

Convergence of a force-based hybrid method in three dimension

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Abstract

We study a force-based hybrid method that couples atomistic model with Cauchy-Born elasticity model. We show the proposed scheme converges to the solution of the atomistic model with second order accuracy, as the ratio between lattice parameter and the characteristic length scale of the deformation tends to zero. Convergence is established for the three dimensional system without defects, with general finite range atomistic potential and simple lattices structure. The proof is based on consistency and stability analysis. General tools for stability analysis are developed in the framework of pseudo-difference operators in arbitrary dimension. © 2000 Wiley Periodicals, Inc.

1 Introduction

Multiscale methods for mechanical deformation of materials have been intensively investigated in recent years. The main spirit of these methods is to use atomistic models for regions containing defects, and continuum models in regions where the material is smoothly deformed. We refer to the recent review [28] for various methods and the book [20] for general discussion of multiscale modeling.

There are two different ways of coupling atomistic and continuum models. One is based on energy, and the other is based on force. The energy-based method defines an energy that is a mixture of atomistic energy and continuum elastic energy. The energy functional is then minimized to obtain the solution. The force-based method works instead at the level of force balance equations. The forces derived from atomistic and continuum models are coupled together. The force balance equations are solved to obtain the deformed state of the system.

From a numerical analysis point of view, one of the key issues for these multiscale methods is the consistency and stability of the coupled schemes. Taking one of the most successful multiscale methods, the quasicontinuum (QC) method [26, 40] for example, one of the main issues is the so called ghost force problem [37],

which are the artificial non-zero forces that the atoms experience at their equilibrium states. In the language of numerical analysis, it means that the scheme lacks consistency at the interface between atomistic and continuum regions [16]. In [29], it was shown that the ghost forces may lead to a finite size error of the gradient of the solution.

The stability analysis for the coupling schemes is mostly limited to one dimensional systems, in which a direct calculation is possible thanks to the simple one dimensional lattice structure and the pairwise interaction potential. This is no longer the case in two and three dimensions, and the extension is by no means easy. New tools for stability analysis are required to understand more general multiscale hybrid methods. This is the emphasis of the current work. We also remark that recently Ortner and Shapeev obtained a convergence result for an energy-based method for the two-dimensional model with pairwise interaction but allows for a point defect [32, 36].

In this work, based on existing ideas in the literature, we formulate a force-based hybrid scheme for general finite range potentials in three dimension. This hybrid method is a representative of a general class of multiscale methods. Under certain natural assumptions, we prove the solution of the proposed method converges to the solution of the atomistic model with second order accuracy as the ratio between lattice parameter and the characteristic length scale of the mechanical deformation goes to zero. To the best of our knowledge, this is the first convergence result for multiscale methods coupling atomistic and continuum models in three dimension.

The convergence result is based on the analysis of consistency and linear stability, following the Strang's trick [39]. To achieve this, we study the linearized operator in the framework of pseudo-difference operators. We obtain the stability estimate combining regularity estimate of pseudo-difference operators, consistency of the linearized operator, and stability of the continuous problem. These tools may help in understanding more general multiscale methods.

Before we formulate the method and state the main theorem in Section 1.3, we introduce some preliminaries and notations.

1.1 Lattice function and norms

We will only consider Bravais lattices in this work (see [3] for a definition). They take the form

$$\mathbb{L} = \{x \in \mathbb{R}^d \mid x = \sum_j n_j a_j, n \in \mathbb{Z}^d\},$$

where $\{a_j\}_{j=1}^d \subset \mathbb{R}^d$ are the basis vectors of \mathbb{L} , and d is the dimension. The unit cell of \mathbb{L} , denoted as Γ , is defined by

$$\Gamma = \{x \in \mathbb{R}^d \mid x = \sum_j c_j a_j, 0 \leq c_j < 1, j = 1, \dots, d\}.$$

Let $\{b_j\}_{j=1}^d \subset \mathbb{R}^d$, be the reciprocal basis vectors, which satisfy $a_j \cdot b_k = 2\pi\delta_{jk}$, where δ_{jk} is the standard Kronecker delta. The reciprocal lattice \mathbb{L}^* takes the form

$$\mathbb{L}^* = \{x \in \mathbb{R}^d \mid x = \sum_j n_j b_j, n \in \mathbb{Z}^d\}.$$

The unit cell of \mathbb{L}^* is denoted as Γ^* that is defined by

$$\Gamma^* = \{x \in \mathbb{R}^d \mid x = \sum_j c_j b_j, -1/2 \leq c_j < 1/2, j = 1, \dots, d\}.$$

For $\varepsilon = 1/n, n \in \mathbb{Z}_+$, we will consider lattice system $\varepsilon\mathbb{L}$ inside domain $\Omega = \Gamma \subset \mathbb{R}^d$, denoted as $\Omega_\varepsilon = \Omega \cap \varepsilon\mathbb{L}$. Note that the lattice constant is ε , so that the number of points in Ω_ε is $1/\varepsilon^d$. We will restrict to periodic boundary conditions in this work, general boundary conditions will be left to future publications. For a lattice function u defined on $\varepsilon\mathbb{L}$, we say it is Ω_ε -periodic if

$$u(x) = u(x'), \quad \forall x, x' \in \varepsilon\mathbb{L}, x - x' = a_j \text{ for some } j \in \{1, \dots, d\}.$$

In particular, an Ω_ε -periodic function is determined by its restriction on Ω_ε . Functions defined on Ω_ε can be easily extended to Ω_ε -periodic functions defined on $\varepsilon\mathbb{L}$.

We also define the reciprocal lattice associated with Ω_ε . Let $\mathbb{L}_\varepsilon^* = \mathbb{L}^* \cap (\Gamma^*/\varepsilon)$. Define K_ε a subset of \mathbb{Z}^d , which is given by

$$K_\varepsilon = \{\mu \in \mathbb{Z}^d \mid \sum_j \varepsilon \mu_j b_j \in \Gamma^*\},$$

hence \mathbb{L}_ε^* is given by

$$\mathbb{L}_\varepsilon^* = \{x \in \mathbb{R}^d \mid x = \sum_j \mu_j b_j, \mu \in K_\varepsilon\}.$$

For $\mu \in \mathbb{Z}^d$, the translation operator T_ε^μ is defined as

$$(T_\varepsilon^\mu u)(x) = u(x + \varepsilon \mu_j a_j) \quad \text{for } x \in \mathbb{R}^d.$$

We define the forward and backward discrete gradient operators as

$$D_{\varepsilon,s}^+ = \varepsilon^{-1}(T_\varepsilon^\mu - I) \quad \text{and} \quad D_{\varepsilon,s}^- = \varepsilon^{-1}(I - T_\varepsilon^{-\mu}),$$

where $s = \sum_i \mu_i a_i$ and I denotes the identity operator. It is easy to see $D_{\varepsilon,-s}^+ = -D_{\varepsilon,s}^-$.

We say α is a multi-index if $\alpha \in \mathbb{Z}^d$ and $\alpha \geq 0$. Define $|\alpha| = \alpha_1 + \dots + \alpha_d$. For a multi-index α , the difference operator D_ε^α is given by

$$D_\varepsilon^\alpha = \prod_{j=1}^d (D_{\varepsilon,a_j}^+)^{\alpha_j}.$$

When no confusion occurs, we will omit the subscript ε in the notations $T_\varepsilon^\mu, D_{\varepsilon,s}^+, D_{\varepsilon,s}^-$ and D_ε^α for simplicity.

We will use various norms for functions defined on Ω_ε . For a nonnegative integer k , we define the difference norm

$$\|u\|_{\varepsilon,k}^2 = \sum_{0 \leq |\alpha| \leq k} \varepsilon^d \sum_{x \in \Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)|^2.$$

It is clear that $\|\cdot\|_{\varepsilon,k}$ is a discrete analog of Sobolev norm $H^k(\Omega)$. We denote the corresponding spaces of lattice functions as $H_\varepsilon^k(\Omega)$ and $L_\varepsilon^2(\Omega)$ when $k = 0$. We also need the uniform norms on Ω_ε , which is given by

$$\begin{aligned} \|u\|_{L_\varepsilon^\infty} &= \max_{x \in \Omega_\varepsilon} |u(x)|, \\ \|u\|_{W_\varepsilon^{k,\infty}} &= \sum_{0 \leq |\alpha| \leq k} \max_{x \in \Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)|. \end{aligned}$$

In the above definitions, we have identified lattice function u with its Ω_ε -periodic function defined on $\varepsilon\mathbb{L}$, and hence the differences are well defined. These norms may be extended to vector-valued functions as usual.

Define the discrete Fourier transform for lattice function f as

$$(1.1) \quad \widehat{f}(\xi) = \varepsilon^d (2\pi)^{-d/2} \sum_{x \in \Omega_\varepsilon} e^{-i\xi \cdot x} f(x) \quad \xi \in \mathbb{L}_\varepsilon^*,$$

and its inversion is

$$(1.2) \quad f(x) = (2\pi)^{d/2} \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{i\xi \cdot x} \widehat{f}(\xi) \quad x \in \Omega_\varepsilon.$$

We will use a symbol introduced by Nirenberg in [31], which plays the same role for the difference operators as $\Lambda^2(\xi) = 1 + \Lambda_0^2(\xi) = 1 + |\xi|^2$ for the differential operators. For $\varepsilon > 0$, $\xi \in \mathbb{L}_\varepsilon^*$, let

$$\Lambda_{j,\varepsilon}(\xi) = \frac{1}{\varepsilon} |e^{i\varepsilon\xi_j} - 1|, \quad j = 1, \dots, d,$$

and

$$\Lambda_\varepsilon^2(\xi) = 1 + \Lambda_{0,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \Lambda_{j,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \frac{4}{\varepsilon^2} \sin^2\left(\frac{\varepsilon\xi_j}{2}\right).$$

It is not hard to check for any $\xi \in \mathbb{L}_\varepsilon^*$, it holds

$$(1.3) \quad c\Lambda^2(\xi) \leq \Lambda_\varepsilon^2(\xi) \leq \Lambda^2(\xi),$$

where the positive constant c depends on $\{b_j\}$.

The L_ε^2 norm of lattice function can be rewritten as

$$(1.4) \quad \|f\|_{\varepsilon,0}^2 = (2\pi)^d \sum_{\xi \in \mathbb{L}_\varepsilon^*} |\widehat{f}(\xi)|^2.$$

Moreover, notice that for $\xi \in \mathbb{L}_\varepsilon^*$, we have

$$\widehat{D_{\varepsilon,a_j}^+ f}(\xi) = \frac{1}{\varepsilon} (e^{i\varepsilon\xi \cdot a_j} - 1) \widehat{f}(\xi).$$

Therefore, the discrete Sobolev norms have equivalent representations using discrete Fourier transform:

$$c\|f\|_{\varepsilon,k}^2 \leq \sum_{\xi \in \mathbb{L}_\varepsilon^*} \Lambda_\varepsilon^{2k}(\xi) |\widehat{f}(\xi)|^2 \leq C\|f\|_{\varepsilon,k}^2$$

with the positive constants c and C depending on k and $\{a_j\}$.

For $k > d/2$, we have the following discrete Sobolev imbedding inequality [24, Proposition 6]:

$$\|f\|_{L_\varepsilon^\infty} \leq C\|f\|_{\varepsilon,k},$$

where C depends on k and Ω .

1.2 Atomistic model and Cauchy-Born rule

In this work, we will restrict to the classical empirical potentials. For atoms located at $\{y_1, \dots, y_N\}$, the interaction potential energy is given by $V(y_1, \dots, y_N)$, where V often takes the form:

$$V(y_1, \dots, y_N) = \sum_{i,j} V_2(y_i/\varepsilon, y_j/\varepsilon) + \sum_{i,j,k} V_3(y_i/\varepsilon, y_j/\varepsilon, y_k/\varepsilon) + \dots,$$

where we have omitted interactions of more than three atoms.

Different potentials are chosen for different materials. In this paper, we will work with general atomistic models, and we will make the following assumptions on the potential function V as in [19]:

- (1) V is translation invariant.
- (2) V is invariant with respect to rigid body motion.
- (3) V is smooth in a neighborhood of the equilibrium state.
- (4) V has finite range and consequently we will consider only interactions that involve a finite number of atoms.

The first two assumptions are general [8], while the latter two are specific technical assumptions.

For simplicity of notation and clarity of presentation, our presentation will be limited to potentials that contain only two-body and three-body potentials. Actually, we will only make explicit the three-body term in the expressions for the potential, as it includes the two-body term as a special case. It is straightforward to extend our results to potentials with interactions of more atoms that satisfy the above conditions, following the discussion on the three-body term. By [25], the potential function V is a function of atom distances and angles by invariance with respect to rigid body motion. Therefore, we may write

$$V_3(y_i, y_j, y_k) = V_3(|y_i - y_j|^2, |y_i - y_k|^2, \langle y_i - y_j, y_i - y_k \rangle),$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product over \mathbb{R}^d . We write the two-body and three-body potentials in this way to make the formula in our calculations easier to read.

We assume that the atoms located at Ω_ε are in equilibrium, with $x \in \Omega_\varepsilon$ the equilibrium position. Positions of the atoms under deformation will be viewed as

a function defined over Ω_ε , denote as $y(x) = x + u(x)$. Hence, $u : \Omega_\varepsilon \rightarrow \mathbb{R}^d$ is the displacement of the atoms. We extend u as an Ω_ε -periodic function defined on $\varepsilon\mathbb{L}$. Define the space of atom positions y as

$$X_\varepsilon = \{y : \varepsilon\mathbb{L} \rightarrow \mathbb{R}^d \mid y = x + u, u \text{ } \Omega_\varepsilon\text{-periodic, } \sum_{x \in \Omega_\varepsilon} u(x) = 0\}.$$

Any $y \in X_\varepsilon$ satisfies

$$y(x) - y(x') = x - x', \quad \forall x, x' \in \varepsilon\mathbb{L}, x - x' = a_j \text{ for some } j \in \{1, \dots, d\}.$$

The atomistic problem is formulated as follows. Given $f_\varepsilon : \Omega_\varepsilon \rightarrow \mathbb{R}^d$, find $y \in X_\varepsilon$ such that

$$(1.5) \quad y = \arg \min_{z \in X_\varepsilon} I_{\text{at}}(z),$$

where

$$I_{\text{at}}(z) = \frac{1}{3!} \varepsilon^d \sum_{x \in \Omega_\varepsilon} \sum_{(s_1, s_2) \in S} V_{(s_1, s_2)}[z] - \varepsilon^d \sum_{x \in \Omega_\varepsilon} f_\varepsilon(x) z(x),$$

and

$$V_{(s_1, s_2)}[z] = V(|D_{s_1}^+ z(x)|^2, |D_{s_2}^+ z(x)|^2, \langle D_{s_1}^+ z(x), D_{s_2}^+ z(x) \rangle).$$

Here S is the set of all possible (s_1, s_2) within the range of the potential. By our assumptions, S is a finite set. We only make explicit the three-body terms in the potential as addressed before. In I_{at} , ε^d is a normalization factor, so that I_{at} is actually the energy of the system per atom.

The Euler-Lagrange equation for the atomistic problem is

$$(1.6) \quad \mathcal{F}_{\text{at}}[y](x) = f_\varepsilon(x) \quad x \in \Omega_\varepsilon,$$

where

$$\begin{aligned} \mathcal{F}_{\text{at}}[y](x) = & \sum_{(s_1, s_2) \in S} \left(D_{s_1}^- (2\partial_1 V_{(s_1, s_2)}[y](x) D_{s_1}^+ y(x) + \partial_3 V_{(s_1, s_2)}[y](x) D_{s_2}^+ y(x)) \right. \\ & \left. + D_{s_2}^- (2\partial_2 V_{(s_1, s_2)}[y](x) D_{s_2}^+ y(x) + \partial_3 V_{(s_1, s_2)}[y](x) D_{s_1}^+ y(x)) \right), \end{aligned}$$

where for $i = 1, 2, 3$, we denote

$$\partial_i V_{(s_1, s_2)}[y](x) = \partial_i V(|D_{s_1}^+ y(x)|^2, |D_{s_2}^+ y(x)|^2, \langle D_{s_1}^+ y(x), D_{s_2}^+ y(x) \rangle)$$

the partial derivative with respect to the i -th argument of V .

To guarantee the uniqueness of the solution of (1.6), we assume that f_ε takes the following special form: for $x \in \Omega_\varepsilon$,

$$f_\varepsilon(x) \equiv \varepsilon^{-d} \int_{x + \varepsilon\Gamma} f(z) \, dz,$$

where $f(x)$ is a function defined on Ω with zero mean. This makes sure that $f_\varepsilon(x)$ satisfies

$$\sum_{x \in \Omega_\varepsilon} f_\varepsilon(x) = \varepsilon^{-d} \int_{\Omega} f(x) \, dx = 0.$$

To introduce the Cauchy-Born elasticity problem [8, 21, 22], we fix more notations. For any positive integer k , we denote by $W^{k,p}(\Omega; \mathbb{R}^d)$ the Sobolev space of mappings $y: \Omega \rightarrow \mathbb{R}^d$ such that $\|y\|_{W^{k,p}}$ is finite. In particular, we denote by $W_{\#}^{k,p}(\Omega; \mathbb{R}^d)$ the Sobolev space of periodic functions whose distributional derivatives of order less than k are in the space $L^p(\Omega)$. For any $p > d$ and $m \geq 0$, we define X as

$$X = \{y: \Omega \rightarrow \mathbb{R}^d \mid y = x + v, v \in W^{m+2,p}(\Omega; \mathbb{R}^d) \cap W_{\#}^{1,p}(\Omega; \mathbb{R}^d), \int_{\Omega} v = 0\}.$$

As in [19], the Cauchy-Born elasticity problem can be formulated as follows: find $y \in X$ such that

$$(1.7) \quad y = \arg \min_{z \in X} I(z),$$

where the total energy functional I is given by

$$I(z) = \int_{\Omega} (W_{\text{CB}}(\nabla v(x)) - f(x)z(x)) \, dx,$$

where $v(x) = z(x) - x$ and the Cauchy-Born stored energy density W_{CB} is given by

$$W_{\text{CB}}(A) = \frac{1}{3!} \sum_{(s_1, s_2) \in S} W_{(s_1, s_2)}(A),$$

where for $A \in \mathbb{R}^{d \times d}$,

$$W_{(s_1, s_2)}(A) = V(|s_1 + s_1 A|^2, |s_2 + s_2 A|^2, \langle s_1 + s_1 A, s_2 + s_2 A \rangle).$$

The range S is the same as that in the atomistic potential function. We have used the deformed position y instead of the more standard displacement field u as the unknown variables in (1.7) in order to be parallel with the atomistic problem.

The Euler-Lagrange equation for the Cauchy-Born elasticity model is

$$(1.8) \quad \mathcal{F}_{\text{CB}}[y](x) = f(x),$$

where

$$\mathcal{F}_{\text{CB}}[y](x) = -\nabla \cdot (D_A W_{\text{CB}}(\nabla v(x))) \quad \text{and} \quad v(x) = y(x) - x.$$

Here $D_A W_{\text{CB}}(A)$ denotes differentiation of $W_{\text{CB}}(A)$ with respect to A .

Since we are primarily interested in the coupling between the atomistic and continuum models, we will take the finite element mesh $\mathcal{T}_{\varepsilon}$ as a triangulation of Ω_{ε} with each atom site as an element vertex. The triangulation is translational invariant. The approximation space \tilde{X}_{ε} is defined as

$$\tilde{X}_{\varepsilon} = \{y \in W_{\#}^{1,p}(\Omega; \mathbb{R}^d) \mid y|_T \in P_1(T), \forall T \in \mathcal{T}_{\varepsilon}\},$$

where $P_1(T)$ is the space of linear functions on the element T .

1.3 Force-based hybrid method

We are ready to formulate the force-based hybrid method. We take $\rho : \Omega \rightarrow [0, 1]$ as a smooth cutoff function. The atomistic region corresponds to the zero level set of ρ : $\Omega_a = \{x \mid \rho(x) = 0\}$, and the continuum region corresponds to the region that ρ equals to 1: $\Omega_c = \{x \mid \rho(x) = 1\}$. The region in between is a buffer between the atomistic and the continuum regions.

The force-based hybrid method is given as follows. For $y(x) \in X_\varepsilon$, we define the force on $x \in \Omega_\varepsilon$ as

$$(1.9) \quad \mathcal{F}_{\text{hy}}[y](x) \equiv (1 - \rho(x))\mathcal{F}_{\text{at}}[y](x) + \rho(x)\mathcal{F}_\varepsilon[y](x) \quad x \in \Omega_\varepsilon,$$

where \mathcal{F}_ε is the force from finite element approximation of the Cauchy-Born elasticity problem (1.7). Due to the choice of ρ , in the atomistic region Ω_a , the force acting on the atom is just that of atomistic model, while in the continuum region Ω_c , the force is calculated from finite element approximation of the Cauchy-Born elasticity.

For given loading f_ε , we solve $y \in X_\varepsilon$ such that

$$(1.10) \quad (\Pi_\varepsilon \mathcal{F}_{\text{hy}}[y])(x) = f_\varepsilon(x) \quad x \in \Omega_\varepsilon,$$

where for Ω_ε -periodic function g , Π_ε projects g to the function with zero mean:

$$(1.11) \quad (\Pi_\varepsilon g)(x) = g(x) - \varepsilon^3 \sum_{x' \in \Omega_\varepsilon} g(x').$$

As noted in [11], the projection Π_ε is necessary here, as the force $\mathcal{F}_{\text{hy}}[y]$ might not be zero mean, which is however required by the periodic boundary condition.

The proposed scheme works in dimension $d \leq 3$ for general finite range interaction potentials. The main result of this work is the following second order convergence rate for the force-based hybrid method.

Theorem 1.1 (Convergence). *Under Assumption A, there exist positive constants δ and M , so that for any $p > d$ and $f \in W^{17,p}(\Omega) \cap W_{\#}^{1,p}(\Omega)$ with $\|f\|_{W^{17,p}} \leq \delta$, we have*

$$(1.12) \quad \|y_{\text{hy}} - y_{\text{at}}\|_{\varepsilon,2} \leq M\varepsilon^2.$$

Remark 1.2. While we do not attempt in this work to optimize the regularity assumption on f , we note that it is easy to relax the assumption to $f \in W^{5,p}(\Omega)$ with $p > d$ following the remarks in the proof.

Remark 1.3. The sharp stability Assumption A for the atomistic model will be given in Section 3. This assumption is quite natural and physical. We refer to Section 3 and also [19] for more discussions on the stability conditions and its link to physics literature.

The proof of Theorem 1.1, which will be viewed as a convergence result for nonlinear finite difference schemes, follows the spirit of Strang's work [39]. In

short, consistency and linear stability imply convergence. The heart of the matter lies in the analysis of consistency and stability, which will be the focus of the proof.

The rest of the paper is organized as follows. In the next subsection, we review some related works. Section 2 discusses the consistency of the scheme. The linear stability is proved in Section 4. The stability estimate is based on the regularity estimate of finite difference schemes in Section 3, which is established in the framework of pseudo-difference operators [9, 27, 42]. With the preparation of consistency and linear stability analysis, the proof is concluded in Section 5.

1.4 Related works

Recently there are a lot of papers discussing various atomistic/continuum coupling strategies as summarized in the reviews [10, 15, 28, 34], we will only mention the work that are closely related to ours and refer the readers to these reviews and the references therein.

The hybrid method resembles several methods in the literature. The most closely related method is the quasicontinuum method [26, 40], which is among the most popular methods for modeling the mechanical deformation of crystalline solids. The QC method contains the following ingredients: decomposition of the whole domain into atomistic and continuum regions, with the defects covered by the atomistic region; degree of freedom reduction by adaptive selection of representative atoms, with fewer atoms selected in regions with smooth deformation; and the application of the Cauchy-Born elasticity in the continuum region to reduce the complexity involved in computing the total energy of the system.

Both the proposed method and QC method couple the atomistic model with the Cauchy-Born elasticity model. In some sense, the proposed method can be viewed as a smoothed modification of the force-based QC method. Indeed, the original force-based QC method amounts to take ρ as a characteristic function so that there is no buffer region. The force-based QC is free of ghost force, and it was proven in [12, 30] that, for one-dimensional problem, the force-based method converges. However, its convergence behavior remains open for high dimensional problem. As will be proved later in the paper, the proposed method is stable and also converges in three dimension. The framework developed here also provides tools to understand the original force-based QC, which will be investigated in future works.

The Arlequin method [5, 7] and the bridging domain method [6] also adopt a smooth transition between atomistic and continuum regions. These methods are energy-based, so that the coupling is done at the energy level, while the current method is force-based. Moreover, these two methods enforce consistency between the atomistic and the continuum regions by imposing certain constraints, while there is no such constraints in our method. These methods suffer from ghost force problems as shown in [28], while the proposed method is consistent at the interface.

The proposed method also shares certain common traits with the concurrent AtC coupling method (AtC) in [4]. The AtC method also uses a smooth transition

between atomistic and continuum regions and is force-based. However, the proposed method differs from AtC in the following aspects: (1) our method employs Cauchy-Born elasticity while AtC uses linear elasticity; and (2) our method is free of ghost force while AtC is plagued by ghost force as demonstrated in [28].

Most of the analysis of these multiscale methods limits to QC. In [19], the Cauchy-Born rule for crystalline solids is verified under sharp stability conditions. In the language of QC, the authors in [19] actually proved the convergence of the local QC in the sense that the whole computational domain is treated as local region. Explicit convergence rate for the local QC can be found in [17, 18].

For the QC method that couples the atomistic and the continuum models (non-local QC method in short), the error estimate can be found in [13, 29] and the references therein. Most of the previous attentions are however restricted to one-dimensional problem, except some recent efforts devoted to the two-dimensional problem with pairwise interactions [32, 36] and consistency of 2D energy-based method [33].

To the best of the authors' knowledge, there is no convergence analysis for the nonlocal QC method or other coupling schemes for high-dimensional problems with general potential (usually, many-body potential function). The main difficulties lie in the analysis of the consistency and stability. For one-dimensional problem, the lattice structure is very simple and the pairwise potential function can be handled by a direct calculation. However, such an approach cannot be easily extended to high-dimensional problem with general potential function because the lattice structure and the potential function for high-dimensional problem are much more involved. One of the main contributions of the current paper is the development of general tools for the analysis of consistency and stability.

Finally, we remark that in this work the analysis of the proposed method, especially the stability analysis, is based on analysis of finite difference schemes. The readers might wonder why the analysis is *not* done in the framework of finite element method, as after all, we are dealing with static problems, the systems to be solved are "elliptic"; and moreover, the continuum region is discretized by finite element method. The reason actually lies in the atomistic part, since the equilibrium equations derived from energy of discrete lattice systems are intrinsically of finite difference type. To the best of our knowledge, there has not been yet a successful way to put the atomistic equations into the framework of finite element analysis. Therefore, we also view the finite element approximation in the continuum region as a finite difference approximation for consistency. The proof hence relies on the analysis of finite difference schemes. This may give a reminiscence of the early history about finite element analysis. At that time the finite element method was also analyzed in the framework of finite difference schemes [38]. Since the theory of adaptive mesh is well-established for finite element method, it is an interesting question whether one can adopt the finite element framework to analyze these multiscale coupling methods.

2 Consistency

We study the consistency of the force-based hybrid method in this section. The key is the following lemma, which is a refined version of [19, Lemma 5.1].

Lemma 2.1 (Consistency of Cauchy-Born rule). *For any $y = x + u(x)$, we have*

$$(2.1) \quad \|\mathcal{F}_{\text{at}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2 \|u\|_{W^{18,\infty}},$$

where the constant C depends on V and $\|u\|_{L^\infty}$, but is independent of ε .

Remark 2.2. The consistency estimate (2.1) is crucial for Proposition 3.4. A bound involves less order of derivatives of u is possible. In fact, it is not hard to show

$$(2.2) \quad \|\mathcal{F}_{\text{at}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2,$$

where C depends on V and $\|u\|_{W^{6,\infty}}$. The price is however the dependence of C on $\|u\|_{W^{6,\infty}}$ is nonlinear.

Proof. For any $x \in \Omega_\varepsilon$, and for $i = 1, 2$, Taylor expansion at x gives

$$D_{s_i}^+ y(x) = \nabla_{s_i}^1 [y](x) + \varepsilon \nabla_{s_i}^2 [y](x) + \varepsilon^2 R_{2,s_i} [y](x),$$

where we have introduced the shorthand for the Taylor series and its remainder:

$$\begin{aligned} \nabla_{s_i}^j [y](x) &= \frac{1}{j!} (s_i \cdot \nabla)^j y(x), \quad j = 1, 2, \\ R_{k,s_i} [y](x) &= \int_0^1 (k+1)(1-t)^k \nabla_{s_i}^{k+1} [y](x + \varepsilon t s_i) dt, \quad k \in \mathbb{N}, \end{aligned}$$

provided that the terms on the right hand side are well defined. We may write

$$(2.3) \quad D_{s_i}^+ = \nabla_{s_i}^1 + \varepsilon \nabla_{s_i}^2 + \varepsilon^2 R_{2,s_i}, \quad D_{s_i}^- = \nabla_{s_i}^1 - \varepsilon \nabla_{s_i}^2 - \varepsilon^2 R_{2,-s_i}.$$

For $i = 1, 2, 3$ and $t \in [0, 1]$, let

$$\begin{aligned} F_i(t) &= \partial_i V_{(s_1, s_2)} \left(|t D_{s_1}^+ y(x) + (1-t)(s_1 \cdot \nabla) y(x)|^2, \right. \\ &\quad |t D_{s_2}^+ y(x) + (1-t)(s_2 \cdot \nabla) y(x)|^2, \\ &\quad \langle t D_{s_1}^+ y(x) + (1-t)(s_1 \cdot \nabla) y(x), \\ &\quad \left. t D_{s_2}^+ y(x) + (1-t)(s_2 \cdot \nabla) y(x) \rangle \right). \end{aligned}$$

Using Taylor expansion, we get

$$(2.4) \quad F_i(1) = F_i(0) + F_i'(0) + R_1[F_i](0).$$

Here for $F_i : [0, 1] \rightarrow \mathbb{R}$, we have used a similar shorthand for the remainder

$$R_k[F_i](0) = \int_0^1 \frac{(1-t)^k}{k!} \nabla^{k+1} F_i(t) dt.$$

By definition we have

$$\begin{aligned}
F_i(1) &= \partial_i V_{(s_1, s_2)} (|D_{s_1}^+ y(x)|^2, |D_{s_2}^+ y(x)|^2, \langle D_{s_1}^+ y(x), D_{s_2}^+ y(x) \rangle) \\
&= \partial_i V_{(s_1, s_2)} [y](x), \\
F_i(0) &= \partial_i V_{(s_1, s_2)} (|(s_1 \cdot \nabla) y(x)|^2, |(s_2 \cdot \nabla) y(x)|^2, \langle (s_1 \cdot \nabla) y(x), (s_2 \cdot \nabla) y(x) \rangle) \\
&= \partial_i W_{(s_1, s_2)} (\nabla u(x)).
\end{aligned}$$

Therefore, we can rewrite (2.4) as

$$\begin{aligned}
(2.5) \quad \partial_i V_{(s_1, s_2)} [y](x) &= \partial_i W_{(s_1, s_2)} (\nabla u(x)) + \varepsilon a_j \partial_{ij} W_{(s_1, s_2)} (\nabla u(x)) \\
&\quad + (\varepsilon^2 b_j \partial_{ij} W_{(s_1, s_2)} (\nabla u(x)) + R_1 [F_i](0)) \\
&\equiv \mathcal{Q}_{i, (s_1, s_2)} [\nabla u](x).
\end{aligned}$$

Here, for $j = 1, 2$,

$$\begin{aligned}
a_j &= 2 \langle (s_j \cdot \nabla) y, \nabla_{s_j}^2 [y] \rangle, \quad b_j = 2 \langle (s_j \cdot \nabla) y, R_{2, s_j} [y] \rangle \\
a_3 &= \langle (s_1 \cdot \nabla) y, \nabla_{s_2}^2 [y] \rangle + \langle (s_2 \cdot \nabla) y, \nabla_{s_1}^2 [y] \rangle, \\
b_3 &= \langle (s_1 \cdot \nabla) y, R_{2, s_2} [y] \rangle + \langle (s_2 \cdot \nabla) y, R_{2, s_1} [y] \rangle.
\end{aligned}$$

Substituting (2.3) and (2.5) into $\mathcal{F}_{\text{at}} [y](x)$, we obtain

$$\begin{aligned}
\mathcal{F}_{\text{at}} [y](x) &= \\
&\sum_{(s_1, s_2) \in \mathcal{S}} (\nabla_{s_1}^1 - \varepsilon \nabla_{s_1}^2 - \varepsilon^2 R_{2, -s_1}) \left\{ 2 \mathcal{Q}_{1, (s_1, s_2)} [\nabla u] (\nabla_{s_1}^1 + \varepsilon \nabla_{s_1}^2 + \varepsilon^2 R_{2, s_1}) [y] \right. \\
&\quad \left. + \mathcal{Q}_{3, (s_1, s_2)} [\nabla u] (\nabla_{s_2}^1 + \varepsilon \nabla_{s_2}^2 + \varepsilon^2 R_{2, s_2}) [y] \right\} \\
&+ (\nabla_{s_2}^1 - \varepsilon \nabla_{s_2}^2 - \varepsilon^2 R_{2, -s_2}) \left\{ 2 \mathcal{Q}_{2, (s_1, s_2)} [\nabla u] (\nabla_{s_2}^1 + \varepsilon \nabla_{s_2}^2 + \varepsilon^2 R_{2, s_2}) [y] \right. \\
&\quad \left. + \mathcal{Q}_{3, (s_1, s_2)} [\nabla u] (\nabla_{s_1}^1 + \varepsilon \nabla_{s_1}^2 + \varepsilon^2 R_{2, s_1}) [y] \right\}.
\end{aligned}$$

Collecting the terms of the same order, we get

$$(2.6) \quad \mathcal{F}_{\text{at}} [y](x) = \mathcal{L}_0 [u](x) + \varepsilon \mathcal{L}_1 [u](x) + \varepsilon^2 \mathcal{L}_2 [u](x) + \mathcal{O}(\varepsilon^3).$$

Since each atom site in the lattice \mathbb{L} is a center of inversion symmetry, i.e., if $s \in \mathbb{L}$, then $-s \in \mathbb{L}$, and thus $\mathcal{L}_1 = 0$. Therefore, we have

$$\mathcal{F}_{\text{at}} [y](x) = \mathcal{L}_0 [u](x) + \varepsilon^2 \mathcal{L}_2 [u](x) + \mathcal{O}(\varepsilon^4).$$

The explicit form of \mathcal{L}_0 can be written as

$$\begin{aligned} \mathcal{L}_0[u](x) = & - \sum_{(s_1, s_2) \in \mathcal{S}} \left\{ 2 \sum_{j=1}^2 (s_j \cdot \nabla) [(s_j + (s_j \cdot \nabla)u) \partial_j W_{(s_1, s_2)}(\nabla u(x))] \right. \\ & + (s_1 \cdot \nabla) [(s_2 + (s_2 \cdot \nabla)u) \partial_3 W_{(s_1, s_2)}(\nabla u(x))] \\ & \left. + (s_2 \cdot \nabla) [(s_1 + (s_1 \cdot \nabla)u) \partial_3 W_{(s_1, s_2)}(\nabla u(x))] \right\}. \end{aligned}$$

We see that $\mathcal{L}_0[u](x) = \mathcal{F}_{\text{CB}}[y]$ with $y = x + u(x)$.

To prove (2.1), it remains to estimate terms of $\mathcal{O}(\varepsilon^2)$, which is a combination of the form: for $\alpha, \beta = 1, 2$,

$$\begin{aligned} & (s_\alpha \cdot \nabla)^k \left(\partial_i W_{(s_1, s_2)}(\nabla u) (s_\beta \cdot \nabla)^l u \right), \quad l+k=4, \quad l, k \in \mathbb{N}, \\ & (s_\alpha \cdot \nabla)^k \left(a_j \partial_{ij} W_{(s_1, s_2)}(\nabla u) (s_\beta \cdot \nabla)^l u \right), \quad l+k=3, \quad l, k \in \mathbb{N}, \\ & (s_\alpha \cdot \nabla) \left(b_j \partial_{ij} W_{(s_1, s_2)}(\nabla u) (s_\beta \cdot \nabla) u + R_1[F_i](0) (s_\beta \cdot \nabla) u \right). \end{aligned}$$

We only estimate the first term, and the other two terms can be bounded similarly. Due to the chain rule and to Leibniz's rule, $(s_\alpha \cdot \nabla)^k \left(\partial_i W_{(s_1, s_2)}(\nabla u) (s_\beta \cdot \nabla)^l u \right)$ is a linear combination of terms T of the form

$$T = \nabla^{|\gamma|} \left(\partial_i W_{(s_1, s_2)}(\nabla u) \right) (s_\beta \cdot \nabla)^{4-|\gamma|} u \prod_{j=1}^3 (s_\alpha \cdot \nabla)^{\gamma_j} P_j,$$

where γ is a multi-index with $|\gamma| \leq 3$, and

$$P_1 = |s_1 + (s_1 \cdot \nabla)u|^2, \quad P_2 = |s_2 + (s_2 \cdot \nabla)u|^2, \quad P_3 = \langle s_1 + (s_1 \cdot \nabla)u, s_2 + (s_2 \cdot \nabla)u \rangle.$$

Using the chain rule once again, we get, for $k, j = 1, 2, 3$ and $\alpha = 1, 2$,

$$\|(s_\alpha \cdot \nabla)^k P_j\|_{L^\infty} \leq C(s_\alpha) \left((1 + \|\nabla u\|_{L^\infty}) \|\nabla^{k+1} u\|_{L^\infty} + \|\nabla^k u\|_{L^\infty} \|\nabla^2 u\|_{L^\infty} \right).$$

Using Gagliardo-Nirenberg inequality [31],

$$\|\nabla^j u\|_{L^\infty} \leq C \|\nabla^m u\|_{L^\infty}^{j/m} \|u\|_{L^\infty}^{1-j/m}, \quad 0 < j < m,$$

we have, for $k, j = 1, 2, 3$ and $\alpha = 1, 2$,

$$\|(s_\alpha \cdot \nabla)^k P_j\|_{L^\infty} \leq C(s_\alpha) \left(\|u\|_{L^\infty} \|\nabla^{k+2} u\|_{L^\infty} + \|\nabla^{k+1} u\|_{L^\infty} \right).$$

Using the above inequality, we conclude

$$\begin{aligned} \|T\|_{L^\infty} &\leq C \max_{2 \leq |\gamma| \leq 4} \|\partial_\gamma \mathcal{W}_{(s_1, s_2)}(\nabla u)\|_{L^\infty} \|\nabla^{4-|\gamma|} u\|_{L^\infty} \\ &\times \left\{ (1 + \|u\|_{L^\infty}^3) \prod_{i=1}^3 \|\nabla^{\gamma_i+2} u\|_{L^\infty} + \prod_{i=1}^3 \|\nabla^{\gamma_i+1} u\|_{L^\infty} \right. \\ &\quad \left. + \sum_{m=1}^2 (1 + \|u\|_{L^\infty}^m) \sum_{i,j,k=1}^3 \|\nabla^{\gamma_i+2} u\|_{L^\infty} \|\nabla^{\gamma_j+m} u\|_{L^\infty} \|\nabla^{\gamma_k+1} u\|_{L^\infty} \right\}. \end{aligned}$$

Invoking Gagliardo-Nirenberg inequality again, we obtain

$$\|T\|_{L^\infty} \leq C \sum_{i=3}^6 \|u\|_{L^\infty}^i \|u\|_{W^{10,\infty}}.$$

Proceeding along the same line, we can obtain the similar bounds for the other terms, while $\|u\|_{W^{18,\infty}}$ arises from the estimate of

$$R_{2,s_\alpha}(R_1[F_i](0)(\nabla u)R_{2,s_\beta}[y]), \quad \alpha, \beta = 1, 2.$$

Summing up all terms of $\mathcal{O}(\varepsilon^2)$, we get (2.1). □

Corollary 2.3 (Consistency of finite element discretization). *For any $y = x + u(x)$ with u smooth, we have*

$$\|\mathcal{F}_\varepsilon[y] - \mathcal{F}_{\text{CB}}[y]\|_{L^\infty} \leq C\varepsilon^2 \|u\|_{W^{18,\infty}},$$

where the constant C depends on V and $\|u\|_{L^\infty}$, but is independent of ε .

Proof. The corollary follows from Lemma 2.1 and the following observation: We can view the energy functional of the finite element discretization as a particular form of the atomistic energy.

Let us consider the case $d = 2$, and the same argument applies to $d = 3$ with certain complication of notations.

Let $y_\varepsilon \in \tilde{X}_\varepsilon$ be the approximation of y so that $y_\varepsilon(x) = y(x)$ for any $x \in \Omega_\varepsilon$. Let $u_\varepsilon = y_\varepsilon - x$. Obviously, we have $u_\varepsilon(x) = u(x)$ for any $x \in \Omega_\varepsilon$.

Now, for each $T \in \mathcal{T}_\varepsilon$, $\nabla u_\varepsilon|_T$ is a linear function of y_ε on the vertices of T . Denote the three vertices of T as x_0, x_1, x_2 , and $s_1 = (x_1 - x_0)/\varepsilon$, $s_2 = (x_2 - x_0)/\varepsilon$, then $\nabla u_\varepsilon|_T$ is the solution of the linear system

$$\begin{cases} s_1 + s_1 A = D_{\varepsilon, s_1}^+ y_\varepsilon(x_0), \\ s_2 + s_2 A = D_{\varepsilon, s_2}^+ y_\varepsilon(x_0). \end{cases}$$

Therefore, let us denote

$$\nabla u_\varepsilon|_T = A_{(s_1, s_2)}(y_\varepsilon(x_0)/\varepsilon, y_\varepsilon(x_1)/\varepsilon, y_\varepsilon(x_2)/\varepsilon)$$

as the solution of the above system. Due to linearity, the map $A_{(s_1, s_2)}$ is independent of ε . Hence, for $x \in T$, we can write

$$(2.7) \quad \begin{aligned} W_{\text{CB}}(\nabla u_\varepsilon(x)) &= W_{\text{CB}}\left(A_{(s_1, s_2)}(y_\varepsilon(x_0)/\varepsilon, y_\varepsilon(x_1)/\varepsilon, y_\varepsilon(x_2)/\varepsilon)\right) \\ &= W_{\text{FE}, (s_1, s_2)}(y_\varepsilon(x_0)/\varepsilon, y_\varepsilon(x_1)/\varepsilon, y_\varepsilon(x_2)/\varepsilon), \end{aligned}$$

where $W_{\text{FE}, (s_1, s_2)} \equiv W_{\text{CB}} \circ A_{(s_1, s_2)}$. Denote S_{FE} as the set of all pairs (s_1, s_2) such that $\{x_0, x_0 + \varepsilon s_1, x_0 + \varepsilon s_2\}$ forms the vertices of an element $T \in \mathcal{T}_\varepsilon$ containing x_0 (it is easy to see that S_{FE} is independent of ε). Using (2.7), we have

$$\begin{aligned} \int_{\Omega} W_{\text{CB}}(\nabla u_\varepsilon(x)) \, dx &= \sum_{T \in \mathcal{T}_\varepsilon} |T| W_{\text{CB}}(\nabla u_\varepsilon|_T) \\ &= \frac{1}{3!} \sum_{x \in \Omega_\varepsilon} \sum_{(s_1, s_2) \in S_{\text{FE}}} \varepsilon^d |T_{(s_1, s_2)}| W_{\text{FE}, (s_1, s_2)}\left(\frac{y_\varepsilon(x)}{\varepsilon}, \frac{y_\varepsilon(x + \varepsilon s_1)}{\varepsilon}, \frac{y_\varepsilon(x + \varepsilon s_2)}{\varepsilon}\right) \\ &= \frac{1}{3!} \varepsilon^d \sum_{x \in \Omega_\varepsilon} \sum_{(s_1, s_2) \in S_{\text{FE}}} V_{\text{FE}, (s_1, s_2)}\left(\frac{y_\varepsilon(x)}{\varepsilon}, \frac{y_\varepsilon(x + \varepsilon s_1)}{\varepsilon}, \frac{y_\varepsilon(x + \varepsilon s_2)}{\varepsilon}\right), \end{aligned}$$

where $V_{\text{FE}, (s_1, s_2)} = |T_{(s_1, s_2)}| W_{\text{FE}, (s_1, s_2)}$ and $T_{(s_1, s_2)}$ is the triangle formed by vectors s_1 and s_2 . This indicates that we can view the energy functional in the finite element discretization as a particular atomistic potential model, given by three-body interactions $V_{\text{FE}, (s_1, s_2)}$, by identifying the value of y on nodes as the deformed atom positions.

It is clear that the Cauchy-Born energy density corresponding to the atomic potential constructed above is just W_{CB} . Indeed, for a homogeneously deformed system with deformation gradient A , by definition, the energy of the system is just $W_{\text{CB}}(A)|\Omega|$, and hence the Cauchy-Born energy density is given again by $W_{\text{CB}}(A)$.

With this viewpoint of the finite element discretization as an atomic potential, the conclusion follows from Lemma 2.1. \square

Corollary 2.4 (Local truncation error). *For any $y = x + u(x)$, we have*

$$(2.8) \quad \|\mathcal{F}_\varepsilon[y] - \mathcal{F}_{\text{at}}[y]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2 \|u\|_{W^{18, \infty}},$$

$$(2.9) \quad \|\mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{at}}[y]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2 \|u\|_{W^{18, \infty}},$$

and

$$(2.10) \quad \|\mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_\varepsilon^\infty} \leq C\varepsilon^2 \|u\|_{W^{18, \infty}},$$

where the constant C depends on V and $\|u\|_{L^\infty}$, but is independent of ε .

Proof. The inequality (2.8) is a combination of Lemma 2.1, Corollary 2.3, and the triangle inequality. As $\rho(x) \in [0, 1]$, we have

$$\begin{aligned} \|\mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{at}}[y]\|_{L_\varepsilon^\infty} &= \|\mathcal{F}_{\text{hy}}[y] - \Pi_\varepsilon \mathcal{F}_{\text{at}}[y]\|_{L_\varepsilon^\infty} \\ &\leq 2\|\rho(x)(\mathcal{F}_\varepsilon[y](x) - \mathcal{F}_{\text{at}}[y](x))\|_{L_\varepsilon^\infty} \\ &\leq 2\|\mathcal{F}_\varepsilon[y] - \mathcal{F}_{\text{at}}[y]\|_{L_\varepsilon^\infty}, \end{aligned}$$

where the first equality follows from that $\mathcal{F}_{\text{at}}[y]$ is zero mean. This gives (2.9). Finally, the inequality (2.10) follows from Lemma 2.1 and (2.9). \square

3 Regularity estimate

To analyze the stability of the proposed method, we use the framework of pseudo-difference operators [27, 42]. In this section, we will establish the regularity estimate Theorem 3.9 for the force-based hybrid method. This will be one of the key ingredients used to prove the stability estimate in the next section.

Let us denote $\mathcal{H}_{\text{hy}}[u]$ the linearization of \mathcal{F}_{hy} at state u :

$$\mathcal{H}_{\text{hy}}[u] = \left. \frac{\delta \mathcal{F}_{\text{hy}}}{\delta y} \right|_{y=x+u},$$

which is a linear operator, and for any lattice function w ,

$$\mathcal{H}_{\text{hy}}[u]w = \lim_{t \rightarrow 0} \frac{\partial \mathcal{F}_{\text{hy}}}{\partial t} [x + u + tw].$$

It is convenient to write \mathcal{H}_{hy} in the form of a pseudo-difference operator as

$$\mathcal{H}_{\text{hy}}[u] = \sum_{\mu \in \mathcal{A}} h_{\text{hy}}[u](x, \mu) T^\mu,$$

where, for each x and μ , the coefficient $h_{\text{hy}}[u](x, \mu)$ is a d by d (probably asymmetric) matrix, which is given by

$$(3.1) \quad (h_{\text{hy}}[u])_{\alpha\beta}(x, \mu) = \left. \frac{\partial (\mathcal{F}_{\text{hy}}[y])_\alpha(x)}{\partial (T^\mu y)_\beta(x)} \right|_{y=x+u}, \quad \alpha, \beta = 1, \dots, d,$$

where \mathcal{A} is the range of the pseudo-difference operator stencil (note that $0 \in \mathcal{A}$), which is finite by the assumptions on the potential function. By the definition of \mathcal{F}_{hy} , we have

$$(3.2) \quad h_{\text{hy}}[u](x, \mu) = (1 - \rho(x)) h_{\text{at}}[u](x, \mu) + \rho(x) h_\varepsilon[u](x, \mu),$$

where $h_{\text{at}}[u]$ and $h_\varepsilon[u]$ are given by similar equations as (3.1) with \mathcal{F}_{hy} replaced by \mathcal{F}_{at} and \mathcal{F}_ε , respectively.

Define $\tilde{h}_{\text{hy}}[u](x, \xi)$ as the symbol of the pseudo-difference operator $\mathcal{H}_{\text{hy}}[u]$:

$$\tilde{h}_{\text{hy}}[u](x, \xi) = \sum_{\mu \in \mathcal{A}} h_{\text{hy}}[u](x, \mu) \exp(i\varepsilon \sum_j \mu_j a_j \cdot \xi) \quad \text{for } \xi \in \mathbb{L}_\varepsilon^*,$$

and similar expressions are valid for $\tilde{h}_\varepsilon[u]$ and $\tilde{h}_{\text{at}}[u]$. By definition, we have, for any $x \in \Omega_\varepsilon$,

$$(\mathcal{H}_{\text{hy}}[u] e_k e^{ix \cdot \xi})_j(x) = (\tilde{h}_{\text{hy}}[u])_{jk}(x, \xi) e^{ix \cdot \xi}, \quad j, k = 1, \dots, d.$$

Similar expressions are valid for $\tilde{h}_\varepsilon[u]$ and $\tilde{h}_{\text{at}}[u]$. Here $\{e_k\}_{k=1}^d$ is the canonical basis of \mathbb{R}^d . It is clear that (3.2) implies

$$(3.3) \quad \tilde{h}_{\text{hy}}[u](x, \xi) = (1 - \rho(x)) \tilde{h}_{\text{at}}[u](x, \xi) + \rho(x) \tilde{h}_\varepsilon[u](x, \xi).$$

When the linearization is performed around the equilibrium state $u = 0$, we get a simplified expression as

$$\mathcal{H}_{\text{hy}} = \mathcal{H}_{\text{hy}}[0], \quad h_{\text{hy}} = h_{\text{hy}}[0], \quad \tilde{h}_{\text{hy}} = \tilde{h}_{\text{hy}}[0],$$

and similarly for those defined for the atomistic model and the finite element discretization. We observe that by the translation invariance of the total energy I_{at} at the state $u = 0$, the coefficients are independent of position x , i.e.,

$$h_{\text{at}}(x, \mu) = h_{\text{at}}(\mu), \quad h_{\varepsilon}(x, \mu) = h_{\varepsilon}(\mu).$$

Similarly, $\tilde{h}_{\text{at}}(x, \mu) = h_{\text{at}}(\mu)$ and $\tilde{h}_{\varepsilon}(x, \mu) = \tilde{h}_{\varepsilon}(\mu)$.

We also denote $\tilde{\mathcal{H}}_{\text{CB}}$ as the linearized operator of \mathcal{F}_{CB} at the equilibrium state $u = 0$, and define $\tilde{h}_{\text{CB}} = \tilde{h}_{\text{CB}}(x, \xi)$ as its symbol. Due to the periodic boundary condition imposed on Ω , ξ here only takes value in \mathbb{L}^* . Again, due to the translation invariance of the total energy, \tilde{h}_{CB} is independent of x .

Let us start the analysis with the operator \mathcal{H}_{hy} . We observe that the matrix \tilde{h}_{hy} is Hermitian. We omit the elementary proof of the following lemma.

Lemma 3.1. *The matrices $\tilde{h}_{\text{at}}(\xi)$, $\tilde{h}_{\varepsilon}(\xi)$ and $\tilde{h}_{\text{hy}}(x, \xi)$ are Hermitian for any $\varepsilon > 0$, $x \in \Omega_{\varepsilon}$ and $\xi \in \mathbb{L}_{\varepsilon}^*$.*

We make the following stability assumption about the atomistic potential.

Assumption A. The matrix $\tilde{h}_{\text{at}}(\xi)$ is positive definite and there exists a positive constant a_{at} such that for any $\varepsilon > 0$ and any $\xi \in \mathbb{L}_{\varepsilon}^*$,

$$\det \tilde{h}_{\text{at}}(\xi) \geq a_{\text{at}} \Lambda_{0, \varepsilon}^{2d}(\xi).$$

Assumption A will be assumed in the sequel without further indication.

Remark 3.2. This assumption is quite natural and physical. In fact, for Bravais lattice, Assumption A is just the phonon stability conditions identified in [19], here we rephrase it by the notion of symbol of difference operator. From a mathematical point of view, Assumption A can be seen as the uniform ellipticity of the difference operator.

As a consequence of Assumption A, for sufficiently small ε , the finite element approximation is also linearly stable.

Lemma 3.3. *There exist constants $a, \varepsilon_0 > 0$ that for any $\varepsilon \in (0, \varepsilon_0)$, $\tilde{h}_{\varepsilon}(\xi)$ is positive definite and for any $\xi \in \mathbb{L}_{\varepsilon}^*$,*

$$\det \tilde{h}_{\varepsilon}(\xi) \geq a \Lambda_{0, \varepsilon}^{2d}(\xi).$$

Lemma 3.3 is a direct consequence of the following proposition.

Proposition 3.4. *There exists $\varepsilon_0 > 0$ and $s > 0$ such that for any $\varepsilon \leq \varepsilon_0$ and $\xi \in \mathbb{L}_{\varepsilon}^*$, we have*

$$|\tilde{h}_{\varepsilon}(\xi) - \tilde{h}_{\text{at}}(\xi)| \leq C \varepsilon^2 (|\xi| + 1)^s.$$

Proof. By definition, for $1 \leq j, k \leq d$,

$$(\tilde{h}_\varepsilon)_{jk}(\xi) = \mathcal{H}_\varepsilon(e_k f_\xi)_j(0) \quad \text{and} \quad (\tilde{h}_{\text{at}})_{jk}(\xi) = \mathcal{H}_{\text{at}}(e_k f_\xi)_j(0),$$

where $f_\xi(x) = e^{ix \cdot \xi}$ for $x \in \Omega$ and we have used the translational symmetry. Hence, taking difference, we obtain

$$|\tilde{h}_\varepsilon(\xi) - \tilde{h}_{\text{at}}(\xi)| \leq C \sup_{1 \leq k \leq d} \|\mathcal{H}_\varepsilon(e_k f_\xi) - \mathcal{H}_{\text{at}}(e_k f_\xi)\|_{L^\infty}.$$

By the definitions of the linearized operators \mathcal{H}_ε and \mathcal{H}_{at} , we have

$$\mathcal{H}_\varepsilon(e_k f_\xi) - \mathcal{H}_{\text{at}}(e_k f_\xi) = \lim_{t \rightarrow 0^+} \frac{1}{t} (\mathcal{F}_\varepsilon[x + t(e_k f_\xi)] - \mathcal{F}_{\text{at}}[x + t(e_k f_\xi)]).$$

Hence,

$$\begin{aligned} \|\mathcal{H}_\varepsilon(e_k f_\xi) - \mathcal{H}_{\text{at}}(e_k f_\xi)\|_{L^\infty} &= \lim_{t \rightarrow 0^+} \frac{1}{t} \|\mathcal{F}_\varepsilon[x + t(e_k f_\xi)] - \mathcal{F}_{\text{at}}[x + t(e_k f_\xi)]\|_{L^\infty} \\ &\leq C\varepsilon^2 \|e_k f_\xi\|_{W^{18, \infty}} \\ &\leq C\varepsilon^2 \|e_k f_\xi\|_{H^s} \leq C\varepsilon^2 (1 + |\xi|)^s, \end{aligned}$$

where s is chosen so that the Sobolev inequality

$$\|f\|_{W^{18, \infty}(\Omega)} \leq C \|f\|_{H^s(\Omega)}$$

holds for any $f \in H^s(\Omega)$ (s depends on the dimension). Here we have used Corollary 2.4 and the fact that $\|te_k f_\xi\|_{L^\infty}$ is uniformly bounded for ξ as $t \rightarrow 0^+$. This concludes the proof. \square

As a consequence of the stability assumption, the continuous Cauchy-Born elasticity problem is also elliptic. We omit the proof, which is analogous to that of Lemma 3.3.

Corollary 3.5. *The matrix $\tilde{h}_{\text{CB}}(\xi)$ is positive definite and there exists a positive constant a_{CB} such that for any $\xi \in \mathbb{L}^*$,*

$$\det \tilde{h}_{\text{CB}}(\xi) \geq a_{\text{CB}} \Lambda_0^{2d}(\xi).$$

As a result of Assumption A and Lemma 3.3, we establish a lower bound for the symbol \tilde{h}_{hy} , which is crucial for the regularity and stability estimates.

Lemma 3.6. *For any $\varepsilon > 0$, $x \in \Omega_\varepsilon$ and any $\xi \in \mathbb{L}_\varepsilon^*$, we have*

$$\det \tilde{h}_{\text{hy}}(x, \xi) \geq \min(a, a_{\text{at}}) \Lambda_{0, \varepsilon}^{2d}(\xi).$$

Proof. For any $x, \rho(x) \in [0, 1]$, we have

$$\begin{aligned} \det \tilde{h}_{\text{hy}}(x, \xi) &= \det((1 - \rho(x))\tilde{h}_{\text{at}}(\xi) + \rho(x)\tilde{h}_\varepsilon(\xi)) \\ &\geq (\det \tilde{h}_{\text{at}}(\xi))^{1 - \rho(x)} (\det \tilde{h}_\varepsilon(\xi))^{\rho(x)} \\ &\geq a_{\text{at}}^{1 - \rho(x)} a^{\rho(x)} \Lambda_{0, \varepsilon}^{2d}(\xi) \\ &\geq \min(a, a_{\text{at}}) \Lambda_{0, \varepsilon}^{2d}(\xi), \end{aligned}$$

where the first inequality follows from the log-concavity of the function $A \mapsto \det(A)$ for positive definite matrix A [23]. \square

With these preparations, we are ready to establish the regularity estimate of the quasi-continuum approximation. The regularity of the discrete elliptic systems is understood by a fundamental result of finite difference approximation by Bube and Strikwerda [9]. They extended the regularity estimate of Thomée and Westergren [41] from a single elliptic equation to the elliptic system.

Following [9], we introduce the regular discrete elliptic system. The concept is parallel to the regular continuous elliptic system [1].

Definition 3.7 (Regular discrete elliptic system). For $i, j = 1, \dots, d$, let L_{ij} be a difference operator with symbol $l_{ij}(x, \xi)$. The system of difference equations

$$(3.4) \quad \sum_{j=1}^d L_{ij} v_j(x) = f_i(x), \quad i = 1, \dots, d,$$

is a *regular discrete elliptic system*, if there are set of integers $\{\sigma_i\}_{i=1}^d$ and $\{\tau_j\}_{j=1}^d$ such that each L_{ij} is a difference operator of order at most $\sigma_i + \tau_j$, and if there are positive constants C, ξ_0 and ε_0 such that

$$|\det l_{ij}(x, \xi)| \geq C \Lambda_\varepsilon^{2p}(\xi)$$

for $0 < \varepsilon \leq \varepsilon_0$, $\xi \in \mathbb{L}_\varepsilon^*$, and $\max_{1 \leq i \leq d} |\xi_i| \geq \xi_0$, where $2p = \sum_i (\sigma_i + \tau_i)$. We will call that the system (3.4) is a regular elliptic of order (σ, τ) .

By Lemma 3.6, we immediately have

Proposition 3.8. *Under Assumption A, the finite difference system*

$$(3.5) \quad \mathcal{H}_{\text{hy}} v = f$$

is a regular discrete elliptic system of order $(0, 2)$.

For the regular discrete elliptic system (3.5), we have the following regularity estimate.

Theorem 3.9. *Under Assumption A, for any $v \in H_\varepsilon^2(\Omega)$, we have*

$$(3.6) \quad \|v\|_{\varepsilon, 2} \leq C(\|\mathcal{H}_{\text{hy}} v\|_{\varepsilon, 0} + \|v\|_{\varepsilon, 0}).$$

The constant C is independent of v and ε .

Remark 3.10. Theorem 3.9 is analogous to the interior regularity estimate for elliptic partial differential equations in [2]. The statement of the theorem is just rewriting Theorem 2.1 in [9] by the current notation. We note that in [9], Bube and Strikwerda proved the interior regularity estimates, which clearly implies the *a priori* estimate for the periodic case.

4 Stability

The main theorem we will prove in this section is the following stability estimate.

Theorem 4.1 (Stability). *Under Assumption A, for any $v \in H_\varepsilon^2(\Omega)$ such that*

$$\sum_{x \in \Omega_\varepsilon} v(x) = 0,$$

we have

$$(4.1) \quad \|v\|_{\varepsilon,2} \leq C \|\mathcal{H}_{\text{hy}} v\|_{\varepsilon,0}.$$

Let us make some remarks about the stability result. In general, we do not know whether a stability estimate like (4.1) is valid for the force-based quasicontinuum method in high dimension (see [11, 14] for works in one dimension). From a pseudo-difference operator point of view, the continuity in x variable of the symbol of the linearized operator is crucial for the validity of the strong stability. This is also the main motivation to use a smooth transition function $\rho(x)$ in the current scheme. The strong stability property of the scheme will facilitate the numerical solution based on iterative methods.

We also note that the strong stability is also crucial for the extension of the current scheme to the time-dependent case. It plays the role of Gårding inequality. We will leave this to future publications.

To obtain the stability estimate from the regularity estimate of Theorem 3.9, we need to eliminate $\|v\|_{\varepsilon,0}$ on the right hand side of (3.6). In one dimension problem, this can be achieved by the discrete maximum principle for the finite difference equation. This is however no longer the case for higher dimension, as then we are dealing with an elliptic system. The argument we will use is similar in spirit to the argument used in [1, 35] for passing from regularity estimate to uniqueness results for elliptic systems. The difficulty however is that a compactness argument as in [35] can not apply to the finite difference system, as we need a uniform estimate for different ε . Therefore, instead of using the compactness, the proof is based on the uniqueness of the continuous elliptic system, the consistency of the finite difference schemes to the continuous system, and the regularity estimate Theorem 3.9.

To connect the finite difference system with PDE, we need to extend grid functions on Ω_ε to continuous functions defined in Ω . For this purpose, let us define an interpolation operator Q_ε as follows.¹ For any lattice function u on Ω_ε , we define $Q_\varepsilon u \in L^2(\Omega)$ by

$$(4.2) \quad (Q_\varepsilon u)(x) = (2\pi)^{d/2} \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \xi} \widehat{u}(\xi) \quad x \in \Omega.$$

Comparing with (1.2), we know that $Q_\varepsilon u$ agrees with u on Ω_ε . We have the following properties of Q_ε .

¹The usual linear interpolation is not sufficient for our purpose as we need high regularity of the interpolant.

Lemma 4.2. For $k \geq 0$, there exists constants $c_k, C_k > 0$, such that for any u ,

$$c_k \|u\|_{\varepsilon, k} \leq \|Q_\varepsilon u\|_{H^k(\Omega)} \leq C_k \|u\|_{\varepsilon, k}.$$

Proof. The conclusion follows immediately from (4.2) and (1.3). \square

For simplicity of notation, we will denote

$$\bar{u}_\varepsilon = Q_\varepsilon u_\varepsilon$$

for lattice function u_ε on Ω_ε .

To prove Theorem 4.1, we need a consistency result in the following form, which follows easily from Lemma 2.1.

Proposition 4.3. For $\{v_\varepsilon\}_{\varepsilon>0}$ that $v_\varepsilon \in H_\varepsilon^s(\Omega)$ and $\|v_\varepsilon\|_{\varepsilon, s}$ is uniformly bounded for some large enough s , we have

$$(4.3) \quad \lim_{\varepsilon \rightarrow 0^+} \|\mathcal{H}_{\text{CB}}^* \mathcal{H}_{\text{CB}} \bar{v}_\varepsilon - \overline{\mathcal{H}_{\text{hy}}^* \mathcal{H}_{\text{hy}} v_\varepsilon}\|_{L^2(\Omega)} = 0.$$

We are now ready to prove Theorem 4.1. The proof is a *reductio ad absurdum*.

Proof of Theorem 4.1. Suppose (4.1) does not hold, then there is a sequence of functions $\{v_k\}$ and $\lambda_k, \varepsilon_k > 0$ such that

$$\begin{aligned} \|v_k\|_{\varepsilon_k, 0} &= 1, & \text{for all } k; \\ \mathcal{H}_{\text{hy}}^* \mathcal{H}_{\text{hy}} v_k &= \lambda_k v_k, & \text{for all } k; \\ \lambda_k &\rightarrow 0, & \text{as } k \rightarrow \infty. \end{aligned}$$

Using Theorem 3.9 and the fact that $\|v_k\|_{\varepsilon_k, 0} = 1$, we have the estimate for any $s \in \mathbb{N}$

$$(4.4) \quad \|v_k\|_{\varepsilon_k, s} \leq C_s$$

uniformly in k .

By the construction of $\{v_k\}$, we have

$$\begin{aligned} (\mathcal{H}_{\text{CB}}^* \mathcal{H}_{\text{CB}} - \lambda_k) \bar{v}_k &= (\mathcal{H}_{\text{hy}}^* \mathcal{H}_{\text{hy}} - \lambda_k) v_k + (\mathcal{H}_{\text{CB}}^* \mathcal{H}_{\text{CB}} \bar{v}_k - \overline{\mathcal{H}_{\text{hy}}^* \mathcal{H}_{\text{hy}} v_k}) \\ &= \mathcal{H}_{\text{CB}}^* \mathcal{H}_{\text{CB}} \bar{v}_k - \overline{\mathcal{H}_{\text{hy}}^* \mathcal{H}_{\text{hy}} v_k}. \end{aligned}$$

By the regularity of v_k from (4.4), we use (4.3) to obtain

$$\|\mathcal{H}_{\text{CB}}^* \mathcal{H}_{\text{CB}} \bar{v}_k - \overline{\mathcal{H}_{\text{hy}}^* \mathcal{H}_{\text{hy}} v_k}\|_{L^2(\Omega)} \rightarrow 0 \quad \text{as } k \rightarrow \infty.$$

Therefore, as $\lambda_k \rightarrow 0$, we obtain

$$\|\mathcal{H}_{\text{CB}}^* \mathcal{H}_{\text{CB}} \bar{v}_k\|_{L^2(\Omega)} \rightarrow 0 \quad \text{as } k \rightarrow \infty.$$

Note also that the average of \bar{v}_k is zero, since $\widehat{\bar{v}_k}(0) = 0$. By the invertibility of $\mathcal{H}_{\text{CB}}^* \mathcal{H}_{\text{CB}}$ on the subspace orthogonal to constant function, $\|\bar{v}_k\|_{L^2(\Omega)} \rightarrow 0$, as $k \rightarrow \infty$. It follows from Lemma 4.2 that $\|v_k\|_{\varepsilon_k, 0} \rightarrow 0$ as $k \rightarrow \infty$. The contradiction with the choice of v_k proves (4.1). \square

The stability still holds when the projection Π_ε is included in the right hand side of (4.1).

Corollary 4.4 (Stability). *Under Assumption A, for any $v \in H_\varepsilon^2(\Omega)$ such that $\sum_{x \in \Omega_\varepsilon} v(x) = 0$, we have*

$$(4.5) \quad \|v\|_{\varepsilon,2} \leq C \|\Pi_\varepsilon \mathcal{H}_{\text{hy}} v\|_{\varepsilon,0}.$$

This is an easy corollary of Theorem 4.1 and the following lemma.

Lemma 4.5. *For $v \in H_\varepsilon^2$, we have*

$$(4.6) \quad \left| \varepsilon^3 \sum_{x \in \Omega_\varepsilon} (\mathcal{H}_{\text{hy}} v)(x) \right| \leq C \varepsilon^2 \|v\|_{\varepsilon,2}.$$

Proof. For $j = 1, \dots, d$, we have

$$\begin{aligned} \varepsilon^3 \sum_{x \in \Omega_\varepsilon} (\mathcal{H}_{\text{hy}} v)_j(x) &= \langle e_j, \mathcal{H}_{\text{hy}} v \rangle_{L_\varepsilon^2(\Omega)} \\ &= \langle e_j, (\rho \mathcal{H}_{\text{at}} + (1 - \rho) \mathcal{H}_\varepsilon) v \rangle_{L_\varepsilon^2(\Omega)} \\ &= \langle \mathcal{H}_{\text{at}}(e_j \rho) + \mathcal{H}_\varepsilon(e_j(1 - \rho)), v \rangle_{L_\varepsilon^2(\Omega)}, \end{aligned}$$

where we have used the fact that \mathcal{H}_{at} and \mathcal{H}_ε are symmetric. Note that

$$0 = \mathcal{H}_{\text{at}} e_j = \mathcal{H}_{\text{at}}(e_j \rho) + \mathcal{H}_{\text{at}}(e_j(1 - \rho)).$$

Therefore,

$$\begin{aligned} \varepsilon^3 \sum_{x \in \Omega_\varepsilon} (\mathcal{H}_{\text{hy}} v)_j(x) &= \langle (\mathcal{H}_\varepsilon - \mathcal{H}_{\text{at}})(e_j(1 - \rho)), v \rangle_{L_\varepsilon^2(\Omega)} \\ &\leq \|(\mathcal{H}_\varepsilon - \mathcal{H}_{\text{at}})(e_j(1 - \rho))\|_{L_\varepsilon^\infty} \|v\|_{L_\varepsilon^\infty} \\ &\leq C(\rho) \varepsilon^2 \|v\|_{\varepsilon,2}, \end{aligned}$$

where the last inequality follows from the consistency of \mathcal{H}_ε and \mathcal{H}_{at} , and the Sobolev inequality. \square

Using a perturbation argument, we may extend Theorem 4.1 and Corollary 4.4 to a deformed state u .

Theorem 4.6 (Stability). *Under Assumption A, there exists $\delta > 0$, such that for any $\varepsilon > 0$ and u , $\|u\|_{W_\varepsilon^{2,\infty}} \leq \delta$ and any $v \in H_\varepsilon^2(\Omega)$ with $\sum_{x \in \Omega_\varepsilon} v(x) = 0$, we have*

$$(4.7) \quad \|v\|_{\varepsilon,2} \leq C \|\Pi_\varepsilon \mathcal{H}_{\text{hy}}[u] v\|_{\varepsilon,0},$$

where the constant depends on δ , but is independent of u , v and ε .

Proof. Denote by v_0 the solution of

$$\Pi_\varepsilon \mathcal{H}_{\text{hy}}[0] v_0 = f.$$

We immediately have

$$\Pi_\varepsilon \mathcal{H}_{\text{hy}}[0](v - v_0) = (\Pi_\varepsilon \mathcal{H}_{\text{hy}}[0] - \Pi_\varepsilon \mathcal{H}_{\text{hy}}[u]) v.$$

Using Theorem 4.1, we have

$$\|v - v_0\|_{\varepsilon,2} \leq C \|\Pi_\varepsilon (\mathcal{H}_{\text{hy}}[0] - \mathcal{H}_{\text{hy}}[u]) v\|_{\varepsilon,0} \leq C \|\nabla u\|_{W_\varepsilon^{1,\infty}} \|v\|_{\varepsilon,2}.$$

By the triangle inequality, we have

$$\begin{aligned} \|v\|_{\varepsilon,2} &\leq \|v_0\|_{\varepsilon,2} + \|v - v_0\|_{\varepsilon,2} \\ &\leq C \|\Pi_\varepsilon \mathcal{H}_{\text{hy}}[0] v_0\|_{\varepsilon,0} + C \|\nabla u\|_{W_\varepsilon^{1,\infty}} \|v\|_{\varepsilon,2} \\ &\leq C \|\Pi_\varepsilon \mathcal{H}_{\text{hy}}[u] v\|_{\varepsilon,0} + C \|\nabla u\|_{W_\varepsilon^{1,\infty}} \|v\|_{\varepsilon,2} \\ &\leq C \|\Pi_\varepsilon \mathcal{H}_{\text{hy}}[u] v\|_{\varepsilon,0} + C \delta \|v\|_{\varepsilon,2}, \end{aligned}$$

which gives (4.7) by choosing $\delta = 1/(2C)$. \square

5 Convergence of the force-based hybrid method

With the consistency and stability results proved in the last three sections, we are now ready to prove the main result Theorem 1.1. The proof follows the same line of Strang's convergence proof of nonlinear finite difference schemes [39].

As a direct consequence of Corollary 2.4, we have the following

Corollary 5.1 (Higher order expansion). *Under the same assumptions of Theorem 1.1, there exist positive constants δ and M , so that for any $p > d$ and $f \in W^{17,p}(\Omega) \cap W_{\#}^{1,p}(\Omega)$ with $\|f\|_{W^{17,p}} \leq \delta$, denote $\tilde{y} = x + u(x)$ with u the solution of the Cauchy-Born elasticity problem (1.8), we then have*

$$\|\Pi_\varepsilon \mathcal{F}_{\text{hy}}[\tilde{y}] - f_\varepsilon\|_{L_\varepsilon^\infty} \leq M \varepsilon^2.$$

Remark 5.2. Using the remark under Lemma 2.1, the regularity assumption of f can be relaxed to $W^{5,p}(\Omega)$ with $p > d$.

Proof. By the construction of \tilde{y} , we have

$$\mathcal{F}_{\text{CB}}[\tilde{y}] = f.$$

Using the definition of f_ε , we have for all $x \in \Omega_\varepsilon$,

$$|(\mathcal{F}_{\text{CB}}[\tilde{y}])(x) - f_\varepsilon(x)| \leq \varepsilon^{-d} \left| \int_{x+\varepsilon\Gamma} [f(x) - f(y)] dy \right| \leq C \varepsilon^2 \|f\|_{W^{2,\infty}}.$$

Hence, using (2.10) of Corollary 2.4 and the regularity of f , we have

$$\|\mathcal{F}_{\text{hy}}[\tilde{y}] - f_\varepsilon\|_{L_\varepsilon^\infty} \leq C \varepsilon^2.$$

The proof is concluded by noting that

$$\|\Pi_\varepsilon \mathcal{F}_{\text{hy}}[\tilde{y}] - f_\varepsilon\|_{L_\varepsilon^\infty} = \|\Pi_\varepsilon \mathcal{F}_{\text{hy}}[\tilde{y}] - \Pi_\varepsilon f_\varepsilon\|_{L_\varepsilon^\infty} \leq 2 \|\mathcal{F}_{\text{hy}}[\tilde{y}] - f_\varepsilon\|_{L_\varepsilon^\infty},$$

where the first equality is valid as f_ε is zero mean. \square

We are now ready to prove the main result of the paper.

Proof of Theorem 1.1. We take \tilde{y} be that given by Corollary 5.1. It is easy to see

$$\int_0^1 \Pi_\varepsilon \mathcal{H}_{\text{hy}}[ty + (1-t)\tilde{y}](x) dt \cdot (y - \tilde{y}) = \Pi_\varepsilon \mathcal{F}_{\text{hy}}[y] - \Pi_\varepsilon \mathcal{F}_{\text{hy}}[\tilde{y}].$$

Hence y is the solution of (1.10) if and only if

$$\int_0^1 \Pi_\varepsilon \mathcal{H}_{\text{hy}}[ty + (1-t)\tilde{y}](x) dt \cdot (y - \tilde{y}) = f_\varepsilon - \Pi_\varepsilon \mathcal{F}_{\text{hy}}[\tilde{y}].$$

For any $\kappa \in (3/2, 2)$, we define

$$B = \{y \in X_\varepsilon \mid \|y - \tilde{y}\|_{\varepsilon,2} \leq \varepsilon^\kappa\}.$$

We define a map $T : B \rightarrow B$ as follows: for any $y \in B$, let $T(y)$ be the solution of the linear system

$$(5.1) \quad \int_0^1 \Pi_\varepsilon \mathcal{H}_{\text{hy}}[ty + (1-t)\tilde{y}](x) dt \cdot (T(y) - \tilde{y}) = f_\varepsilon - \Pi_\varepsilon \mathcal{F}_{\text{hy}}[\tilde{y}].$$

We first show that T is well defined. Since

$$\|ty + (1-t)\tilde{y} - \tilde{y}\|_{\varepsilon,2} \leq t\|y - \tilde{y}\|_{\varepsilon,2} \leq \varepsilon^\kappa,$$

which gives that for sufficiently small ε and $d \leq 3$, there holds

$$\|ty + (1-t)\tilde{y} - \tilde{y}\|_{W_\varepsilon^{2,\infty}} \leq \varepsilon^{\kappa-d/2} < \delta,$$

where the constant δ appears in Theorem 4.6. It follows from Theorem 4.6 that the problem (5.1) is solvable and

$$(5.2) \quad \|T(y) - \tilde{y}\|_{\varepsilon,2} \leq C\|f_\varepsilon - \Pi_\varepsilon \mathcal{F}_{\text{hy}}[\tilde{y}]\|_{\varepsilon,0} \leq C\varepsilon^2,$$

where we have used Corollary 5.1. For sufficiently small ε , we have

$$\|T(y) - \tilde{y}\|_{\varepsilon,2} \leq \varepsilon^\kappa.$$

Therefore, $T(y) \in B$ and T is well-defined, which in turn implies $T(B) \subset B$ for sufficiently small ε . Now the existence of y follows from the Brouwer fixed point theorem. The solution y is locally unique since the Hessian at y is nondegenerate. Let us denote the solution as y_{hy} , we then have from (5.2) that

$$(5.3) \quad \|\tilde{y} - y_{\text{hy}}\|_{\varepsilon,2} \leq C\varepsilon^2.$$

Proceeding along the same line that leads to (5.2) and using Lemma 2.1, we get

$$(5.4) \quad \|\tilde{y} - y_{\text{at}}\|_{\varepsilon,2} \leq C\varepsilon^2.$$

Finally, we conclude that y_{hy} satisfies (1.12) by combining (5.3) and (5.4). \square

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