho(\xi - x) \\
=\ & \beta(x)\partial W(\nabla z(x)) - \sum_{\xi\in\mathbb{Z}^d} \beta(\xi) \sum_{\rho\in\mathcal{R}} \big[\bar{V}_{,\rho} \otimes \rho\big]\omega_\rho(\xi - x) \\
& - \sum_{\xi\in\mathbb{Z}^d} \beta(\xi) \sum_{\rho,\varsigma\in\mathcal{R}} \big[\bar{V}_{,\rho\varsigma}(D_\varsigma z - \nabla_\varsigma z)\big] \otimes \rho\,\omega_\rho(\xi - x) + O(\epsilon_2^2) \\
=:\ & \mathrm{T}_1 - \mathrm{T}_2 + O(\epsilon_2^2).
\end{aligned} \tag{6.6}$$

We expand $\beta(\xi) = \beta + \nabla\beta\cdot(\xi - x) + O(\delta_2)$, and employ (4.18) to estimate

$$\begin{aligned}
\mathrm{T}_1 &= \beta\partial W(\nabla z(x)) - \sum_{\xi\in\mathbb{Z}^d} \Big(\beta + \nabla\beta\cdot(\xi - x)\Big) \sum_{\rho\in\mathcal{R}} \big[\bar{V}_{,\rho} \otimes \rho\big]\omega_\rho(\xi - x) + O(\delta_2) \\
&= \beta\partial W(\nabla z(x)) - \beta \sum_{\rho\in\mathcal{R}} \big[\bar{V}_{,\rho} \otimes \rho\big] \\
&\quad - \nabla\beta \cdot \sum_{\rho\in\mathcal{R}} \big[\bar{V}_{,\rho} \otimes \rho\big] \sum_{\xi\in\mathbb{Z}^d} (\xi - x)\omega_\rho(\xi - x) + O(\delta_2).
\end{aligned}$$

Since $\sum_{\rho\in\mathcal{R}} \big[\bar{V}_{,\rho} \otimes \rho\big] = \partial W(\nabla z(x))$ and $\sum_{\xi\in\mathbb{Z}^d}(\xi - x)\omega_\rho(\xi - x) = -\frac{1}{2}\rho$ by (4.19), we further obtain

$$\mathrm{T}_1 = -\frac{1}{2}\sum_{\rho\in\mathcal{R}} \big[\bar{V}_{,\rho} \otimes \rho\big](\nabla\beta\cdot\rho) + O(\delta_2) = O(\delta_2),$$

where the sum over $\mathcal{R}$ cancels due to the point symmetry assumption (2.6).

To estimate T_2 we expand β and use expansion (4.6), (4.18), and (4.19) to obtain

$$\begin{aligned}\mathrm{T}_2 &= \sum_{\xi\in\mathbb{Z}^d}\Big(\beta + \nabla\beta\cdot(\xi - x)\Big)\sum_{\rho,\varsigma\in\mathcal{R}}\big[\bar V_{,\rho\varsigma}(\nabla_\varsigma\nabla_{\xi-x}z + \tfrac12\nabla_\varsigma^2 z)\big]\otimes\rho\,\omega_\rho(\xi - x) + O(\delta_2+\varepsilon_3)\\ &= \beta\sum_{\rho,\varsigma\in\mathcal{R}}\big[\bar V_{,\rho\varsigma}(-\tfrac12\nabla_\varsigma\nabla_\rho z + \tfrac12\nabla_\varsigma^2 z)\big]\otimes\rho + O\big(|\nabla\beta|\,|\nabla^2 z|\big) + O(\delta_2+\varepsilon_3)\end{aligned}$$

Using again (2.6) we observe that the sum over $\rho,\varsigma\in\mathcal{R}$ cancels, and hence we obtain that $|\mathrm{T}_2| \lesssim |\nabla\beta|\,|\nabla^2 z| + \delta_2 + \varepsilon_3$.

Combining this with the estimate for T_1, we obtain the stated result. □

We now convert the pointwise estimate (6.5) into a global estimate.

Lemma 6.5. *Under the conditions of Theorem 4.5, we have*

$$\big\|\mathsf{R}^\beta(\tilde y;x)\big\|_{L^2} \le C\big(\|\nabla^2\beta\|_{L^2} + \|\nabla\beta\|_{L^\infty}\|\nabla^2\tilde y\|_{L^2(\Omega^\beta)} + \|\nabla^3\tilde y\|_{L^2(\Omega^c)} + \|\nabla^2\tilde y\|^2_{L^4(\Omega^c)}\big), \quad (6.7)$$

where C depends on $M_\epsilon^{(\boldsymbol\rho)}(y), \boldsymbol\rho\in\mathcal{R}^j, j = 1,\dots,3$.

Proof. The main point of this proof is to use the inverse estimates from § 5.4 to obtain L^q-type bounds from the L^∞ bounds provided by Lemma 6.4.

Let $r(x) := \mathsf{R}^{\tilde\beta}(\hat y^x;x)$ and $\mathsf{F}(x) := \nabla\hat y^x(x)$, then we begin by estimating

$$\begin{aligned}\|\mathsf{R}^\beta(\tilde y) - r\|_{L^2} &\le \|\beta\partial W(\nabla\tilde y) - \tilde\beta\partial W(\mathsf{F})\|_{L^2}\\ &\lesssim \big(\|\beta-\tilde\beta\|_{L^2}\big) + \big\|\beta\big(\partial W(\nabla\tilde y) - \partial W(\mathsf{F})\big\|_{L^2}\\ &\lesssim \big(\|\nabla^2\beta\|_{L^2} + \|\beta(\nabla\tilde y - \mathsf{F})\|_{L^2}\big),\end{aligned} \quad (6.8)$$

where we used $\|\beta - \tilde\beta\|_{L^2} \le C\|\nabla^2\beta\|_{L^2}$. Let $x\in\mathrm{supp}(\beta)\cap Q^x$ where $Q^x = \xi + [0,1)^d$, and let $\xi\in\mathbb{Z}^d$. Then

$$|\nabla\tilde y - \mathsf{F}(x)| \le \|\nabla\tilde y - \nabla\hat y^x\|_{L^2(Q)} \lesssim \|\nabla^3\tilde y\|_{L^2(Q)}.$$

Integrating over x yields

$$\int\beta(x)^2|\nabla\tilde y - \mathsf{F}(x)|^2\,\mathrm{d}x \le \int\beta(x)\|\nabla^3\tilde y\|^2_{L^2(Q^x)}\,\mathrm{d}x \lesssim \|\nabla^3\tilde y\|^2_{L^2(\Omega^c)}, \quad (6.9)$$

using an argument analogous to the one in [34, App.A]. Together with (6.8) we obtain

$$\|\mathsf{R}^\beta(\tilde y) - r\|_{L^2} \lesssim \big(\|\nabla^2\beta\|_{L^2} + \|\nabla^3\tilde y\|_{L^2(\Omega^c)}\big). \quad (6.10)$$

Using Lemma 6.4 with β replaced with $\tilde\beta$ and $z = \hat y^x$, defining $\nu_x^\beta := \nu_x\cap\mathrm{supp}(\nabla\tilde\beta)$, and recalling (5.10), we obtain

$$\begin{aligned}|r(x)|^2 &\lesssim \Big(\|\nabla^2\tilde\beta\|^2_{L^\infty(\nu_x)} + \|\nabla\tilde\beta\|^2_{L^\infty}\|\nabla^2\hat y^x\|^2_{L^\infty(\nu_x^\beta)} + \|\nabla^3\hat y^x\|^2_{L^\infty(\nu_x)} + \|\nabla^2\hat y^x\|^4_{L^\infty(\nu_x)}\Big)\\ &\lesssim \Big(\|\nabla^2\tilde\beta\|^2_{L^2(\nu_x)} + \|\nabla\tilde\beta\|^2_{L^\infty}\|\nabla^2\hat y^x\|^2_{L^2(\nu_x^\beta)} + \|\nabla^3\hat y^x\|^2_{L^2(\nu_x)} + \|\nabla^2\hat y^x\|^4_{L^4(\nu_x)}\Big).\end{aligned}$$

Using Lemma 2.1, the results of § 5.4, and techniques similar to those used to prove (6.9), we deduce that

$$\|r\|_{L^2} \lesssim \|\nabla^2\beta\|_{L^2} + \|\nabla\beta\|_{L^\infty}\|\nabla^2\tilde y\|_{L^2(\Omega^\beta)} + \|\nabla^3\tilde y\|_{L^2(\Omega^c)} + \|\nabla^2\tilde y\|^2_{L^4(\Omega^c)}.$$

Together with (6.10), this yields the desired result. □

Proof of Theorem 4.5. The result follows upon combining Lemma 6.3 and Lemma 6.5. □

6.3. **B-QCE energy error estimate.** We assume that all conditions of Theorem 3.1 hold. Let y^{a} be a solution to (2.11) and let y_h^{bqce} be the solution to (3.2) guaranteed by Theorem 3.1. For ease of notation, we write $y := y^{\mathrm{a}}$ and $y_h := y_h^{\mathrm{bqce}}$. Further, we define

$$V'(Dy) := V(Dy) - V(Dy_0) \qquad \text{and} \qquad W'(\nabla y) := W(\nabla y) - W(\nabla y_0).$$

Let

$$\tilde{\mathscr{E}} := \sum_{\ell\in\mathbb{Z}^d}(1-\beta(\ell))V'(Dy(\ell)) + \int_{\mathbb{R}^d}[Q_h\beta]W'(\nabla\tilde{y})\,\mathrm{d}x,$$

then we split the energy error into

$$\begin{aligned}\mathscr{E}^{\mathrm{a}}(y) - \mathscr{E}_h^{\beta}(y_h) &= \big[\mathscr{E}^{\mathrm{a}}(y) - \tilde{\mathscr{E}}\big] + \big[\tilde{\mathscr{E}} - \mathscr{E}_h^{\beta}(\Pi_h y)\big] + \big[\mathscr{E}_h^{\beta}(\Pi_h y) - \mathscr{E}_h^{\beta}(y_h)\big] \\ &=: T_1 + T_2 + T_3.\end{aligned}$$

Since y_h is a minimiser we obtain

$$|T_3| \lesssim \|\nabla\Pi_h u - \nabla u_h\|_{L^2}^2, \tag{6.11}$$

which we already estimated in Theorem 3.1.

6.3.1. *Estimate for T_1.* The term T_1 contains the main "modelling error" contribution. For $f : \mathbb{R}^d \to \mathbb{R}$ let $I_1 f := \bar{f}$ denote the P1 nodal interpolant with respect to the atomistic mesh $\mathscr{T}$. Then, using the fact that

$$\sum_{\xi\in\mathbb{Z}^d}\beta(\xi)W'(\nabla\tilde{y}(\xi)) = \int_{\mathbb{R}^d} I_1[\beta W'(\nabla\tilde{y})]\,\mathrm{d}x,$$

we rewrite T_1 as

$$\begin{aligned}T_1 &= \sum_{\xi\in\mathbb{Z}^d}\beta(\xi)V'\big(Dy(\xi)\big) - \int[Q_h\beta]W'(\nabla\tilde{y})\,\mathrm{d}x \\ &= \sum_{\xi\in\mathbb{Z}^d}\beta(\xi)\Big(V'\big(Dy(\xi)\big) - W'\big(\nabla\tilde{y}(\xi)\big)\Big) + \int\Big([Q_h\beta]W'(\nabla\tilde{y}) - I_1[\beta W'(\nabla\tilde{y})]\Big)\,\mathrm{d}x \\ &=: T_{1,1} + T_{1,2}.\end{aligned}$$

$T_{1,2}$ is essentially a quadrature error estimate, since both the integrals $\int Q_h[\beta W'(\nabla\tilde{y})]\,\mathrm{d}x$ and $\int I_1[\beta W'(\nabla\tilde{y})]\,\mathrm{d}x$ are second-order quadrature approximations to $\int \beta W'(\nabla\tilde{y})\,\mathrm{d}x$:

$$\begin{aligned}|T_{1,2}| \lesssim{}& \|\nabla^2\beta\|_{L^2}\|\nabla\tilde{u}\|_{L^2(\Omega^c)} + \|\nabla\beta\|_{L^\infty}\|\nabla\tilde{u}\|_{L^2(\Omega^c)}\|\nabla^2 y_0\|_{L^2(\Omega^c)} + \|\nabla\beta\|_{L^2}\|\nabla^2\tilde{u}\|_{L^2(\Omega^c)} \\ &+ \|\nabla\tilde{u}\|_{L^2(\Omega^c)}\big(\|\nabla^3 y_0\|_{L^2(\Omega^c)} + \|\nabla^2 y_0\|_{L^4(\Omega^c)}^2\big) + \|\nabla^2\tilde{u}\|_{L^2(\Omega^c)}^2 \\ &+ \|\nabla^2\tilde{u}\|_{L^2}\|\nabla^2 y_0\|_{L^2(\Omega^c)} + \|\nabla^3\tilde{u}\|_{L^1(\Omega^c)}.\end{aligned} \tag{6.12}$$

We will later see that most of these terms are dominated by other terms occuring in the energy error estimate.

Proof of (6.12). Fix an atomistic element $T \in \mathscr{T}$. If $\beta \not\equiv 1$ in T, then $T \in \mathcal{T}_h$ as well, so $Q_h\beta = Q_1\beta$, where Q_1 denotes the P0 midpoint nodal interpolant with respect to the atomistic mesh $\mathscr{T}$. In the other case, where $\beta \equiv 1$ in T, we also have $Q_h\beta = Q_1\beta = 1$.

We estimate the integral defining $\mathrm{T}_{1,2}$ restricted to T; call it

$$\mathrm{T}_{1,2}^T := \int_T\Big([Q_1\beta]W'(\nabla\tilde{y}) - I_1[\beta W'(\nabla\tilde{y})]\Big)\,\mathrm{d}x.$$

First, we replace $\tilde y$ with $\hat y^T := \hat y^{x_T}$, y_0 with $\hat y_0^T := \hat y_0^{x_T}$ where x_T is the barycentre of T, and β with $\tilde\beta$. Also, let $y_0^T := y_0^{x_T}$ and $W'(\nabla \hat y^T) = W(\nabla \hat y^T) - W(\nabla \hat y_0^T)$. Then, a brief computation shows that

$$\begin{aligned}\big\|W'(\nabla y^T) - W'(\nabla \hat y^T)\big\|_{L^\infty} &\lesssim \big\||\nabla y_0^T - \nabla \hat y_0^T|\,|\nabla \tilde u|\big\|_{L^\infty(T)} \lesssim \|\nabla \tilde u\|_{L^2(T)}\|\nabla^3 y_0\|_{L^2(T)},\\ \|(\beta-\tilde\beta)W'(\nabla\tilde y)\|_{L^\infty(T)} &\le \|\nabla^2\beta\|_{L^2(T)}\|\nabla\tilde u\|_{L^2(T)},\end{aligned}$$

and hence,

$$\begin{aligned}\big|\mathrm{T}_{1,2}^T\big| &\lesssim \bigg|\int_T \Big([Q_1\tilde\beta]W'(\nabla\hat y^T) - I_1[\tilde\beta W'(\nabla \hat y^T)]\Big)\,\mathrm{d}x\bigg|\\ &\qquad + \|\nabla\tilde u\|_{L^2(T)}(\|\nabla^3 y_0\|_{L^2(T)} + \|\nabla^2\beta\|_{L^2(T)})\\ &=: \big|\hat{\mathrm{T}}_{1,2}^T\big| + \|\nabla\tilde u\|_{L^2(T)}(\|\nabla^3 y_0\|_{L^2(T)} + \|\nabla^2\beta\|_{L^2(T)}),\end{aligned}$$

We estimate the term $\hat{\mathrm{T}}_{1,2}^T$ as follows:

$$\begin{aligned}\big|\hat{\mathrm{T}}_{1,2}^T\big| &\le \bigg|\int_T [Q_1\tilde\beta]\big(W'(\nabla y^T) - Q_1[W'(\nabla y^T)]\big)\,\mathrm{d}x\bigg| + \bigg|\int_T (Q_1 - I_1)[\tilde\beta W'(\nabla\tilde y)]\,\mathrm{d}x\bigg|\\ &\lesssim \|\nabla^2[\tilde\beta W'(\nabla\hat y^T)]\|_{L^\infty(T)}\\ &\lesssim \|(\nabla^2\tilde\beta)W'(\nabla\hat y^T)\|_{L^\infty(T)} + \|\nabla\tilde\beta\otimes\nabla W'(\nabla\hat y^T)\|_{L^\infty(T)} + \|\tilde\beta\nabla^2 W'(\nabla\hat y^T)\|_{L^\infty(T)}\\ &\lesssim \|\nabla^2\tilde\beta\|_{L^\infty}\|\nabla\tilde u\|_{L^\infty(T)} + \|\nabla\tilde\beta\|_{L^\infty}\Big(\|\nabla\tilde u\nabla^2\hat y_0\|_{L^\infty(T)} + \|\nabla^2\tilde u\|_{L^\infty(T)}\Big)\\ &\qquad + \Big(\big\||\nabla\tilde u|\,|\nabla^2\hat y_0|^2\big\|_{L^\infty(T)} + \big\||\nabla^2\tilde u|\,|\nabla^2\hat y_0|\big\|_{L^\infty(T)} + \big\||\nabla^2\tilde u|^2\big\|_{L^\infty(T)}\\ &\qquad\quad + \|\nabla^3\tilde u\|_{L^\infty(T)} + \big\||\nabla\tilde u|\,|\nabla^3\hat y_0|\big\|_{L^\infty(T)}\Big),\end{aligned}$$

where we used the fact that $\nabla\hat y^T - \nabla\hat y_0^T = \nabla\tilde u$ and identities along the lines of

$$\begin{aligned}\nabla W'(\nabla\hat y^T) &= \nabla\big(W(\nabla\hat y^T) - W(\nabla\hat y_0^T)\big) = \partial W(\nabla\hat y^T) : \nabla^2\hat y^T - \partial W(\nabla\hat y_0^T) : \nabla^2\hat y_0^T\\ &= \big(\partial W(\nabla\hat y^T) - \partial W(\nabla\hat y_0^T)\big) : \nabla^2\hat y_0^T + \partial W(\nabla\hat y^T) : \big(\nabla^2\hat y^T - \nabla^2\hat y_0^T\big),\end{aligned}$$

and its lower and higher order analogues.

Applying suitable inverse inequalities (cf. § 5.4), summing over $T\in\mathscr{T}$, and being careful to only collect those terms for that actually occur in a given element yields (6.12). ☐

To estimate $T_{1,1}$ we perform a basic Taylor expansion, using the tools developed in § 4.2.1 and § 4.2.2.

Lemma 6.6. *Let $\xi\in\mathbb{Z}^d\setminus B_{R^{\mathrm{a}}}$, and $y\in\mathscr{Y}$, then*

$$\begin{aligned}\big|V'(Dy(\xi)) - W'(\nabla\tilde y(\xi))\big| \lesssim \Big(&\|\nabla^3\tilde u\|_{L^1(\nu_\xi)} + \|\nabla^2\tilde u\|_{L^2(\nu_\xi)}^2 + \|\nabla^2\tilde u\|_{L^2(\nu_\xi)}\|\nabla^2 y_0\|_{L^2(\nu_\xi)}\\ &+ \|\nabla\tilde u\|_{L^2(\nu_\xi)}\big(\|\nabla^3 y_0\|_{L^2(\nu_\xi)} + \|\nabla^2 y_0\|_{L^4(\nu_\xi)}^2\big)\Big).\end{aligned} \tag{6.13}$$

Proof. All derivatives and finite differences below are evaluated at ξ, so we omit the argument, writing Du for $Du(\xi)$, for example. Let $z := \hat y^\xi$ and $z_\theta := \hat y_0^\xi + \theta\tilde u$, so that $z = z_1$, $V'(Dz) = V(Dz) - V(Dz_0)$ and $W'(\nabla z) = W(\nabla z) - W(\nabla z_0)$. Then

$$V'(Dz) - W'(\nabla z) = \int_{\theta=0}^1 \Big(\langle\delta V(Dz_\theta), Du\rangle - \langle\partial W(\nabla z_\theta), \nabla\tilde u\rangle\Big)\,\mathrm{d}\theta.$$

Expanding $\langle \delta V(Dz_\theta), Du\rangle$ analogously to the proof of Lemma 6.4, with $\varepsilon_j := \|\nabla^j z_\theta\|_{L^\infty(\nu_\xi)}$ and $\tilde\varepsilon_j := \|\nabla^j \tilde u\|_{L^\infty(\nu_\xi)}$, we obtain

$$\begin{aligned}
\langle \delta V(Dz_\theta), Du\rangle &= \sum_{\rho\in\mathcal{R}} V_{,\rho}(Dz_\theta) D_\rho u \\
&= \sum_{\rho\in\mathcal{R}} \Big(V_{,\rho} + \sum_{\varsigma\in\mathcal{R}} V_{,\rho\varsigma} \tfrac12 \nabla_\varsigma^2 z_\theta + O(\varepsilon_3 + \varepsilon_2^2)\Big) D_\rho u \\
&= \sum_{\rho\in\mathcal{R}} V_{,\rho}\big(\nabla_\rho \tilde u + \tfrac12 \nabla_\rho^2 \tilde u\big) + \sum_{\rho,\varsigma\in\mathcal{R}} \langle V_{,\rho\varsigma} \nabla_\rho \tilde u, \tfrac12 \nabla_\varsigma^2 z_\theta\rangle \\
&\qquad + O(\tilde\varepsilon_3) + O(\varepsilon_2\tilde\varepsilon_2) + O\big(\tilde\varepsilon_1(\varepsilon_3 + \varepsilon_2^2)\big).
\end{aligned}$$

We now observe that $\sum_{\rho\in\mathcal{R}} V_{,\rho}\nabla_\rho \tilde u = \partial W(\nabla z_\theta) : \nabla \tilde u$, and that, due to the point symmetry (2.6), both

$$\sum_{\rho\in\mathcal{R}} V_{,\rho} \tfrac12 \nabla_\rho^2 \tilde u = 0 \qquad \text{and} \qquad \sum_{\rho,\varsigma\in\mathcal{R}} \langle V_{,\rho\varsigma}\nabla_\rho \tilde u, \nabla_\varsigma^2 z_\theta\rangle = 0.$$

We combine the foregoing calculations to obtain

$$\begin{aligned}
\big|V'(Dz) - W'(\nabla z)\big| \leq C\Big(&\|\nabla^3 \tilde u\|_{L^\infty(\nu_\xi)} + \|\nabla^2\tilde u\|_{L^\infty(\nu_\xi)} \|\nabla^2 z_0\|_{L^\infty(\nu_\xi)} + \|\nabla^2 \tilde u\|^2_{L^\infty(\nu_\xi)} \\
&+ \|\nabla\tilde u\|_{L^\infty(\nu_\xi)}\big(\|\nabla^3 z_0\|_{L^\infty(\nu_\xi)} + \|\nabla^2 z_0\|^2_{L^\infty(\nu_\xi)}\big)\Big).
\end{aligned}$$

Using appropriate inverse estimates, and incorporating the error $\nabla z_\theta - \nabla\tilde y$, similarly (e.g.) as in the proof of (6.12) (this yields additional $\|\nabla \tilde u\|_{L^2}\|\nabla^3 \tilde y_0\|_{L^2}$ terms), we obtain the stated result. ∎

Summing (6.13) over all $\xi \in \mathbb{Z}^d$ with $\beta(\xi) > 0$ it is straightforward now to prove that

$$\begin{aligned}
|T_{1,1}| \leq C\Big(&\|\nabla^3 \tilde u\|_{L^1(\Omega^c)} + \|\nabla^2 \tilde u\|^2_{L^2(\Omega^c)} + \|\nabla^2 \tilde y\|_{L^2(\Omega^c)} \|\nabla^2 \tilde y\|_{L^2(\Omega^c)} \\
&+ \|\nabla \tilde u\|_{L^2(\Omega^c)}\big(\|\nabla^3 y_0\|_{L^2(\Omega^c)} + \|\nabla^2 y_0\|^2_{L^4(\Omega^c)}\big)\Big).
\end{aligned} \tag{6.14}$$

This completes the estimate for T_1

6.3.2. *Estimate for* T_2. We begin by recalling that $\mathcal{T}_h$ and Π_h are defined in such a way that $\Pi_h y(\xi) = y(\xi)$ in a sufficiently large neighbourhood so that

$$\begin{aligned}
\mathrm{T}_2 &= \int \Big([Q_h\beta] W'(\nabla\tilde y) - Q_h\big[\beta W'(\nabla \Pi_h y)\big]\Big)\,\mathrm{d}x \\
&= \int [Q_h\beta]\big(W'(\nabla\tilde y) - Q_h W'(\nabla\Pi_h y)\big)\,\mathrm{d}x \\
&= \int [Q_h\beta]\big(W'(\nabla\tilde y) - W'(\nabla\Pi_h y)\big)\,\mathrm{d}x \\
&\qquad + \int [Q_h\beta]\big(W'(\nabla\Pi_h y) - Q_h W'(\nabla\Pi_h y)\big)\,\mathrm{d}x \\
&=: \mathrm{T}_{2,1} + \mathrm{T}_{2,2}.
\end{aligned}$$

The term $T_{2,1}$ is an approximation error, while $T_{2,2}$ is a quadrature error.

First, we prove that

$$|T_{2,1}| \lesssim \big\|\big(|\nabla\tilde u| + |\nabla u^{\mathrm{lin}}|^2\big)(\nabla\tilde u - \nabla\Pi_h u)\big\|_{L^1(\Omega^c)} + \|\nabla^3 \tilde u\|_{L^1(\Omega^c)} + \|\nabla\tilde u - \nabla\Pi_h u\|_{L^2(\Omega^c)}, \tag{6.15}$$

where we set $u^{\rm lin} \equiv 0$ in the case (pPt).

Proof of (6.15). We first note that, with $e_h := \nabla\tilde{u} - \nabla\Pi_h u$ we have

$$\begin{aligned}
|T_{2,1}| &= \bigg| \int [Q_h\beta]\big(W(\nabla\tilde{y}) - W(\nabla\tilde{y} - \nabla e_h)\big)\,{\rm d}x \bigg| \\
&\leq \bigg| \int [Q_h\beta]\big(\partial W(\nabla\tilde{y})\nabla e_h\big)\,{\rm d}x \bigg| + C\|\nabla e_h\|_{L^2}^2 \\
&=: |T_{2,1}'| + C\|\nabla e_h\|_{L^2}^2.
\end{aligned}$$

Let $e_h = [\nabla\tilde{u} - \nabla\bar{u}] + [\nabla\bar{u} - \nabla\Pi_h u] =: e_h' + e_h''$, then $\|[Q_h\beta]\nabla e_h'\|_{L^1} \lesssim \|\nabla^3\tilde{u}\|_{L^1(\Omega^{\rm c})}$ and $e_h'' = 0$ in Ω^β, hence

$$\begin{aligned}
|T_{2,1}'| &\leq \bigg| \int [Q_h\beta]\big(\partial W(\nabla\tilde{y})\nabla e_h''\big)\,{\rm d}x \bigg| + C\|\nabla^3\tilde{u}\|_{L^1(\Omega^{\rm c})} \\
&= \bigg| \int \big[\partial W(\nabla\tilde{y}) - \mathsf{S}^{\rm lin}\big]\nabla e_h''\,{\rm d}x \bigg| + C\|\nabla^3\tilde{u}\|_{L^1(\Omega^{\rm c})},
\end{aligned}$$

where, setting $u^{\rm lin} \equiv 0$ in the case (pPt),

$$\mathsf{S}^{\rm lin} = \partial W(\mathsf{A}) + \mathbb{C} : \nabla u^{\rm lin},$$

We can now estimate

$$\big|\partial W(\nabla\tilde{y}) - \mathsf{S}^{\rm lin}\big| \lesssim |\nabla\tilde{u}| + |\nabla u^{\rm lin}|^2,$$

which yields

$$\begin{aligned}
|T_{2,1}'| &\lesssim \Big(\big\|\big(|\nabla\tilde{u}| + |\nabla u^{\rm lin}|^2\big)\nabla e_h''\big\|_{L^1(\Omega^{\rm c})}^2 + \|\nabla^3\tilde{u}\|_{L^1(\Omega^{\rm c})} \\
&\lesssim \big\|\big(|\nabla\tilde{u}| + |\nabla u^{\rm lin}|^2\big)\nabla e_h\big\|_{L^1(\Omega^{\rm c})}^2 + \|\nabla^3\tilde{u}\|_{L^1(\Omega^{\rm c})},
\end{aligned}$$

estimating again that $\|\nabla e_h'\|_{L^1(\Omega^{\rm c})} \leq \|\nabla^3\tilde{u}\|_{L^1(\Omega^{\rm c})}$.

This completes the proof of (6.15). □

The final term to complete the estimate for the B-QCE energy error is $T_{2,2}$, which we can bound by

$$\begin{aligned}
|T_{2,2}| &\lesssim \Big(\|h^2\nabla^3 y_0\|_{L^2(\Omega^{\rm c})} + \|h\nabla^2 y_0\|_{L^4(\Omega^{\rm c})}^2\Big)\|\nabla\Pi_h u\|_{L^2(\Omega^{\rm c})} &(6.16)\\
&\lesssim \Big(\|h^2\nabla^3 y_0\|_{L^2(\Omega^{\rm c})} + \|h\nabla^2 y_0\|_{L^4(\Omega^{\rm c})}^2\Big)\Big(\mathbf{E}^{\rm apx}(y) + \|\nabla\tilde{u}\|_{L^2(\Omega^{\rm c})}\Big) &(6.17)
\end{aligned}$$

The proof of this estimate follows much along the same lines as that of (6.12), exploiting the fact that

$$\begin{aligned}
&W'(\nabla\Pi_h y) - Q_h W'(\nabla\Pi_h y) \\
&\quad= \int_{\theta=0}^1 \Big(\partial W(\nabla y_0 + \theta\nabla\Pi_h u) - \partial W\big(Q_h[\nabla y_0] + \theta\nabla\Pi_h u\big)\Big){\rm d}\theta : \nabla\Pi_h u.
\end{aligned}$$

6.3.3. *Completing the energy error estimate.* Combining the estimates (6.12), (6.14), (6.15) and (6.17), ignoring any terms that are dominated by others, we arrive at

$$\begin{aligned}
\big|\mathscr{E}^{\mathrm{a}}(y) - \mathscr{E}_h^{\beta}(y_h)\big| \leq C\Big\{ & \mathbf{E}^{\mathrm{apx}}(y)^2 + \mathbf{E}^{\mathrm{cb}}(y)^2 + \mathbf{E}^{\mathrm{int}}(y)^2 \\
& + \|\nabla^2\beta\|_{L^2}\|\nabla\tilde{u}\|_{L^2(\Omega^{\mathrm{c}})} + \|\nabla\beta\|_{L^2}\|\nabla^2\tilde{u}\|_{L^2(\Omega^{\mathrm{c}})} \\
& \qquad + \mathbf{E}^{\mathrm{apx}}(y)\big(\|\nabla\tilde{u}\|_{L^2(\Omega^{\mathrm{c}})} + \|\nabla u^{\mathrm{lin}}\|^2_{L^4(\Omega^{\mathrm{c}})}\big) \\
& + \|\nabla^3\tilde{u}\|_{L^1(\Omega^{\mathrm{c}})} + \|\nabla^2\tilde{u}\|^2_{L^2(\Omega^{\mathrm{c}})} \\
& + \Big(\|h^2\nabla^3 y_0\|_{L^2(\Omega^{\mathrm{c}})} + \|h\nabla^2 y_0\|^2_{L^4(\Omega^{\mathrm{c}})}\Big)\Big(\mathbf{E}^{\mathrm{apx}}(y) + \|\nabla\tilde{u}\|_{L^2(\Omega^{\mathrm{c}})}\Big) \\
& + \|\nabla^2\tilde{u}\|_{L^2(\Omega^{\mathrm{c}})}\|\nabla^2 y_0\|_{L^2(\Omega^{\mathrm{c}})} + \|\nabla\beta\|_{L^\infty}\|\nabla\tilde{u}\|_{L^2(\Omega^{\mathrm{c}})}\|\nabla^2 y_0\|_{L^2(\Omega^{\mathrm{c}})}\Big\}.
\end{aligned} \tag{6.18}$$

A slight rearrangement yields the statement of Proposition 3.2.

6.4. **B-QCF Consistency analysis.**

6.4.1. *Consistency error estimate, part 1.* Recall the definition of the B-QCF operator (3.4) and assume that $y_h(\xi) = y(\xi)$ for $\xi \in \Lambda^{\rm a}$, then we have

$$\langle \mathscr{F}_h^\beta(y_h), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v\rangle = \langle \delta\mathscr{E}^{\rm a}(y), (1-\beta)v_h - v\rangle + \langle \delta\mathscr{E}_h^{\rm c}(y_h), I_h[\beta v_h]\rangle.$$

Similar to the B-QCE case in § 6.2, we choose a specially adapted test function $v := \Pi_h'' v_h$, as defined in (4.25), for the "weak form" of the atomistic force $\langle \delta\mathscr{E}^{\rm a}(y), v\rangle$. That is,

$$v = (1-\beta)v_h|_{\mathbb{Z}^d} + w^*, \quad \text{where} \quad w(\xi) := \big(\bar\zeta * w_h\big)(\xi) \text{ and } w_h := I_h[\beta v_h]. \tag{6.19}$$

Standard quasi-interpolation error estimates (see e.g. [5] for an analogous result) yield

$$\|\nabla \bar w - \nabla w_h\|_{L^2} + \|\bar w - w_h\|_{L^2} \lesssim \|\nabla w_h\|_{L^2}. \tag{6.20}$$

Applying the stress form of $\delta\mathscr{E}^{\rm a}(y)$ in (4.15), with $\mathsf{S}^{\rm a} = \mathsf{S}^{\rm a}(y;x)$, we can now compute

$$\begin{aligned}
&\langle \mathscr{F}_h^\beta(y_h), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v\rangle \\
&\quad= \langle \delta\mathscr{E}^{\rm a}(y), (1-\beta)v_h - v\rangle + \langle \delta\mathscr{E}_h^{\rm c}(y_h), I_h[\beta v_h]\rangle \\
&\quad= -\langle \delta\mathscr{E}^{\rm a}(y), w^*\rangle + \langle \delta\mathscr{E}_h^{\rm c}(y_h), w_h\rangle = \langle \delta\mathscr{E}_h^{\rm c}(y_h), w_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), w^*\rangle \\
&\quad= \int \Big[Q_h\big[\partial W(\nabla y_h) : \nabla w_h\big] - \mathsf{S}^{\rm a} : \nabla \bar w\Big]\,{\rm d}x \\
&\quad= \int Q_h\Big[\partial W(\nabla y_h) - \partial W(\nabla \tilde y)\Big] : \nabla w_h\,{\rm d}x + \int \big(Q_h - {\rm Id}\big)\big[\partial W(\nabla\tilde y) : \nabla w_h\big]\,{\rm d}x \\
&\qquad + \int \partial W(\nabla \tilde y) : \big(\nabla w_h - \nabla \bar w\big)\,{\rm d}x + \int \big(\partial W(\nabla\tilde y) - \mathsf{S}^{\rm a}\big) : \nabla \bar w\,{\rm d}x \\
&\quad=: T_1 + T_2 + T_3 + T_4.
\end{aligned}$$

Applying Lemma 6.1 and Lemma 6.2 with $\beta \equiv 1$, and exploiting the fact that ${\rm supp}(w_h), {\rm supp}(\bar w) \subset \Omega^{\rm c}$ we obtain

$$\begin{aligned}
|T_1| &\lesssim \|\nabla u_h - \nabla \tilde u\|_{L^2(\Omega^{\rm c})}\|\nabla w_h\|_{L^2}, \\
|T_2| &\lesssim \|h^2\nabla^2\partial W(\tilde y)\|_{L^2(\Omega^{\rm c})}\|\nabla w_h\|_{L^2}, \quad \text{and} \\
|T_3| &\lesssim \|\nabla\,{\rm div}\,\partial W(\tilde y)\|_{L^2(\Omega^{\rm c})}\|\nabla w_h\|_{L^2}.
\end{aligned}$$

Finally, the fourth term is the Cauchy–Born modelling error estimated in Lemma 4.3 combined with the quasi-interpolation error estimates in (6.20). Applying Lemma 6.5 with $\beta \equiv 1$ and exploiting again that ${\rm supp}(\bar w) \subset \Omega^{\rm c}$, we obtain

$$|T_4| \lesssim \big(\|\nabla^3\tilde y\|_{L^2(\Omega^{\rm c})} + \|\nabla^2\tilde y\|_{L^4(\Omega^{\rm c})}^2\big)\|\nabla w_h\|_{L^2}.$$

Combining the estimates for the terms $\mathrm{T}_1, \dots, \mathrm{T}_4$ and then arguing as in Lemma 6.3 we arrive at

$$\big|\langle \mathscr{F}_h^\beta(y_h), v_h\rangle - \langle \delta\mathscr{E}^{\rm a}(y), v\rangle\big| \lesssim \big(\mathbf{E}^{\rm apx}(y) + \mathbf{E}^{\rm cb}(y)\big)\|\nabla w_h\|_{L^2}. \tag{6.21}$$

In particular, we have proven (4.26).

It now remains to estimate $\|\nabla w_h\|_{L^2}$, where $w_h = I_h[\beta v_h]$ in terms of $\|\nabla v_h\|_{L^2}$.

6.4.2. *The trace inequality.* Our aim is to prove (4.27). For the sake of argument, suppose $w_h \sim \beta v_h$ (we dropped the interpolant), so that $\nabla w_h \sim \beta \nabla v_h + v_h \otimes \nabla \beta$. Thus, we need to estimate v_h in the support of $\nabla \beta$ (i.e., in the blending region) in terms of ∇v_h in Ω_h. The key ingredient to obtain such an estimate is the following trace inequality.

Lemma 6.7. *Let $d \geq 2$ and $0 < r_0 < r_1$, then*

$$\|u\|^2_{L^2(\partial B_{r_0})} \leq C_1 \|\nabla u\|^2_{L^2(B_{r_1} \setminus B_{r_0})} \quad \text{for all } u \in H^1(B_{r_1} \setminus B_{r_0}), u|_{\partial B_{r_1}} = 0, \tag{6.22}$$

$$\text{where } C_1 = \begin{cases} 2r_0 \left| \log \frac{r_1}{r_0} \right|, & d = 2, \\ 2r_0/(d-2), & d \geq 3. \end{cases} \tag{6.23}$$

Proof. The result follows from minor modifications to remove the constraint $r_1 < 1$ of the proof of [20, Lemma 5.1]; up to [20, Eq. (5.4)] and choosing $s = r_1$ from the beginning. □

Corollary 6.8. *Under the conditions of Lemma 6.7, we have*

$$\|v_h\|^2_{L^2(\Omega^\beta)} \leq \big((R^\beta)^2 - (R^{\rm a})^2\big) C_1' \|\nabla v_h\|^2_{L^2(\Omega_h)} \qquad \forall v_h \in \mathscr{U}_h,$$

$$\text{where} \qquad C_1' = \begin{cases} \log \left| \frac{R^{\rm o}}{R^{\rm a}} \right|, & d = 2, \\ 1, & d = 3. \end{cases}$$

Proof. Recalling that $\Omega^\beta \subset B_{R^\beta} \setminus B_{R^{\rm a}}$ we write

$$\|v_h\|^2_{L^2(\Omega^\beta)} \leq \int_{r=R^{\rm a}}^{R^\beta} \|v_h\|^2_{L^2(\partial B_r)} \, {\rm d}r.$$

Applying (6.22) yields the stated result. □

Proof of Lemma 4.6. If $T \in \mathcal{T}_h$ with $\beta|_T \equiv 1$, then $I_h[\beta v_h] = v_h$, and hence $\|\nabla I_h[\beta v_h]\|_{L^2(T)} \leq \|\nabla v_h\|_{L^2(T)}$.

Conversely, if $\beta|_T \not\equiv 1$, then $h_T \lesssim 1$ and hence standard nodal interpolation error estimates [6] imply

$$\begin{aligned} \|\nabla I_h[\beta v_h]\|_{L^2(T)} &\leq \|\nabla I_h[\beta v_h] - \nabla(\beta v_h)\|_{L^2(T)} + \|\nabla(\beta v_h)\|_{L^2(T)} \\ &\lesssim \|\nabla^2(\beta v_h)\|_{L^2(T)} + \|\nabla(\beta v_h)\|_{L^2(T)}. \end{aligned}$$

Since $v_h|_T \in$ P1(T), so $\nabla^2 v_h = 0$, for each such element T we have

$$\begin{aligned} \|\nabla I_h[\beta v_h]\|_{L^2(T)} &\lesssim \|\nabla^2 \beta\|_{L^\infty(T)} \|v_h\|_{L^2(T)} + 2\|\nabla \beta\|_{L^\infty(T)} \|\nabla v_h\|_{L^2(T)} \\ &\qquad + \|\beta \nabla v_h\|_{L^2(T)} + \|v_h \otimes \nabla \beta\|_{L^2(T)} \\ &\lesssim \|\nabla \beta\|_{W^{1,\infty}(T)} \|v_h\|_{L^2(T)} + (1 + \|\nabla \beta\|_{L^\infty(T)}) \|\nabla v_h\|_{L^2(T)}. \end{aligned}$$

Recall that Ω^β is constructed in such a way that ${\rm supp} \nabla \beta \cap T \neq \emptyset$ implies that $T \subset \Omega^\beta$. Thus, summing over all $T \subset \Omega^\beta$, and also recalling that $\|\nabla \beta\|_{L^\infty} \lesssim 1$ and then applying Corollary 6.8, we obtain

$$\begin{aligned} \|\nabla I_h[\beta v_h]\|_{L^2} &\lesssim \|\nabla \beta\|_{W^{1,\infty}} \|v_h\|_{L^2(\Omega^\beta)} + \|\nabla v_h\|_{L^2} \\ &\lesssim \Big(C_1' \big[(R^\beta)^2 - (R^{\rm a})^2\big]^{1/2} \|\nabla \beta\|_{W^{1,\infty}} + 1\Big) \|\nabla v_h\|_{L^2}, \end{aligned} \tag{6.24}$$

where C_1' is the constant from Lemma 6.8.

Recall now that in (3.6) we assumed that the blending function β satisfies $\|\nabla^j \beta\|_{L^\infty} \lesssim (R^\beta)^{-j}$ for $j = 1, 2$. Inserting this assumption into (6.24) finally completes the proof of Lemma 4.6. □

7. Stability Proofs

7.1. BQCE stability.

Proof of Lemma 4.9. Assume, for contradiction, that there exists a sequence of B-QCE approximations, characterized by β_n, $\mathscr{T}_{h,n}$, $v_{h,n} \in \mathscr{U}_{h,n}$, etc., with $R_n^{\rm a} \to \infty$, as well as test functions $v_{h,n}$ satisfying $\|\nabla v_{h,n}\|_{L^2}^2 = 1$ and

$$\lim_{n\to\infty} \langle \delta^2[\mathscr{E}_{h,n}^\beta(\Pi_{h,n}y) + \mathscr{P}(\Pi_{h,n}y)]v_{h,n}, v_{h,n}\rangle =: \tilde{\gamma}_h^\beta < \min\big\{\gamma^{\rm a}(y), \gamma_h^\beta(\mathsf{A}x)\big\}.$$

In what follows, we will drop the index h in $\mathscr{U}_{h,n}$, $\mathscr{T}_{h,n}$, $\Pi_{h,n}$, $\mathscr{E}_{h,n}^\beta$, and so forth.

Upon extracting a subsequence (which is still denoted by v_n), we have $\nabla v_n \rightharpoonup \nabla \bar{v}_0$ in L^2 for some lattice function $v_0 : \mathbb{Z}^d \to \mathbb{R}^m$. Further, similarly to [13, Lemma 4.9], there exists a sequence $\check{r}_n \to \infty$, $\check{r}_n < \frac{1}{2}R_n^{\rm a}$, such that, defining $w_n := \overline{\eta_n v_n}$, where η_n is a smooth cut-off function satisfying

$$\eta_n(\xi) = 1 \quad (|\xi| \le \check{r}_n + 2r_{\rm cut}) \qquad \text{and} \qquad \eta_n(\xi) = 0 \quad (|\xi| \ge 2\check{r}_n - 2r_{\rm cut}),$$

(cf. the definition of the truncation operator T_R in (4.20)) and $z_n := v_n - w_n$, then

$$\begin{aligned} Dw_n &\to Dv_0 \text{ in } \ell^2, & \nabla w_n &\to \nabla \bar{v}_0 \text{ in } L^2, \\ Dz_n &\rightharpoonup 0 \text{ in } \ell^2, & \nabla z_n &\rightharpoonup 0 \text{ in } L^2, \end{aligned}$$

$$Dw_n(\xi) = \begin{cases} Dv_n(\xi), & |\xi| \le \check{r}_n, \\ 0, & |\xi| \ge 2\check{r}_n, \end{cases} \qquad \text{and} \qquad \nabla w_n(x) = \begin{cases} \nabla v_n(x), & |x| \le \check{r}_n, \\ 0, & |x| \ge 2\check{r}_n. \end{cases}$$

We note that $w_n = 0$ on $\Omega^{\rm c}$ and hence w_n is an admissible displacement, $w_n \in \mathscr{U}_n$, which also ensures that $z_n \in \mathscr{U}_n$. The statement that $Dz_n \rightharpoonup 0$ follows from the fact that, for any fixed $\varphi \in \mathscr{U}^{\rm c}$, $\langle Dz_n, D\varphi\rangle \to 0$ as $\Lambda^{\rm a}$ will eventually enclose the support of φ for sufficiently large n.

Hence we have

$$\begin{aligned} \langle \delta^2[\mathscr{E}_n^\beta + \mathscr{P}](\Pi_n y)v_n, v_n\rangle &= \langle \delta^2\mathscr{E}_n^\beta(\Pi_n y)w_n + \delta^2\mathscr{P}(y)w_n, w_n\rangle \\ &\quad + 2\langle \delta^2\mathscr{E}_n^\beta(\Pi_n y)w_n, z_n\rangle + \langle \delta^2\mathscr{E}_n^\beta(\Pi_n y)z_n, z_n\rangle \\ &=: a_n + 2b_n + c_n. \end{aligned}$$

Here we used the fact that, for n large enough, $\mathscr{P}(\Pi_n y) = \mathscr{P}(y)$ and is supported outside $\mathrm{supp}(Dz_n)$ or $\mathrm{supp}(\nabla z_n)$.

Due to $\check{r}_n < \frac{1}{2}R_n^{\rm a}$ and the stability assumption (4.29) we have that

$$a_n = \langle \delta^2[\mathscr{E}^{\rm a} + \mathscr{P}](\Pi_n y)w_n, w_n\rangle = \langle \delta^2[\mathscr{E}^{\rm a} + \mathscr{P}](y)w_n, w_n\rangle \ge \gamma^{\rm a}(y)\|\nabla w_n\|_{L^2}^2.$$

Similarly, since $Dw_n(\xi)$ can be nonzero only for ξ such that $\beta(\xi) = 1$, we have that

$$\begin{aligned} b_n &= \langle \delta^2\mathscr{E}_n^\beta(\Pi_n y)w_n, z_n\rangle = \langle \delta^2\mathscr{E}^{\rm a}(y)w_n, z_n\rangle \\ &= \sum_{\xi\in\mathbb{Z}^d} \langle \delta^2 V(Dy(\xi))Dw_n(\xi), Dz_n(\xi)\rangle. \end{aligned}$$

Since $\delta^2V(Dy)Dw_n \to \delta^2V(Dy)Dv_0$ in ℓ^2 and $Dz_n \rightharpoonup 0$ in ℓ^2 it follows that $b_n \to 0$.

Finally, the fact that $\|\nabla\Pi_n y - \mathsf{A}\|_{L^\infty(\mathbb{R}^d\setminus B_{\check{r}_n})} \to 0$ as $\check{r}_n \to \infty$ and the Lipschitz regularity of $\delta^2 V$ and $\partial^2 W$ imply that

$$\|\delta^2V(D\Pi_n y) - \delta^2V(\mathsf{A}\mathcal{R})\|_{\ell^\infty(\mathrm{supp}(Dz_n))} \le \|\delta^2V(D\Pi_n y) - \delta^2V(\mathsf{A}\mathcal{R})\|_{\ell^\infty(\mathbb{Z}^d\setminus B_{\check{r}_n})} \to 0, \quad \text{and}$$

$$\|\partial^2W(\nabla\Pi_n y) - \partial^2W(\mathsf{A})\|_{L^\infty(\mathrm{supp}(\nabla z_n))} \le \|\partial^2W(\nabla\Pi_n y) - \partial^2W(\mathsf{A})\|_{L^\infty(\mathbb{R}^d\setminus B_{\check{r}_n})} \to 0$$

which, upon writing out $\delta^2\mathscr{E}_n^\beta(\Pi_n y) - \delta^2\mathscr{E}_n^\beta(\mathsf{A}x)$ and estimating $\|Dz_n\|_{\ell^2}$ by $\|\nabla z_n\|_{L^2}$, allow us to conclude that

$$c_n = \langle \delta^2\mathscr{E}_n^\beta(\mathsf{A}x)z_n, z_n\rangle + o(1)\|\nabla z_n\|_{L^2}^2 \geq (\gamma_h^\beta(\mathsf{A}x) + o(1))\|\nabla z_n\|_{L^2}^2,$$

where $o(1)$ denotes a sequence that converges to 0 as $n \to \infty$.

It remains only to observe that

$$\begin{aligned}
\gamma^{\mathrm{a}}(y)\|\nabla w_n\|_{L^2}^2 &+ (\gamma_h^\beta(\mathsf{A}x) + o(1))\|\nabla z_n\|_{L^2}^2 \\
&\geq \min\{\gamma^{\mathrm{a}}(y), \gamma_h^\beta(\mathsf{A}x) + o(1)\}\,(\|\nabla w_n\|_{L^2}^2 + \|\nabla z_n\|_{L^2}^2) \\
&= \min\{\gamma^{\mathrm{a}}(y), \gamma_h^\beta(\mathsf{A}x) + o(1)\}\,(\|\nabla v_n\|_{L^2}^2 - 2(\nabla w_n, \nabla z_n)_{L^2}) \\
&= \min\{\gamma^{\mathrm{a}}(y), \gamma_h^\beta(\mathsf{A}x)\} + o(1),
\end{aligned}$$

where we used again that fact that ∇w_n converges strongly while $\nabla z_n \rightharpoonup 0$.

Thus, we have arrived at a contradiction to our original assumption, and have therefore established the result. $\square$

In the proof of Lemma 4.10 we will use the following auxiliary result.

Lemma 7.1. *If $\beta : \mathbb{R}^d \to \mathbb{R}$ satisfies* (3.7) *then $\sqrt{\beta}, \sqrt{1-\beta} \in W^{1,\infty}$ and*

$$\max\left\{\|\nabla\sqrt{\beta}\|_{L^\infty}, \|\nabla\sqrt{1-\beta}\|_{L^\infty}\right\} \leq \sqrt{\|\nabla^2\beta\|_{L^\infty}/2}.$$

Proof. It is proved in [15] that $\sqrt{\beta}$ is continuously differentiable on $\Omega = \{x \mid \beta(x) \neq 0 \text{ or } \nabla^2\beta(x) = 0\}$ and $\|\nabla\sqrt{\beta}\|_{L^\infty(\Omega)} \leq \sqrt{\|\nabla^2\beta\|_{L^\infty}/2}$. It remains to notice that Ω is everywhere dense, hence $\sqrt{\beta}$ is Lipschitz everywhere, i.e., $\sqrt{\beta} \in W^{1,\infty}$. The result for $\sqrt{1-\beta}$ follows similarly. $\square$

Proof of Lemma 4.10. As in the proof of Lemma 4.9 we assume, for contradiction, that there exists a sequence β_n, $\mathscr{T}_n$, $v_n \in \mathscr{U}_n$, $\|\nabla v_n\|_{L^2} = 1$ etc. (again, we omit the subscript h) such that

$$\lim_{n\to\infty} \left\langle \delta^2\mathscr{E}_n^\beta(\mathsf{A}x)v_n, v_n\right\rangle < \gamma^{\mathrm{a}} = \gamma^{\mathrm{a}}(\mathsf{A}x). \tag{7.1}$$

We introduce the parameter $\varepsilon_n = 1/R_n^{\mathrm{a}} \to 0$, rescale variables,

$$x \mapsto \varepsilon_n x, \quad \xi \mapsto \varepsilon_n \xi, \quad v_n \mapsto \varepsilon_n^{1-d/2} v_n, \quad \Omega_n \mapsto \varepsilon_n\Omega_n,$$

and define $\|w_n\|_{\ell^2(\varepsilon_n\mathbb{Z}^d)}^2 := \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} |w_n(\xi)|^2$. We observe that $\|\nabla v_n\|_{L^2} = 1$ is preserved under this rescaling, while (7.1) now reads $\lim_{n\to\infty}\langle H_n v_n, v_n\rangle < \gamma^{\mathrm{a}}$, where

$$\langle H_n v_n, v_n\rangle := \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi))\langle A\, D_n v_n(\xi), D_n v_n(\xi)\rangle + \int_{\Omega_n} (Q_n\beta_n)(\mathbb{C}:\nabla v_n):\nabla v_n\,\mathrm{d}x,$$

$$A := \delta^2 V(\mathsf{A}\mathcal{R}), \quad \mathbb{C} := \partial^2 W(\mathsf{A}), \quad \text{and} \quad D_n w(\xi) = \left(\frac{w(\xi+\varepsilon_n\rho) - w(\xi)}{\varepsilon_n}\right)_{\rho\in\mathcal{R}}. \tag{7.2}$$

Upon extracting a subsequence we have that $\nabla v_n \rightharpoonup \nabla v_0$ in L^2 for some $v_0 \in H^1_{\mathrm{loc}}(\mathbb{R}^d)$. Hence we define $w_n := \Pi_h(\eta_{r_n} * v_0) \in \mathscr{U}_n$ and split $v_n = w_n + z_n$, where $\eta_r \in C^\infty(\mathbb{R}^d)$ is a family of mollifiers, and the sequence $r_n \to 0$ will be chosen later. Since $\nabla w_n \to \nabla v_0$ in L^2, we have that $\nabla z_n \rightharpoonup 0$ in L^2.

Step 1: estimating $\langle H_n z_n, z_n\rangle$.

Step 1.1: continuum contribution. We start by bounding the continuum contribution from $\langle H_n z_n, z_n \rangle$,

$$\int_{\Omega_n} (Q_n\beta_n)(\mathbb{C}\colon\nabla z_n)\colon\nabla z_n \,\mathrm{d}x.$$

Due to rescaling $\beta_n(x) \mapsto \beta_n(\varepsilon_n^{-1}x)$ and $\varepsilon_n = 1/R_n^{\mathrm{a}}$, we now have a uniform bound $|\nabla^2\beta_n| \le C_2^\beta$. Hence, the error of interpolation of β_n tends to zero due to the assumption (3.8), i.e., $\|Q_n\beta_n - \beta_n\|_{L^\infty} \to 0$, which enables us to replace $Q_n\beta_n$ by β_n while making at most $o(1)$ error as $n \to \infty$.

For ease of notation, let $\hat{R} := C_1^\beta$, so that $\varepsilon_n R_n^\beta = R_n^\beta/R_n^{\mathrm{a}} \le \hat{R}$, and $\hat{B} := B_{\hat{R}}$; cf. (3.6).

Upon shifting the test function we may assume that $\fint_{\hat{B}} v_n \,\mathrm{d}x = 0$. (Note that the shifted test function does not satisfy the homogeneous Dirichlet boundary condition, but this is irrelevant for the following estimates.) Therefore, due to (i) norm equivalence $\|v_n\|_{H^1(\hat{B})} \lesssim \|\nabla v_n\|_{L^2(\hat{B})}$ and (ii) the compactness of the embedding $L^2(\hat{B}) \subset H^1(\hat{B})$, we have that $\|z_n\|_{L^2(\hat{B})} \to 0$. Further, (3.7) implies that $\sqrt{\beta_n} =: \varphi_n \in W^{1,\infty}$ and that it satisfies the bound $\|\nabla\varphi_n\|_{L^\infty} \le \sqrt{\|\nabla^2\beta_n\|_{L^\infty}/2} \le \sqrt{C_2^\beta/2}$, as we have proved in Lemma 7.1.

Noting that $\mathrm{supp}(\varphi_n) \subset \hat{B}$, we have that

$$\begin{aligned}
&\left| \int_{\Omega_n} \beta_n(\mathbb{C}\colon\nabla z_n)\colon\nabla z_n - \int_{\Omega_n} (\mathbb{C}\colon\nabla(\varphi_n z_n))\colon\nabla(\varphi_n z_n) \right| \\
&= \left| 2\int_{\Omega_n} (\mathbb{C}\colon(\nabla\varphi_n \otimes z_n))\colon\nabla(\varphi_n z_n) + \int_{\Omega_n} (\mathbb{C}\colon(\nabla\varphi_n \otimes z_n))\colon(\nabla\varphi_n \otimes z_n) \right| \\
&\lesssim 2\|z_n\|_{L^2(\hat{B})}\|\nabla z_n\|_{L^2(\hat{B})} + \|z_n\|_{L^2(\hat{B})}^2 \to 0 \quad \text{as } n \to \infty.
\end{aligned}$$

Thus,

$$\begin{aligned}
\int_{\Omega_n} (Q_n\beta_n)(\mathbb{C}\colon\nabla z_n)\colon\nabla z_n &= \int_{\Omega_n} \beta_n(\mathbb{C}\colon\nabla z_n)\colon\nabla z_n + o(1) \\
&= \int_{\Omega_n} (\mathbb{C}\colon\nabla(\varphi_n z_n))\colon\nabla(\varphi_n z_n) + o(1) \\
&\ge \gamma_{\mathrm{c}}\|\nabla(\varphi_n z_n)\|_{L^2}^2 + o(1) \\
&= \gamma_{\mathrm{c}}\big\|\nabla\big(\sqrt{\beta_n} z_n\big)\big\|_{L^2}^2 + o(1). \qquad (7.3)
\end{aligned}$$

In the last estimate we used two facts: (i) the stability (2.12) of the exact solution implies the stability of the far-field [12], that is,

$$\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} \big\langle \delta^2 V(\mathsf{A}\mathcal{R}) D_n w_n(\xi), D_n w_n(\xi) \big\rangle \ge \gamma^{\mathrm{a}}\|\nabla w_n\|_{L^2}^2;$$

and (ii) that atomistic stability implies continuum stability [18], that is,

$$\int (\mathbb{C}\colon\nabla w_n)\colon\nabla w_n \ge \gamma^{\mathrm{c}}\|\nabla w_n\|_{L^2}^2 \qquad \text{where} \quad \gamma^{\mathrm{c}} = \gamma^{\mathrm{c}}(\mathsf{A}) \ge \gamma^{\mathrm{a}}(\mathsf{A}x).$$

Step 1.2. A similar argument can be applied to the atomistic contribution to $\langle H_n z_n, z_n \rangle$. We introduce the translation operator $T_n w_n(\xi) := (w(\xi+\varepsilon_n\rho))_{\rho\in\mathcal{R}}$ and the product $D_n\varphi_n T_n z_n :=$

$((D_n\varphi_n)_\rho(T_nz_n)_\rho)_{\rho\in\mathcal{R}}$. Then, redefining $\varphi_n := \sqrt{1-\beta_n} \in W^{1,\infty}$, $\|\nabla\varphi_n\| \le \sqrt{C_2^\beta/2}$, we obtain

$$\begin{aligned}
&\Big|\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi))\Big\langle A\, D_nz_n(\xi), D_nz_n(\xi)\Big\rangle - \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} \Big\langle A\, D_n(\varphi_nz_n)(\xi), D_n(\varphi_nz_n)(\xi)\Big\rangle\Big| \\
&\quad = \Big|\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} \Big\langle A\,\big(D_n\varphi_nT_nz_n\big)(\xi), 2D_n(\varphi_nz_n)(\xi) + \big(D_n\varphi_nT_nz_n\big)(\xi)\Big\rangle\Big| \\
&\quad \lesssim \big(2\|\nabla\bar z_n\|_{L^2(\operatorname{supp}(\varphi_n))} + \|\bar z_n\|_{L^2(\operatorname{supp}(\varphi_n))}\big)\|\bar z_n\|_{L^2(\operatorname{supp}(\varphi_n))}, \qquad (7.4)
\end{aligned}$$

where we used rescaled versions of the local norm-equivalence and inverse estimates (5.7).

Next, we notice that the mesh $\mathscr{T}_n$ is fully refined on $\operatorname{supp}(\varphi_n)$ (cf. the assumption (3.8)), hence $\bar z_n = z_n$ on $\operatorname{supp}(\varphi_n)$, and therefore (7.4) tends to zero as $n\to\infty$. Thus,

$$\begin{aligned}
&\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi))\Big\langle A\, D_nz_n(\xi), D_nz_n(\xi)\Big\rangle \\
&\qquad = \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} \Big\langle AD_n\big(\varphi_n(\xi)z_n(\xi)\big), D_n\big(\varphi_n(\xi)z_n(\xi)\big)\Big\rangle + o(1) \\
&\qquad \ge \gamma_{\rm a}\big\|\nabla\big(\overline{\varphi_nz_n}\big)\big\|_{L^2}^2 + o(1).
\end{aligned}$$

Next, we need to prove that $\|\nabla(\overline{\varphi_nz_n} - \varphi_nz_n)\|_{L^2} \to 0$. Indeed, $\nabla(\overline{\varphi_nz_n} - \varphi_nz_n)$ can be nonzero only in those $T\in\mathscr{T}_n$ where φ_n is not constant, and all such triangles are contained in $\hat B$, which implies

$$\|\nabla(\overline{\varphi_nz_n} - \varphi_nz_n)\|_{L^2(\mathbb{R}^d)} = \|\nabla(\overline{\varphi_nz_n} - \varphi_nz_n)\|_{L^2(\hat B)}.$$

Upon defining the oscillation operator $\operatorname{osc}_T(f) := \sup_{x,y\in T}|f(x)-f(y)|$ we can estimate the right-hand side, for any $T\in\mathscr{T}_n$, by

$$\begin{aligned}
\|\nabla(\overline{\varphi_nz_n} - \varphi_nz_n)\|_{L^\infty(T)} &\le \operatorname*{osc}_T(\nabla(\varphi_nz_n)) \\
&\le \operatorname*{osc}_T(\nabla\varphi_n\, z_n) + \operatorname*{osc}_T(\varphi_n\nabla z_n) \\
&\le 2\|\nabla\varphi_n\|_{L^\infty(T)}\|z_n\|_{L^\infty(T)} + \operatorname*{osc}_T(\varphi_n)\big|\nabla z_n|_T\big| \\
&\lesssim 2\|\nabla\varphi_n\|_{L^\infty(T)}\|z_n\|_{L^2(T)} + \varepsilon_n\|\nabla\varphi_n\|_{L^\infty(T)}\big|\nabla z_n|_T\big|,
\end{aligned}$$

where in the last step we used the fact that $\operatorname{diam}(T) \lesssim \varepsilon_n$ and that $\|z_n\|_{L^\infty(T)} \lesssim \|z_n\|_{L^2(T)}$ since z_n is a linear function on T.

Then summing the contributions over all $T\subset\hat B$, we obtain

$$\|\nabla(\overline{\varphi_nz_n} - \varphi_nz_n)\|_{L^2(\hat B)} \lesssim 2\|\nabla\varphi_n\|_{L^\infty}\|z_n\|_{L^2(\hat B)} + \varepsilon_n\|\varphi_n\|_{L^\infty}\|\nabla z_n\|_{L^2(\hat B)} \to 0,$$

since $\|z_n\|_{L^2(\hat B)} \to 0$ and $\varepsilon_n \to 0$ as $n\to\infty$.

Thus,

$$\begin{aligned}
\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi))\Big\langle A\, D_nz_n(\xi), D_nz_n(\xi)\Big\rangle &\ge \gamma_{\rm a}\|\nabla(\varphi_nz_n)\|_{L^2}^2 + o(1) \\
&= \gamma_{\rm a}\big\|\nabla\big(\sqrt{1-\beta_n}z_n\big)\big\|_{L^2}^2 + o(1). \qquad (7.5)
\end{aligned}$$

Step 1.3. Combining (7.3) and (7.5),and using $\gamma^{\rm c} \ge \gamma^{\rm a}$, we obtain

$$\langle H_nz_n, z_n\rangle \ge \gamma_{\rm a}\int_{\Omega_h}\Big(\big|\nabla\big(\sqrt{1-\beta_n}\,z_n\big)\big|^2 + \big|\nabla\big(\sqrt{\beta_n}\,z_n\big)\big|^2\Big)\,{\rm d}x + o(1).$$

Then arguing similarly to the above (expanding the gradient of a product and exploiting the fact that $\|z_n\|_{L^2(\hat{B})} \to 0$) we conclude that

$$\int_{\Omega_h} \Big(\big|\nabla\big(\sqrt{1-\beta_n}\, z_n\big)\big|^2 + \big|\nabla\big(\sqrt{\beta_n}\, z_n\big)\big|^2 \Big)\,\mathrm{d}x = \int_{\Omega_h} \big((1-\beta_n)|\nabla z_n|^2 + \beta_n |\nabla z_n|^2 \big)\,\mathrm{d}x + o(1)$$
$$= \int_{\Omega_h} |\nabla z_n|^2\,\mathrm{d}x + o(1).$$

Summarizing, in Step 1 we proved that

$$\langle H_n z_n, z_n\rangle \geq \gamma_{\mathrm{a}} \|\nabla z_n\|_{L^2}^2 + o(1). \tag{7.6}$$

Step 2: estimating $\langle H_n w_n, w_n\rangle$.

Since $\mathrm{supp}(\beta_n)$ is contained in $\hat{B}$ and $\nabla^2 \beta_n$ is uniformly bounded, we have that, up to extracting a subsequence, $\beta_n \to \beta_0$ in C^1 for some $\beta_0 \in C^1(\mathbb{R}^d)$. Due to the strong convergence $Q_n\beta_n \to \beta_0$ in L^∞ and $w_n \to v_0$ in L^2, it is straightforward to evaluate the limit of the continuum contribution to $\langle H_n w_n, w_n\rangle$:

$$\int_{\Omega_n} (Q_n\beta_n)(\mathbb{C}:\nabla w_n):\nabla w_n\,\mathrm{d}x = \int_{\Omega_n} \beta_0(\mathbb{C}:\nabla v_0):\nabla v_0\,\mathrm{d}x + o(1). \tag{7.7}$$

To evaluate the limit of the atomistic contribution to $\langle H_n w_n, w_n\rangle$, recall the definition (7.2) of D_n and notice that for a fixed $r > 0$, $\|D_n(\eta_r * v_0) - \nabla_{\mathcal{R}}(\eta_r * v_0)\|_{\ell^2(\varepsilon_n\mathbb{Z}^d)} \to 0$ as $D_n(\eta_r * v_0)$ is a finite difference approximation to the derivative of a smooth function, $\nabla_{\mathcal{R}}(\eta_r * v_0)$. Hence, since $\|\beta_n - \beta_0\|_{\ell^\infty(\varepsilon_n\mathbb{Z}^d)} \leq \|\beta_n - \beta_0\|_{L^\infty(\mathbb{R}^d)} \to 0$, we obtain

$$\lim_{n\to\infty} \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi)) \Big\langle A D_n(\eta_r * v_0)(\xi), D_n(\eta_r * v_0)(\xi) \Big\rangle$$
$$= \lim_{n\to\infty} \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_0(\xi)) \Big\langle A \nabla_{\mathcal{R}}(\eta_r * v_0)(\xi), \nabla_{\mathcal{R}}(\eta_r * v_0)(\xi) \Big\rangle$$
$$= \int_{\mathbb{R}^d} (1-\beta_0) \big\langle A\nabla_{\mathcal{R}}(\eta_r * v_0), \nabla_{\mathcal{R}}(\eta_r * v_0) \big\rangle\,\mathrm{d}x.$$

In the last step we used the fact that a summation rule applied to a smooth function converges to its integral.

Next, we notice that $\nabla(\eta_r * v_0) \to \nabla v_0$ in L^2, as $r \to 0$, hence

$$\lim_{r\to 0}\lim_{n\to\infty} \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi)) \Big\langle A D_n(\eta_r * v_0)(\xi), D_n(\eta_r * v_0)(\xi) \Big\rangle$$
$$= \int_{\mathbb{R}^d} (1-\beta_0) \big\langle A\nabla_{\mathcal{R}} v_0, \nabla_{\mathcal{R}} v_0 \big\rangle\,\mathrm{d}x.$$

Therefore there exists a sequence $r_n \downarrow 0$ (sufficiently slowly) such that

$$\lim_{n\to\infty} \varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi)) \Big\langle A D_n(\eta_{r_n} * v_0)(\xi), D_n(\eta_{r_n} * v_0)(\xi) \Big\rangle$$
$$= \int_{\mathbb{R}^d} (1-\beta_0) \big\langle A\nabla_{\mathcal{R}} v_0, \nabla_{\mathcal{R}} v_0 \big\rangle\,\mathrm{d}x$$
$$= \int_{\Omega_n} (1-\beta_0)(\mathbb{C}:\nabla v_0):\nabla v_0\,\mathrm{d}x.$$

Finally it remains to notice that due to the full refinement of $\mathscr{T}_n$ on $\mathrm{supp}(1-\beta_n)$, $w_n := \Pi_n(\eta_{r_n} * v_0) = \eta_{r_n} * v_0$, hence

$$\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n(\xi))\big\langle A\, D_n w_n(\xi), D_n w_n(\xi)\big\rangle \to \int_{\Omega_n} (1-\beta_0)\,(\mathbb{C}\!:\!\nabla v_0)\!:\!\nabla v_0 \,\mathrm{d}x. \tag{7.8}$$

Combining the estimates for the atomistic contribution (7.8) with that for the continuum contribution (7.7) we finally deduce that

$$\begin{aligned}\langle H_n w_n, w_n\rangle &= \int (\mathbb{C}\!:\!\nabla v_0)\!:\!\nabla v_0 + o(1) \\ &\geq \gamma_{\rm c}\|\nabla v_0\|_{L^2}^2 + o(1) = \gamma_{\rm c}\|\nabla w_n\|_{L^2}^2 + o(1).\end{aligned} \tag{7.9}$$

Step 3: estimating the cross terms $\langle H_n w_n, z_n\rangle$.
Since $\nabla z_n \rightharpoonup 0$ and $\nabla w_n \to \nabla v_0$ in L^2, and $Q_n\beta_n \to \beta_0$ in L^∞, we trivially have that

$$\int_{\Omega_n} (Q_n\beta_n)(\mathbb{C}\!:\!\nabla w_n)\!:\!\nabla z_n \,\mathrm{d}x \to \int_{\Omega_n} \beta_0(\mathbb{C}\!:\!\nabla v_0)\!:\!0\,\mathrm{d}x = 0.$$

To prove that

$$\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n)\langle A D_n w_n, D_n z_n\rangle = o(1) \tag{7.10}$$

we convert the sum to stress-strain form as in § 4.2.3. Let $\bar\zeta_n(\xi) = \varepsilon_n^{-d}\,\bar\zeta(\xi/\varepsilon_n)$ be the rescaled hat function and $\psi_n : \varepsilon\mathbb{Z}^d \to \mathbb{R}^m$ such that $\psi_n^* := (\bar\zeta_n * \bar\psi_n) = z_n$ on $\varepsilon_n\mathbb{Z}^d$, then

$$\varepsilon_n^d \sum_{\xi\in\varepsilon_n\mathbb{Z}^d} (1-\beta_n)\langle A D_n w_n, D_n z_n\rangle = \int \mathsf{S}_n : \nabla\bar\psi_n, \qquad \text{where}$$

$$\mathsf{S}_n(x) = \varepsilon_n^d \sum_{\xi\in\varepsilon\mathbb{Z}^d} (1-\beta_n(\xi)) \sum_{\rho,\varsigma\in\mathcal{R}} \big[(A_{\rho\varsigma} D_{n,\varsigma} w_n(\xi))\otimes\varsigma\big] \fint_{t=0}^{\varepsilon_n} \bar\zeta_n(\xi+t\rho)\,\mathrm{d}t.$$

We can now argue analogously as in Step 2 to prove that

$$\mathsf{S}_n(x) \to (1-\beta_0)\mathbb{C} : \nabla v_0 \qquad \text{strongly in } L^2,$$

again requiring that $r_n \to 0$ sufficiently slowly (possibly at a slower rate than in Step 2). Thus, if we can prove that $\nabla\bar\psi_n \rightharpoonup 0$ in $\hat B$, then (7.10) follows.

To that end, let $\mu \in C_{\rm c}^\infty(\hat B;\mathbb{R}^m)$ be a test function with compact support, then $\|\bar\zeta_n * \nabla\mu - \nabla\mu\|_{L^\infty} \to 0$ as $n\to\infty$ and hence,

$$\begin{aligned}\int \nabla\bar\psi_n : \nabla\mu\,\mathrm{d}x &= \int \nabla\bar\psi_n : (\bar\zeta_n * \nabla\mu)\,\mathrm{d}x + o(1) = \int \nabla\big(\bar\zeta_n * \bar\psi_n\big) : \nabla\mu\,\mathrm{d}x + o(1) \\ &= \int \nabla\psi_n^* : \nabla\mu\,\mathrm{d}x + o(1) = \int \psi_n^*\cdot\Delta\mu\,\mathrm{d}x + o(1).\end{aligned}$$

Due to local norm-equivalence in each element, we have that

$$\|\psi_n^*\|_{L^2(\hat B)} \lesssim \|\psi_n^*\|_{\ell^2(\varepsilon\mathbb{Z}^d\cap\hat B)} = \|z_n\|_{\ell^2(\varepsilon\mathbb{Z}^d\cap\hat B)} \lesssim \|z_n\|_{L^2(\hat B)} \to 0 \quad \text{as } n\to\infty.$$

Hence, it follows that $\int\tilde\psi_n\cdot\Delta\mu\,\mathrm{d}x \to 0$, which completes the proof that $\nabla\bar\psi_n \rightharpoonup 0$, and hence also the proof of (7.10). Thus, we have established that

$$\langle H_n w_n, z_n\rangle \to 0 \qquad \text{as } n\to\infty. \tag{7.11}$$

Step 4: conclusion of the proof. Combining (7.6), (7.9) and (7.11) we obtain

$$\begin{aligned}\langle H_n v_n, v_n\rangle &\geq \gamma_{\rm a}\|\nabla z_n\|_{L^2}^2 + \gamma_{\rm a}\|\nabla w_n\|_{L^2}^2 + o(1)\\ &= \gamma_{\rm a}\|\nabla v_n\|_{L^2}^2 - 2\gamma_{\rm a}(\nabla z_n, \nabla w_n)_{L^2}^2 + o(1)\\ &= \gamma_{\rm a}\|\nabla v_n\|_{L^2}^2 + o(1) = \gamma_{\rm a} + o(1).\end{aligned}$$

Thus, we have a contradiction to our initial assumption that $\lim_{n\to\infty}\langle H_n v_n, v_n\rangle < \gamma^{\rm a}$. $\square$

7.2. **BQCF stability.** The main step towards the proof of Lemma 4.12 is the following estimate.

Lemma 7.2. *There exists C, independent of $(\beta, \mathcal{T}_h)$ such that*

$$|\langle \delta^2\mathscr{E}_h^\beta(y_h)v_h - \delta\mathscr{F}_h^\beta(y_h)v_h, v_h\rangle| \leq CE \qquad \forall v_h \in \mathscr{U}_h,$$

where
$$\begin{aligned}E &:= \|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)}\big(\|\nabla v_h\|_{L^2}^2 + \|v_h\|_{L^2(\Omega^\beta)}\|\nabla v_h\|_{L^2}\|\nabla\beta\|_{L^\infty}\big)\\ &\quad + \|\nabla\beta\|_{W^{1,\infty}}\|\nabla v_h\|_{L^2}^2 + \|\nabla^2\beta\|_{L^\infty}\|v_h\|_{L^2(\Omega^\beta)}\|\nabla v_h\|_{L^2}.\end{aligned} \tag{7.12}$$

Proof. Step 1: reduction to the homogeneous case. Let $\delta^2 V_\xi := \delta^2 V(Dy_h(\xi))$ and $\partial^2 W := \partial^2 W(\nabla y_h(x))$, $A := \delta^2 V(\mathsf{A}\mathcal{R})$ and $\mathbb{C} := \partial^2 W(\mathsf{A})$.

Then, the difference in the linearised operators is given by

$$\begin{aligned}&\langle \delta^2\mathscr{E}_h^\beta(y_h)v_h - \delta\mathscr{F}_h^\beta(y_h)v_h, v_h\rangle\\ &\quad= \sum_{\xi\in\mathbb{Z}^d}(1-\beta(\xi))\big\langle\delta^2 V_\xi Dv_h(\xi), Dv_h(\xi)\big\rangle + \int_{\Omega_h}(Q_h\beta)\big(\partial^2 W : \nabla v_h\big) : \nabla v_h\,{\rm d}x,\\ &\qquad - \sum_{\xi\in\mathbb{Z}^d}\big\langle\delta^2 V_\xi Dv_h(\xi), D((1-\beta)v_h)(\xi)\big\rangle - \int_{\Omega_h}(\partial^2 W : \nabla v_h) : \nabla I_h(\beta v_h)\,{\rm d}x\\ &\quad= \sum_{\xi\in\mathbb{Z}^d}\big\langle\delta^2 V_\xi Dv_h(\xi), \big(-\beta Dv_h + D(\beta v_h)\big)(\xi)\big\rangle\\ &\qquad + \int_{\Omega_h}(\partial^2 W : \nabla v_h) : \big((Q_h\beta)\nabla v_h - \nabla I_h(\beta v_h)\big)\,{\rm d}x\\ &\quad= \sum_{\xi\in\Lambda^\beta}\big\langle\delta^2 V_\xi Dv_h(\xi), \big(-\beta Dv_h + D(\beta v_h)\big)(\xi)\big\rangle\\ &\qquad + \int_{\Omega^\beta}(\partial^2 W : \nabla v_h) : \big((Q_h\beta)\nabla v_h - \nabla I_h(\beta v_h)\big)\,{\rm d}x.\end{aligned}$$

In the last step we used the fact that the summand is nonzero only if $\xi \in \Lambda^\beta$ and the integrand is nonzero only if $x \in \Omega^\beta$, where Λ^β and Ω^β are defined in § 3.2.

For such ξ and x we can estimate $|\delta^2 V(Dy_h(\xi)) - A| \lesssim \|Dy_h - \mathsf{A}\mathcal{R}\|_{\ell^\infty(\Lambda^\beta)} \lesssim \|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)}$ and $|\partial^2 W(\nabla y_h(\xi)) - \partial^2 W(\mathsf{A})| \lesssim \|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)}$. Hence, we can estimate

$$\begin{aligned}&\big|\langle \delta^2\mathscr{E}_h^\beta(y_h)v_h - \delta\mathscr{F}_h^\beta(y_h)v_h, v_h\rangle - \langle \delta^2\mathscr{E}_h^\beta(\mathsf{A}x)v_h - \delta\mathscr{F}_h^\beta(\mathsf{A}x)v_h, v_h\rangle\big|\\ &\quad\lesssim \|Dy_h - \mathsf{A}\mathcal{R}\|_{\ell^\infty(\Lambda^\beta)}\|Dv_h\|_{\ell^2(\Lambda^\beta)}\big(\|\beta\|_{\ell^\infty}\|Dv_h\|_{\ell^2} + \|D\beta\|_{\ell^\infty}\|v_h\|_{\ell^2(\Lambda^\beta)}\big)\\ &\qquad + \|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)}\|\nabla v_h\|_{L^2}\big(\|\nabla\beta\|_{L^\infty}\|v_h\|_{L^2(\Omega^\beta)} + \|\nabla v_h\|_{L^2}\|\beta\|_{L^\infty}\big)\\ &\quad\lesssim \|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)}\|\nabla v_h\|_{L^2}\big(\|\nabla\beta\|_{L^\infty}\|v_h\|_{L^2(\Omega^\beta)} + \|\nabla v_h\|_{L^2}\big)\\ &\quad\lesssim E.\end{aligned} \tag{7.13}$$

Step 2: estimate for the case $y_h = \mathsf{A}x$. It remains to bound $\delta^2\mathscr{E}_h^\beta(\mathsf{A}x) - \delta\mathscr{F}_h^\beta(\mathsf{A}x)$. To that end denote

$$E_\xi := \|\nabla\beta\|_{W^{1,\infty}(\nu_\xi)}\|\nabla v_h\|_{L^2(\nu_\xi)}^2 + \|\nabla^2\beta\|_{L^\infty(\nu_\xi)}\|v_h\|_{L^2(\nu_\xi)}\|\nabla v_h\|_{L^2(\nu_\xi)},$$

where $\nu_\xi = B_{2r_{\rm cut}+\sqrt{d}}(\xi)$ is defined in (4.4), so that $\sum_{\xi\in\Lambda^\beta} E_\xi \lesssim E$.

Further, let $A_{\rho\sigma} = V_{,\rho\sigma}(\mathsf{A}\mathcal{R})$, then we have

$$\begin{aligned}
&\langle\delta^2\mathscr{E}_h^\beta(\mathsf{A}x)v_h - \delta\mathscr{F}_h^\beta(\mathsf{A}x)v_h, v_h\rangle \\
&= \sum_{\xi\in\Lambda^\beta} \big\langle ADv_h(\xi), \big(-\beta Dv_h + D(\beta v_h)\big)(\xi)\big\rangle \\
&\qquad + \int_{\Omega^\beta} (\mathbb{C}\colon\nabla v_h)\colon\big((Q_h\beta)\nabla v_h - \nabla I_h(\beta v_h)\big)\,\mathrm{d}x \\
&= \sum_{\xi\in\Lambda^\beta}\Big(\big\langle ADv_h(\xi), (v_h\nabla\beta)(\xi)\big\rangle + O(E_\xi)\Big) - \int_{\Omega^\beta}(\mathbb{C}\colon\nabla v_h)\colon\big(v_h\otimes\nabla\beta\big)\,\mathrm{d}x \\
&= \sum_{\rho,\sigma\in\mathcal{R}} A_{\rho\varsigma} : \bigg\{\sum_{\xi\in\mathbb{Z}^d} D_\rho v_h(\xi)\otimes v_h(\xi)\nabla_\sigma\beta(\xi) - \int \nabla_\rho v_h\otimes v_h\nabla_\sigma\beta\,\mathrm{d}x\bigg\} + O(E).
\end{aligned} \tag{7.14}$$

Let $v(\xi) := v_h(\xi)$ for all $\xi\in\mathbb{Z}^d$ and recall the definition of v^* from (4.13). We observe that the sum and integral are only taken over a region where $v_h = \bar{v}$ (recall that $\mathscr{T} = \mathcal{T}_h$ in the blending region), hence we can write

$$\begin{aligned}
\sum_{\xi\in\mathbb{Z}^d} D_\rho v(\xi)\otimes v_h(\xi)\nabla_\sigma\beta(\xi) &= \sum_{\xi\in\mathbb{Z}^d} D_\rho v^*(\xi)\otimes v(\xi)\nabla_\sigma\beta(\xi) \\
&\qquad + \sum_{\xi\in\mathbb{Z}^d} D_\rho(v - v^*)(\xi)\otimes v(\xi)\nabla_\sigma\beta(\xi) \\
&=: \mathrm{S}_{\rho\sigma} + \mathrm{T}_{\rho\sigma}.
\end{aligned} \tag{7.15}$$

Step 2.1: Rewriting $\mathrm{S}_{\rho\sigma}$. Employing (4.14) and (4.18) we can write

$$\begin{aligned}
\mathrm{S}_{\rho\sigma} &= \sum_{\xi\in\mathbb{Z}^d}\int_{\mathbb{R}^d}\nabla_\rho\bar{v}(x)\omega_\rho(\xi - x)\,\mathrm{d}x\otimes v(\xi)\nabla_\sigma\beta(\xi) \\
&= \int_{\mathbb{R}^d}\nabla_\rho\bar{v}\otimes\bigg\{\sum_{\xi\in\mathbb{Z}^d}\omega_\rho(\xi - x)v(\xi)\nabla_\sigma\beta(\xi)\bigg\} \\
&= \int_{\mathbb{R}^d}\nabla_\rho\bar{v}\otimes\bigg\{\sum_{\xi\in\mathbb{Z}^d}\omega_\rho(x-\xi)\Big(\bar{v}(x)\nabla_\sigma\beta(x) + O\big(\|\nabla(\bar{v}\nabla_\sigma\beta)\|_{L^\infty(\nu_\xi)}\big)\Big)\bigg\}\,\mathrm{d}x \\
&= \int_{\mathbb{R}^d}\nabla_\rho\bar{v}\otimes\bar{v}(x)\nabla_\sigma\beta(x)\,\mathrm{d}x + O(E).
\end{aligned}$$

Thus, we observe from (7.14) and (7.15) that

$$\langle\delta^2\mathscr{E}_h^\beta(\mathsf{A}x)v_h - \delta\mathscr{F}_h^\beta(\mathsf{A}x)v_h, v_h\rangle = \sum_{\rho,\sigma\in\mathcal{R}} A_{\rho\sigma} : \mathrm{T}_{\rho\sigma} + O(E). \tag{7.16}$$

Step 2.2: Estimating $\mathrm{T}_{\rho\sigma}$. Summation by parts yields

$$\begin{aligned}\big|\mathrm{T}_{\rho\sigma}\big| &= \bigg| -\sum_{\xi\in\mathbb{Z}^d}(v-v_*)(\xi)\otimes D_{-\rho}\big(v\nabla_\sigma\beta\big)(\xi)\bigg| \\ &\lesssim \|v-v_*\|_{\ell^2(\Lambda^\beta)}\|D_{-\rho}(v\nabla_\sigma\beta)\|_{\ell^2(\Lambda^\beta)} \\ &\lesssim \|\nabla v\|_{L^2(\Omega^\beta)}\big(\|\bar v\|_{L^2(\Omega^\beta)}\|\nabla^2\beta\|_{L^\infty} + \|D_{-\rho}v\|_{\ell^2(\Lambda^\beta)}\|\nabla\beta\|_{L^\infty}\big) \\ &\lesssim E.\end{aligned}$$

Recalling (7.16) and (7.13), this completes to proof of the lemma. □

Proof of Lemma 4.12. In view of Lemma 7.2 we only need to verify that $E\to 0$ as $R^{\mathrm{a}}\to\infty$, where E is defined by (7.12). Using Corollary 6.8 we estimate

$$\begin{aligned}E &\le \|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)}\big(\|\nabla v_h\|_{L^2}^2 + \sqrt{C_2}\|\nabla v_h\|_{L^2}^2\|\nabla\beta\|_{L^\infty}\big) \\ &\quad + \|\nabla\beta\|_{W^{1,\infty}}\|\nabla v_h\|_{L^2}^2 + \|\nabla^2\beta\|_{L^\infty}\sqrt{C_2}\|\nabla v_h\|_{L^2}^2,\end{aligned}$$

where $C_2 = \big((R^\beta)^2 - (R^{\mathrm{a}})^2\big)C_1'$ and C_1' is the constant from Lemma 6.8. Then, using $\|\nabla^j\beta\|_{L^\infty}\lesssim (R^\beta)^{-j}$, we have

$$\begin{aligned}E &\lesssim \|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)}\big(\|\nabla v_h\|_{L^2}^2 + \sqrt{C_2}\|\nabla v_h\|_{L^2}^2(R^\beta)^{-1}\big) \\ &\quad + \big((R^\beta)^{-2} + (R^\beta)^{-1}\big)\|\nabla v_h\|_{L^2}^2 + (R^\beta)^{-2}\sqrt{C_2}\|\nabla v_h\|_{L^2}^2, \\ &= I_1 + I_2 + I_3.\end{aligned} \tag{7.17}$$

To complete the estimates we note that $\sqrt{C_2}(R^\beta)^{-1}\lesssim\gamma_{\mathrm{tr}}$ where γ_{tr} is defined in (4.27). Further, the regularity estimates from Lemma 2.3 and (2.10) yield

$$\|\nabla y_h - \mathsf{A}\|_{L^\infty(\Omega^\beta)} \lesssim \begin{cases}(R^{\mathrm{a}})^{-1}, & \text{case (pDis)},\\ (R^{\mathrm{a}})^{-d}, & \text{case (pPt)}.\end{cases}$$

These estimates are combined to yield

$$\begin{aligned}I_1 &\lesssim \begin{cases}(R^{\mathrm{a}})^{-1}(\log R^{\mathrm{a}})^{1/2}, & \text{case (pDis)},\\ (R^{\mathrm{a}})^{-2}(\log R^{\mathrm{a}})^{1/2}, & \text{case (pPt)}, d=2,\\ (R^{\mathrm{a}})^{-3}, & \text{case (pPt)}, d=3,\end{cases} \\ I_2 &\lesssim (R^{\mathrm{a}})^{-1}, \qquad \text{and} \\ I_3 &\lesssim \begin{cases}(R^{\mathrm{a}})^{-1}(\log R^{\mathrm{a}})^{1/2}, & \text{case } d=2,\\ (R^{\mathrm{a}})^{-1}, & \text{case } d=3.\end{cases}\end{aligned}$$

This completes the proof of Lemma 4.12. □

Remark 7. The auxiliary results, Lemmas 4.9 and 4.12, hold under much weaker assumptions. For instance, with extra work, Lemma 4.12 can be proved for the blending width (i.e., the width of $\mathrm{supp}(\nabla\beta)$) scaling slower than R^{a} [20]. However, this would not be important for the practical implementation of the method or for our error estimates. □

References

[1] S. Badia, M. L. Parks, P. B. Bochev, M. Gunzburger, and R. B. Lehoucq. On atomistic-to-continuum coupling by blending. *SIAM J. Multiscale Model. Simul.*, 7(1):381–406, 2008.

[2] P. T. Bauman, H. Ben Dhia, N. Elkhodja, J. T. Oden, and S. Prudhomme. On the application of the Arlequin method to the coupling of particle and continuum models. *Comput. Mech.*, 42(4):511–530, 2008.

[3] T. Belytschko and S. P. Xiao. Coupling methods for continuum model with molecular model. *Intl. J. Multiscale Comp. Engrg.*, 1:115–126, 2003.

[4] X. Blanc, C. Le Bris, and P.-L. Lions. From molecular models to continuum mechanics. *Arch. Ration. Mech. Anal.*, 164(4):341–381, 2002.

[5] C. Carstensen. Quasi-interpolation and a posteriori error analysis in nite element methods. *M2AN Math. Model. Numer. Anal.*, 33:1187–1202, 1999.

[6] P. G. Ciarlet. *The finite element method for elliptic problems*, volume 40 of *Classics in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2002. Reprint of the 1978 original.

[7] L. Beirao da Veiga, A. Buffa, J. Rivas, and G. Sangalli. Some estimates for h–p–k-refinement in Isogeometric Analysis. *Num. Math.*, 118(2):271–305, 2011.

[8] M. Dobson, M. Luskin, and C. Ortner. Sharp stability estimates for force-based quasicontinuum methods. *SIAM J. Multiscale Model. Simul.*, 8:782–802, 2010.

[9] M. Dobson, M. Luskin, and C. Ortner. Stability, instability and error of the force-based quasicontinuum approximation. *Arch. Ration. Mech. Anal.*, 197:179–202, 2010.

[10] M. Dobson, C. Ortner, and A. V. Shapeev. The spectrum of the force-based quasicontinuum operator for a homogeneous periodic chain. *SIAM J. Multiscale Model. Simul.*, 10(3):744–765, 2012.

[11] W. E and P. Ming. Cauchy-Born rule and the stability of crystalline solids: static problems. *Arch. Ration. Mech. Anal.*, 183(2):241–297, 2007.

[12] V. Ehrlacher, C. Ortner, and A. V. Shapeev. Analysis of boundary conditions for crystal defect atomistic simulations. *ArXiv e-prints*, 1306.5334v2, 2013.

[13] V. Ehrlacher, C. Ortner, and A. V. Shapeev. Analysis of boundary conditions for crystal defect atomistic simulations. *ArXiv e-prints*, 1306.5334v1, 2013.

[14] J. Fish, M. A. Nuggehally, M. S. Shephard, C. R. Picu, S. Badia, M. L. Parks, and M. Gunzburger. Concurrent AtC coupling based on a blend of the continuum stress and the atomistic force. *Comput. Methods Appl. Mech. Engrg.*, 196(45-48):4548–4560, 2007.

[15] G. Glaeser. Racine carrée d'une fonction différentiable. In *Annales de l'institut Fourier*, volume 13(2), pages 203–210. Institut Fourier, 1963.

[16] R. J. Hardy. Formulas for determining local properties in molecular dynamics simulations: Shock waves. *J. Chem. Phys.*, 76(622):628, 1982.

[17] J. P. Hirth and J. Lothe. *Theory of Dislocations*. Krieger Publishing Company, Malabar, Florida, 1982.

[18] T. Hudson and C. Ortner. On the stability of Bravais lattices and their Cauchy–Born approximations. *ESAIM:Math. Model. Numer. Anal.*, 46:81–110, 2012.

[19] T. Hudson and C. Ortner. Existence and stability of a screw dislocation under anti-plane deformation. *ArXiV e-prints*, 1304.2500, 2013. to appear in Arch. Ration. Mech. Anal.

[20] X. H. Li, M. Luskin, and C. Ortner. Positive-definiteness of the blended force-based quasicontinuum method. *SIAM J. Multiscale Model. Simul.*, 10:1023–1045, 2012. arXiv:1112.2528v1.

[21] X. H. Li, M. Luskin, C. Ortner, and A. V. Shapeev. Theory-based benchmarking of blended force-based quasicontinuum method. *Comp. Meth. Appl. Mech. Engrg*, 268:763781, 2014.

[22] W. K. Liu, H. Park, D. Qian, W. G. Karpov, H. Kadowaki, and G. J. Wagner. Bridging scale methods for nanomechanics and materials. *Comput. Methods Appl. Mech. Engrg.*, 195:1407–1421, 2006.

[23] J. Lu and P. Ming. Stability of a force-based hybrid method in three dimension with sharp interface. *ArXiv e-prints*, December 2012.

[24] J. Lu and P. Ming. Convergence of a force-based hybrid method in three dimensions. *Comm. Pure Appl. Math.*, 66(1):83–108, 2013.

[25] M. Luskin and C. Ortner. Atomistic-to-continuum-coupling. *Acta Numerica*, 2013.

[26] M. Luskin, C. Ortner, and B. Van Koten. Formulation and optimization of the energy-based blended quasicontinuum method. *Comput. Methods Appl. Mech. Engrg.*, 253, 2013.

[27] C. Makridakis and E. Süli. Finite element analysis of Cauchy–Born approximations to atomistic models. *Arch. Ration. Mech. Anal.*, 207:813–843, 2013.

[28] R. Miller and E. Tadmor. A unified framework and performance benchmark of fourteen multiscale atomistic/continuum coupling methods. *Modelling Simul. Mater. Sci. Eng.*, 17, 2009.

[29] Derek Olson, Pavel Bochev, Mitchell Luskin, and Alexander V. Shapeev. Development of an optimization-based atomistic-to-continuum coupling method. arxiv:1309.5988.

[30] C. Ortner. The role of the patch test in 2D atomistic-to-continuum coupling methods. arXiv:1101.5256v2.

[31] C. Ortner and A. Shapeev. Interpolants of lattice functions for the analysis of atomistic/continuum multiscale methods, 2012. arxiv:1204.3705.

[32] C. Ortner and A. V. Shapeev. Analysis of an Energy-based Atomistic/Continuum Coupling Approximation of a Vacancy in the 2D Triangular Lattice. *Math. Comp.*, 82, 2013.

[33] C. Ortner, A. V. Shapeev, and L. Zhang. Stability of geometry reconstruction-based atomistic-to-continuum coupling method. arXiv:1308.3894v1.

[34] C. Ortner and F. Theil. Justification of the Cauchy–Born approximation of elastodynamics. *Arch. Ration. Mech. Anal.*, 207, 2013.

[35] S. Prudhomme, H. Ben Dhia, P. T. Bauman, N. Elkhodja, and J. T. Oden. Computational analysis of modeling error for the coupling of particle and continuum models by the Arlequin method. *Comput. Methods Appl. Mech. Engrg.*, 197(41-42):3399–3409, 2008.

[36] C. Schwab. *p-and hp-finite element methods: Theory and applications in solid and fluid mechanics.* Clarendon Press Oxford, 1998.

[37] P. Seleson and M. Gunzburger. Bridging methods for atomistic-to-continuum coupling and their implementation. *Comm. Comp. Phys.*, 7:831–876, 2010.

[38] B. Van Koten and M. Luskin. Analysis of energy-based blended quasi-continuum approximations. *SIAM J. Numer. Anal.*, 49(5):2182–2209, 2011.

[39] R. Verfürth. *A Review of A Posteriori Error Estimation and Adaptive Mesh-Refinement Techniques.* John Wiley & Sons, New York, 1996.

[40] R. Verfürth. Error estimates for some quasi-interpolation operators. *M2AN Math. Model. Numer. Anal.*, 33:695–713, 1999.

[41] S. P. Xiao and T. Belytschko. A bridging domain method for coupling continua with molecular dynamics. *Comput. Methods Appl. Mech. Engrg.*, 193(17-20):1645–1669, 2004.

Xingjie Helen Li, The Division of Applied Mathematics at Brown University, 182 George St, Providence, RI, 02912, USA
E-mail address: xingjie_li@brown.edu

Christoph Ortner, Mathematics Institute, Zeeman Building, University of Warwick, Coventry CV4 7AL, UK
E-mail address: christoph.ortner@warwick.ac.uk

Alexander V. Shapeev, School of Mathematics, University of Minnesota, 206 Church St. SE, Minneapolis, MN 55455, USA
E-mail address: alexander@shapeev.com

B. Van Koten, The University of Chicago, Department of Statistics, Eckhart Hall Room 108, 5734 S University Ave, Chicago, IL 60637, USA
E-mail address: vankoten@galton.uchicago.edu