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1 **A POSTERIORI ERROR ESTIMATION AND ADAPTIVE ALGORITHM FOR**
2 **ATOMISTIC/CONTINUUM COUPLING IN 2D***

3 HAO WANG[†], MINGJIE LIAO[‡], PING LIN[§], AND LEI ZHANG[¶]

4 **Abstract.** Atomistic/continuum coupling methods aim to achieve optimal balance between accuracy and efficiency.
5 Adaptivity is the key for the efficient implementation of such methods. In this paper, we carry out a rigorous a posteriori
6 analysis of the residual, the stability constant, and the error bound, for a consistent atomistic/continuum coupling method
7 in 2D. We design and implement the corresponding adaptive mesh refinement algorithm, and the convergence rate with
8 respect to degrees of freedom is optimal compare with a priori error estimates.

9 **Key words.** atomistic models, coarse graining, atomistic-to-continuum coupling, adaptive algorithm, a posteriori
10 error estimate

11 **AMS subject classifications.** 65N12, 65N15, 70C20, 82D25

12 **1. Introduction.** Atomistic/continuum (a/c) coupling methods are a class of computational
13 multiscale methods that aim to combine the accuracy of the atomistic model and the efficiency of the
14 continuum model for crystalline solids with defects [26, 43, 14]. Namely, the atomistic model can be
15 applied in a small neighborhood of the localized defects such as vacancies, dislocations, and cracks,
16 while the continuum model (e.g., Cauchy-Born rule) can be employed away from the defect cores
17 where elastic deformation occurs. The construction and analysis of different a/c coupling methods
18 have attracted considerable attention in the research community in recent years [16, 31, 19, 18]. We
19 refer the readers to [23, 20] for a review of such methods.

20 The goal of the mathematical analysis for a/c coupling methods is to find the optimal relation of ac-
21 curacy vs. degrees of freedom. The a priori analysis has been carried out for several typical a/c coupling
22 methods, for example the QNL (quasi-nonlocal quasicontinuum) method [24, 34], the BQCE (blended
23 energy-based quasi-continuum) method [15], the BQCF (blended force-based quasi-continuum) method
24 [18, 15], the GRAC (geometric reconstruction based atomistic/continuum coupling) method [36] and
25 the BGFC (atomistic/continuum blending with ghost force correction) method [38].

26 In contrast, although adaptivity is the key for the efficient implementation of a/c coupling methods,
27 only few research articles are concerned with the a posteriori error control of these methods. The goal-
28 oriented approach has been utilised in [40] by Prudhomme et al. to provide a posteriori error control
29 for a three dimensional nanoindentation problem with the quantity of interest being the force acting on
30 the indenter. The error estimator is a modification of the rigorously derived residual functional, and its
31 effectiveness is only validated numerically. Arndt and Luskin [2, 3] analyze the goal-oriented approach
32 for a one dimensional Frenkel-Kontorova model, where the a posteriori error estimators are used to
33 optimize the choice of the atomistic region as well as the finite element mesh in the continuum region.
34 All these work employ the original energy-based quasicontinuum method as the underlying model
35 which is later shown to be inconsistent and suffers from the so-called "ghost force" [43, 7, 17, 24, 22].

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36 Recently, Kochmann et al. [47] proposed an adaptivity strategy for the so-call "fully-nonlocal quasi-
 37 continuum" method which apply a discrete model in the entire computational domain without coupling
 38 of different models. This approach aims to minimize the ghost force rather than eliminate it as in the
 39 consistent a/c coupling method.

40 The residual based a posteriori error bounds for a/c coupling schemes are first derived in [32, 27]
 41 by Ortner et al. in 1D. A recent advance in this direction [35] is the a posteriori error analysis of a
 42 consistent energy-based coupling method developed in [41, 42], where the a posteriori error estimators
 43 are proposed both in the energy norm and in energy itself. For complex lattice, a posteriori error
 44 analysis for the QC method in 1D has been carried out in [1].

45 Despite all those developments, the rigorous mathematical justification of a posteriori error esti-
 46 mates beyond 1D is still missing. In this paper, we present a rigorous a posteriori error estimate for
 47 a consistent energy-based a/c method in two dimension, which is of physical significance and has not
 48 been considered so far to the best knowledge of the authors. We use the residual-based approach [48]
 49 to establish the estimate in negative Sobolev norms following [35]. Two features distinguish our prob-
 50 lem from the classic residual-based estimate for finite element approximation of the elliptic equations.
 51 The first one is the existence of the modeling error which is in origin different from the applications
 52 of quadrature rules. The second one is that the mesh may not be further refined when it almost co-
 53 incides with the reference lattice, therefore a model adaptation should be imposed. The analysis and
 54 algorithm rely on the so-called divergence free tensor field, which characterizes the essential difference
 55 of 2D results compared with 1D results in [27, 35] where the analysis can be carried out by explicit
 56 calculations.

57 Similar to the a priori analysis of GRAC in [36], we constrain ourselves to the case of nearest-
 58 neighbor interactions. Although the analysis can be extended to finite range interactions and to other
 59 a/c coupling methods, we decide not to include these so that the main ideas and steps are clearly
 60 presented without the distraction from the unnecessary complexity of the presentation. Instead, we
 61 will make further remarks on this point again in § 5.

62 The paper is organized as follows. In § 2 we set up the atomistic, continuum and coupling models
 63 for point defects. In § 3 we present the main results: the residual estimate, stability bound, and
 64 rigorous a posteriori error estimates for the coupling scheme. We formulate the corresponding adaptive
 65 algorithm and demonstrate numerical results in § 4. We draw conclusions and make suggestions for
 66 future research in § 5. Some auxiliary results are given in § Appendix A.

67 **2. Formulation.** We first give a brief review of a model for crystal defects in an infinite lattice
 68 in the spirit of [11] in § 2.1 and the Cauchy-Born continuum model in § 2.2. We then present a generic
 69 form of a/c coupling schemes in § 2.3. We will introduce the consistent scheme GRAC specifically in
 70 § 2.4.

71 2.1. Atomistic model.

72 **2.1.1. Atomistic lattice and defects.** Given $d \in \{2, 3\}$, $A \in \mathbb{R}^{d \times d}$ non-singular, $\Lambda^{\text{hom}} := AZ^d$ is
 73 the *homogeneous reference lattice* which represents a perfect *single lattice crystal* formed by identical
 74 atoms and possessing no defects. $\Lambda \subset \mathbb{R}^d$ is the *reference lattice* with some *local defects*. The mismatch
 75 between Λ and Λ^{hom} represents possible defects Λ^{def} , which are contained in some localized *defect cores*
 76 D^{def} such that the atoms in $\Lambda \setminus D^{\text{def}}$ do not interact with defects Λ^{def} (see § 2.1.2 and § 2.1.3 regarding
 77 interaction neighbourhood). For example, $\Lambda^{\text{def}} = \{x\}$ for a crystal with a single point defect at x , and
 78 one can choose a proper radius $R^{\text{def}} > 0$ such that $D^{\text{def}} = B_{x, R^{\text{def}}}$, where $B_{x, R} := \{z \in \mathbb{R}^d \mid |z - x| \leq R\}$.
 79 For different types of point defects, we have

- 80 • $\Lambda \subset \Lambda^{\text{hom}}$ for a vacancy at $x \in \Lambda^{\text{hom}}$;
- 81 • $\Lambda \supset \Lambda^{\text{hom}}$ for an interstitial at $x \in \Lambda$ but $x \notin \Lambda^{\text{hom}}$;
- 82 • $\Lambda = \Lambda^{\text{hom}}$ for an impurity at $x \in \Lambda^{\text{hom}}$, the difference of the impurity atom with other atoms
 83 can be characterized by the inhomogeneity of interaction potentials (see § 2.1.3).

84 This characterization of localized defects can be straightforwardly generalized to multiple point defects
 85 and micro-cracks, for example, see the setup of the model problem in § 4.2. Straight screw dislocations
 86 can be enforced through the appropriate choice of boundary conditions [11].

87 **2.1.2. Lattice function and lattice function space.** Given $d \in \{2, 3\}$, $m \in \{1, 2, 3\}$, denote
88 the set of vector-valued *lattice functions* by

$$89 \quad \mathcal{U} := \{v : \Lambda \rightarrow \mathbb{R}^m\}.$$

90 A *deformed configuration* is a *lattice function* $y \in \mathcal{U}$. Let x be the identity map, the *displacement*
91 $u \in \mathcal{U}$ is defined by $u(\ell) = y(\ell) - x(\ell) = y(\ell) - \ell$ for any $\ell \in \Lambda$.

92 For each $\ell \in \Lambda$, we prescribe an *interaction neighbourhood* $\mathcal{N}_\ell := \{\ell' \in \Lambda \mid 0 < |\ell' - \ell| \leq r_{\text{cut}}\}$ with
93 some cut-off radius r_{cut} . The *interaction range* $\mathcal{R}_\ell := \{\ell' - \ell \mid \ell' \in \mathcal{N}_\ell\}$ is defined as the union of lattice
94 vectors defined by the finite difference of lattice points in \mathcal{N}_ℓ and ℓ .

95 To measure the error for lattice functions we need to introduce function norms and function spaces
96 on the lattice. Define the “finite difference stencil” $Dv(\ell) := \{D_\rho v(\ell)\}_{\rho \in \mathcal{R}_\ell} := \{v(\ell + \rho) - v(\ell)\}_{\rho \in \mathcal{R}_\ell}$.
97 Higher-order finite differences, e.g., $D_\rho D_\zeta v$ and $D^2 v$ can be defined in a canonical way. A *lattice*
98 *function norm* can hence be defined using those notations. For $v \in \mathcal{U}$, let the lattice energy-norm (a
99 discrete H^1 -semi-norm) be

$$100 \quad (1) \quad \|Dv\|_{\ell^2} := \left(\sum_{\ell \in \Lambda} \sum_{\rho \in \mathcal{R}_\ell} |D_\rho v(\ell)|^2 \right)^{1/2}.$$

101 The associated *lattice function space* is defined by

$$102 \quad \mathcal{U}^{1,2} := \{u : \Lambda \rightarrow \mathbb{R}^m \mid \|Du\|_{\ell^2} < +\infty\}.$$

104 We choose

$$105 \quad (2) \quad \mathcal{B} := \{(\ell, \ell + \rho) : \ell \in \Lambda, \rho \in \mathcal{R}_\ell\}$$

106 to be the collection of all the nearest neighbour bonds in the reference lattice, and for $b = (\ell, \ell + \rho) \in \mathcal{B}$,
107 denote $\rho_b = \rho$. Then the energy norm can be reformulated as

$$108 \quad (3) \quad \|Dv\|_{\ell^2} := \left(\sum_{b=(\ell, \ell+\rho) \in \mathcal{B}} |D_\rho v(\ell)|^2 \right)^{1/2}.$$

109 The homogeneous lattice $\Lambda^{\text{hom}} = \mathbf{A}\mathbb{Z}^d$ naturally induces a simplicial micro-triangulation \mathcal{T} . In
110 2D, $\mathcal{T}^{\text{a}} = \{\mathbf{A}\xi + \hat{T}, \mathbf{A}\xi - \hat{T} \mid \xi \in \mathbb{Z}^2\}$, where $\hat{T} = \text{conv}\{0, e_1, e_2\}$. Let $\bar{\zeta} \in W^{1,\infty}(\Lambda^{\text{hom}}; \mathbb{R})$ be the P1 nodal
111 basis function associated with the origin; namely, $\bar{\zeta}$ is piecewise linear with respect to \mathcal{T}^{a} , and $\bar{\zeta}(0) = 1$
112 and $\bar{\zeta}(\xi) = 0$ for $\xi \neq 0$ and $\xi \in \Lambda^{\text{hom}}$. The nodal interpolant of $v \in \mathcal{U}$ can be written as

$$113 \quad \bar{v}(x) := \sum_{\xi \in \mathbb{Z}^d} v(\xi) \bar{\zeta}(x - \xi).$$

114 We can introduce the discrete homogeneous Sobolev spaces

$$115 \quad \mathcal{U}^{1,2} := \{u \in \mathcal{U} \mid \nabla \bar{u} \in L^2\},$$

116 with semi-norm $\|\nabla \bar{u}\|_{L^2}$. It is known from [30] that $\mathcal{U}^{1,2}$ and $\mathcal{U}^{1,2}$ are equivalent.

117 **2.1.3. Interaction potential.** For each $\ell \in \Lambda$, let $V_\ell(y)$ denote the *site energy* associated with
118 the lattice site $\ell \in \Lambda$, and we assume that $V_\ell(y) \in C^k((\mathbb{R}^d)^{\mathcal{R}_\ell})$, $k \geq 2$. In this paper, we consider the
119 general multibody interaction potential of the *generic pair functional form* [46]. Namely, the potential
120 is a function of the distances between atoms within interaction range and with no angular dependence.
121 Accordingly, we have the following equivalent forms of interaction potentials of generic pair functional
122 form,

$$123 \quad (4) \quad V_\ell(y) = \hat{V}_\ell(\{D_\rho y(\ell)\}_{\rho \in \mathcal{R}_\ell}) = \tilde{V}_\ell(\{|D_\rho y(\ell)|\}_{\rho \in \mathcal{R}_\ell})$$

124 *Remark 2.1.* For convenience, with a slight abuse of notation, we will use $V_\ell(D_\rho y)$, $V_\ell(|D_\rho y|)$
 125 instead of $\widehat{V}_\ell(\{D_\rho y(\ell)\}_{\rho \in \mathcal{R}_\ell})$, $\widetilde{V}_\ell(\{|D_\rho y(\ell)|\}_{\rho \in \mathcal{R}_\ell})$ when there is no confusion in the context.

126 We assume that V_ℓ is *homogeneous* outside the defect region D^{def} , namely, $V_\ell = V$ and $\mathcal{R}_\ell = \mathcal{R}$
 127 for $\ell \in \Lambda \setminus D^{\text{def}}$. V and \mathcal{R} have the following point symmetry: $\mathcal{R} = -\mathcal{R}$, and $V(\{-g_{-\rho}\}_{\rho \in \mathcal{R}}) = V(g)$.

128 *Remark 2.2.* Notice that both displacement u and deformation y are discrete functions belonging
 129 to \mathcal{U} , however $u \in \mathcal{U}^{1,2}$ while $y \notin \mathcal{U}^{1,2}$. We define the interaction potential V through y for the
 130 convenience of stability analysis, the consistency results are the same either with u or with y .

131 A great number of practical potentials are in the form (4), including the widely used embedded
 132 atom model (EAM) [6] and Finnis-Sinclair model [13]. For example, assuming a finite interaction
 133 neighborhood \mathcal{N}_ℓ and an interaction range \mathcal{R}_ℓ for $\ell \in \Lambda$, EAM potential reads

$$\begin{aligned} 134 \quad V_\ell(y) &:= \sum_{\ell' \in \mathcal{N}_\ell} \phi(|y(\ell) - y(\ell')|) + F\left(\sum_{\ell' \in \mathcal{N}_\ell} \psi(|y(\ell) - y(\ell')|)\right), \\ 135 \quad (5) \quad &= \sum_{\rho \in \mathcal{R}_\ell} \phi(|D_\rho y(\ell)|) + F\left(\sum_{\rho \in \mathcal{R}_\ell} \psi(|D_\rho y(\ell)|)\right). \\ 136 \end{aligned}$$

137 for a pair potential ϕ , an electron density function ψ and an embedding function F .

138 The energy of an infinite configuration is typically ill-defined. However, if we redefine the potential
 139 $V_\ell(y)$ as the difference $V_\ell(y) - V_\ell(\ell)$, which is equivalent to assuming $V_\ell(\ell) = 0$, the energy functional

$$140 \quad (6) \quad \mathcal{E}^a(y) = \sum_{\ell \in \Lambda} V_\ell(y)$$

141 is a meaningful object. Given the point symmetry and smoothness assumptions for the site potentials
 142 V_ℓ , $\mathcal{E}^a(y)$ is well-defined for $y - y^B \in \mathcal{U}^{1,2}$, where $y^B(x) = Bx$. Furthermore, if $V_\ell(y)$ is C^k in its
 143 variables, \mathcal{E}^a is k times Fréchet differentiable. In particular, we define M as the Lipschitz constant of
 144 $\delta^2 \mathcal{E}^a$, by [11, Lemma 2.1].

145 Under the above conditions, the goal of the atomistic problem is to find a *strongly stable* equilibrium
 146 y , such that, given a macroscopic applied strain $B \in \mathbb{R}^{d \times d}$, we aim to compute

$$147 \quad (7) \quad y \in \arg \min \{ \mathcal{E}^a(y) \mid y - y^B \in \mathcal{U}^{1,2} \}.$$

148 y is *strongly stable* if there exists $c_0 > 0$ such that

$$149 \quad \langle \delta^2 \mathcal{E}^a(y)v, v \rangle \geq c_0 \|\nabla v\|_{L^2}^2, \quad \forall v \in \mathcal{U}^{1,2}.$$

150 .

151 It is proven in [11, Theorem 2.3] that, if the homogeneous lattice is stable and $y \in \mathcal{U}$ is a critical
 152 point of \mathcal{E}^a such that $u = y - y^B \in \mathcal{U}^{1,2}$, then $D^j u$ exhibit the following *generic decay*, $j = 0, 1, \dots$,

$$153 \quad (8) \quad |D^j u(\ell)| \lesssim |\ell|^{1-d-j}, \quad \text{and} \quad |u(\ell) - u_\infty| \lesssim |\ell|^{-d+1}.$$

154 where $u_\infty := \lim_{|\ell| \rightarrow \infty} u(\ell)$.

155 **2.2. Continuum model.** To formulate atomistic to continuum coupling schemes, we need a
 156 continuum model which is compatible with (6) and defined through a strain energy density function
 157 $W : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}$. Let V be the homogeneous site potential on Λ^{hom} . A typical choice in the multi-scale
 158 context is the Cauchy–Born continuum model [10, 33], the energy density W is defined by

$$159 \quad W(\mathbf{F}) := \det \mathbf{A}^{-1} V(\mathbf{F}x).$$

160 **2.3. A/C coupling.** We give a generic formulation of the a/c coupling method and employ
161 concepts and notation from various earlier works, such as [26, 43, 44, 21, 37], and we adapt the
162 formulation to the settings in this paper.

163 First, the computational domain $\Omega_R \subset \mathbb{R}^d$ is a simply connected, polygonal and closed set, such
164 that $B_{0,R} \subset \Omega_R \subset B_{0,c_0 R}$ for some $c_0 > 0$. Let R be the radius of Ω_R . We have the following
165 decomposition $\Omega_R = \Omega_R^a \cup \Omega_R^c$, where the atomistic region Ω_R^a is again simply connected and polygonal,
166 and contains the defect core: $D^{\text{def}} \subset \Omega_R^a$. Let R_a be the radius of Ω_R^a . Let $\mathcal{T}_{h,R}^c$ be a shape-regular
167 simplicial partition (triangles for $d = 2$ or tetrahedra for $d = 3$) of the continuum region Ω_R^c .

168 Next, we decompose the set of atoms $\Lambda^{a,i} := \Lambda \cap \Omega_R^a = \Lambda^a \cup \Lambda^i$ into a core atomistic set Λ^a and an
169 interface set Λ^i (typically a few “layers” of atoms surrounding Λ^a) such that $\Lambda \cap D^{\text{def}} \subset \Lambda^a$. Let $\mathcal{T}_{h,R}^a$ be
170 the canonical triangulation induced by $\Lambda^{a,i}$, which may contain “holes” due to the existence of defects,
171 and $\mathcal{T}_{h,R} = \mathcal{T}_{h,R}^c \cup \mathcal{T}_{h,R}^a$. Sometimes, it is also convenient to define $\mathcal{T}_{h,R}^i := \{T \in \mathcal{T}_{h,R} : \Lambda^i \cap T \neq \emptyset\}$.
172 Please see Figure 1 for an illustration of the computational mesh.

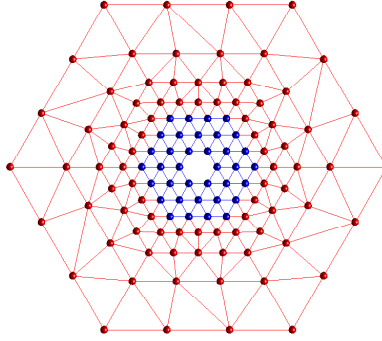


Fig. 1: Illustration of computational mesh. The computational domain is Ω_R , and the corresponding
triangulation is $\mathcal{T}_{h,R}$. Blue nodes in Ω_R are atoms in $\Lambda^{a,i}$. For nearest neighbour interaction, Λ^i is the
set of outmost layer of blue atoms. Red nodes in $\mathcal{T}_{h,R}$ are continuum degrees of freedom. Ω_R^a is the
domain induced by the blue nodes, and $\mathcal{T}_{h,R}^a$ is the corresponding triangulation. Ω_R^c and $\mathcal{T}_{h,R}^c$ are the
respective complements of Ω_R^a and $\mathcal{T}_{h,R}^a$.

173 Let $\Omega_{h,R} = \bigcup_{T \in \mathcal{T}_{h,R}} T$. Notice that $\Omega_{h,R}$ can be multiple-connected, and $\Omega_R \setminus \Omega_{h,R}$ characterizes
174 possible defects. The space of *coarse-grained* displacements is,

$$\mathcal{U}_{h,R} := \left\{ u_h : \Omega_{h,R} \rightarrow \mathbb{R}^m \mid \begin{array}{l} u_h \text{ is continuous and p.w. affine w.r.t. } \mathcal{T}_{h,R}, \\ u_h = 0 \text{ on } \partial\Omega_R \end{array} \right\}.$$

178 We may drop the subscript R in the above definitions, for example, use \mathcal{T}_h instead of $\mathcal{T}_{h,R}$ if there
179 is no confusion. Let \mathcal{N}_h be the set of nodes in \mathcal{T}_h , and \mathcal{F}_h be the set of edges in \mathcal{T}_h .

180 Denote $\text{vor}(\ell)$ as the voronoi cell associated with atom ℓ , the volume of this cell denoted as $|\text{vor}(\ell)|$
181 equals the volume of the unit cell in Λ^{hom} , i.e. $\text{vor}(\ell) = \det(\mathbf{A})$. For each $\ell \in \Lambda^a$, the associated
182 effective volume is $v_\ell = \text{vor}(\ell)$. For $\ell \in \Lambda^i$ the effective volume v_ℓ will depend on the geometry of

183 the interface (see [36]), let $\omega_\ell := \frac{|v_\ell|}{|\text{vor}(\ell)|}$ denote the volume ratio of v_ℓ with respect to vor . For each
184 element $T \in \mathcal{T}_h$ we define the effective volume of T by

$$\omega_T := |T \setminus (\bigcup_{\ell \in \Lambda^a} \text{vor}(\ell)) \setminus (\bigcup_{\ell \in \Lambda^i} v_\ell^i)|.$$

186 We note that $\omega_T = 0$ if $T \in \mathcal{T}_h^a \setminus \mathcal{T}_h^i$, $\omega_T = |T|$ if $T \in \mathcal{T}_h^c \setminus \mathcal{T}_h^i$, and $0 \leq \omega_T < |T|$ if $T \in \mathcal{T}_h^i$. The choices of
187 v_ℓ and ω_T satisfy $\sum_{\ell \in \Lambda^{a,i}} v_\ell + \sum_{T \in \mathcal{T}_h} \omega_T = |\Omega_{h,R}|$.

188 Now we are ready to define the generic a/c coupling energy functional \mathcal{E}^h ,

$$189 \quad (9) \quad \mathcal{E}^h(y_h) := \sum_{\ell \in \Lambda^a} V_\ell(y_h) + \sum_{\ell \in \Lambda^i} \omega_\ell V_\ell^i(y_h) + \sum_{T \in \mathcal{T}_h} \omega_T W(\nabla y_h|_T)$$

191 where V_ℓ^i is a modified interface site potential which satisfies consistency conditions (11) and (12). ω_ℓ
192 and ω_T are suitable coefficients, and their construction will be discussed immediately in Section § 2.4
193 and references therein.

194 The goal of a/c coupling is to find

$$195 \quad (10) \quad y_{h,R} \in \arg \min \{ \mathcal{E}^h(y_h) \mid y_h - y^B \in \mathcal{U}_{h,R} \}.$$

196 The subscript R in $y_{h,R}$ and $\mathcal{U}_{h,R}$ can be omitted if there is no confusion.

197 **2.4. Consistent Atomistic/Continuum Formulation.** The construction of the interface po-
198 tential in (10) is the key for the formulation of atomistic/continuum coupling methods. In order to
199 demonstrate the a posteriori error estimate for the generic a/c coupling methods, we shall restrict
200 ourselves to the GRAC type methods [36].

201 **2.4.1. The patch tests and consistent a/c method.** A key condition that has been widely
202 discussed in the a/c coupling literature is that \mathcal{E}^h should exhibit no “ghost forces”. We call this
203 condition the *force patch test*, namely, for $\Lambda = \Lambda^{\text{hom}}$ and $\Phi_\ell = \Phi$,

$$204 \quad (11) \quad \langle \delta \mathcal{E}^h(y^F), v \rangle = 0 \quad \forall v \in \mathcal{U}_h, \quad \mathbf{F} \in \mathbb{R}^{m \times d}.$$

205 In addition, to guarantee that \mathcal{E}^h approximates the atomistic energy \mathcal{E}^a , it is reasonable to require
206 that the interface potentials satisfy an *energy patch test*

$$207 \quad (12) \quad V_\ell^i(y^F) = V(y^F) \quad \forall \ell \in \Lambda^i, \quad \mathbf{F} \in \mathbb{R}^{m \times d}.$$

208 If an a/c method satisfies the patch test (11) and (12), it is called a *consistent a/c method*.

209 **2.4.2. GRAC: Geometric reconstruction based consistent a/c method.** To complete the
210 construction of the consistent a/c coupling energy (9), we must specify the interface region Λ^i and
211 the interface site potential. The geometric reconstruction approach was pioneered by Shimokawa *et al*
212 [44], and then modified and extended in [9, 36]. We refer to [37] for details of the implementation of
213 geometric reconstruction based consistent atomistic/continuum (GRAC) coupling energy for multibody
214 potentials with general interaction range and arbitrary interfaces. The extension of GRAC to 3D is a
215 work in progress [12].

216 For a prototype implementation of GRAC, we consider the 2D triangular lattice $\Lambda^{\text{hom}} := \mathbf{A}\mathbb{Z}^2$
217 with

$$218 \quad (13) \quad \mathbf{A} = \begin{bmatrix} 1 & \cos(\pi/3) \\ 0 & \sin(\pi/3) \end{bmatrix}.$$

219 Let $a_1 = (1, 0)^T$, then $a_j = \mathbf{A}_6^{j-1} a_1$, $j = 1, \dots, 6$, are the nearest neighbour directions in Λ^{hom} ,
220 where \mathbf{A}_6 is the rotation matrix corresponding to a $\pi/3$ clockwise planar rotation.

221 Given the homogeneous site potential $V(Dy(\ell))$, we can represent V_ℓ^i in terms of V . For each
222 $\ell \in \Lambda^i$, $\rho, \varsigma \in \mathcal{R}_\ell$, let $C_{\ell; \rho, \varsigma}$ be free parameters, and define

$$223 \quad (14) \quad V_\ell^i(y) := V\left(\left(\sum_{\varsigma \in \mathcal{R}_\ell} C_{\ell; \rho, \varsigma} D_\varsigma y(\ell)\right)_{\rho \in \mathcal{R}_\ell}\right)$$

224 A convenient short-hand notation is

$$225 \quad V_\ell^i(y) = V(C_\ell \cdot Dy(\ell)), \quad \text{where} \quad \begin{cases} C_\ell := (C_{\ell; \rho, \varsigma})_{\rho, \varsigma \in \mathcal{R}_\ell}, \quad \text{and} \\ C_\ell \cdot Dy := \left(\sum_{\varsigma \in \mathcal{R}_\ell} C_{\ell; \rho, \varsigma} D_\varsigma y\right)_{\rho \in \mathcal{R}_\ell}. \end{cases}$$

226 We name the parameters $C_{\ell;\rho,\varsigma}$ as the *reconstruction parameters*. They are chosen so that the
 227 resulting energy functional \mathcal{E}^h satisfies the energy and force patch tests (11) and (12). A sufficient
 228 (and likely necessary) condition for the energy patch test is that $\mathbf{F} \cdot \mathcal{R}_\ell = C_\ell \cdot (\mathbf{F} \cdot \mathcal{R})$ for all $\mathbf{F} \in \mathbb{R}^{m \times d}$
 229 and $\ell \in \Lambda^i$. This is equivalent to

$$230 \quad (15) \quad \rho = \sum_{\varsigma \in \mathcal{R}_\ell} C_{\ell;\rho,\varsigma} \varsigma, \quad \forall \ell \in \Lambda^i, \quad \rho \in \mathcal{R}_\ell.$$

231 In addition, optimal condition and stabilisation mechanism were proposed in [37] and [29] to improve
 232 the accuracy and stability of GRAC scheme.

233 **2.4.3. Stress formulation.** The stress tensor based formulation can be obtained from the first
 234 variation of the energy. For any $y \in \mathcal{U}$, and $y_h - y^B \in \mathcal{U}_h$, there exist piecewise constant tensor
 235 fields $\sigma^a(y; \cdot) \in P_0(\mathcal{T}_a)^{2 \times 2}$, $\sigma^c(y_h; \cdot) \in P_0(\mathcal{T}_h)^{2 \times 2}$, and $\sigma^h(y_h; \cdot) \in P_0(\mathcal{T}_h)^{2 \times 2}$, such that they satisfy the
 236 following identities

$$237 \quad (16) \quad \langle \delta \mathcal{E}^a(y), v \rangle = \sum_{T \in \mathcal{T}_a} |T| \sigma^a(y; T) : \nabla_T v, \quad \forall v \in \mathcal{U},$$

$$238 \quad (17) \quad \langle \delta \mathcal{E}^c(y_h), v_h \rangle = \sum_{T \in \mathcal{T}_h} |T| \sigma^c(y_h; T) : \nabla_T v_h, \quad \forall v_h \in \mathcal{U}_h,$$

$$239 \quad (18) \quad \langle \delta \mathcal{E}^h(y_h), v_h \rangle = \sum_{T \in \mathcal{T}_h} |T| \sigma^h(y_h; T) : \nabla_T v_h, \quad \forall v_h \in \mathcal{U}_h.$$

241 here \mathcal{T}_a is the micro-triangulation induced by the reference lattice Λ . We call σ^a an *atomistic stress*
 242 *tensor*, σ^c a *continuum stress tensor*, and σ^h an *a/c stress tensor*. For the nearest neighbour inter-
 243 actions, we can choose the following atomistic stress tensor, continuum stress tensor, and a/c stress
 244 tensor respectively from the first variations (16)-(18),

$$245 \quad (19) \quad \sigma^a(y; T) := \frac{1}{\det \mathbf{A}} \sum_{b=(\ell, \ell+\rho) \in \partial T \cap \mathcal{B}} \partial_\rho V_\ell \otimes a_\rho,$$

$$246 \quad (20) \quad \sigma^c(y_h; T) := \partial W(\nabla_T y_h) = \frac{1}{\det \mathbf{A}} \sum_{j=1}^6 \partial_j V(\nabla_T y_h) \otimes a_j,$$

$$247 \quad (21) \quad \sigma^h(y_h; T) := \sum_{b=(\ell, \ell+\rho) \in \partial T \cap \mathcal{B}} \partial_\rho V_\ell^h(I_a y_h) \otimes a_\rho + \omega_T \sigma^c(y_h; T).$$

249 We call piecewise constant tensor field $\sigma \in P_0(\mathcal{T})^{2 \times 2}$ *divergence free* if

$$250 \quad \sum_{T \in \mathcal{T}} |T| \sigma(T) : \nabla_T v \equiv 0, \quad \forall v \in (P_1(\mathcal{T}))^2.$$

251 By definitions (18), it is easy to know that the force patch test condition (11) is equivalent to that
 252 $\sigma^h(\mathbf{F}x)$ is divergence free for any constant deformation gradient \mathbf{F} .

253 The discrete divergence free tensor fields over the triangulation \mathcal{T} can be characterized by the
 254 non-conforming Crouzeix-Raviart finite elements [36, 28]. The Crouzeix-Raviart finite element space
 255 over \mathcal{T} is defined as

$$256 \quad N_1(\mathcal{T}) = \left\{ c : \bigcup_{T \in \mathcal{T}} \text{int}(T) \rightarrow \mathbb{R} \mid c \text{ is piecewise affine w.r.t. } \mathcal{T}, \text{ and} \right.$$

$$257 \quad \left. \text{continuous in edge midpoints } q_f, \forall f \in \mathcal{F} \right\}$$

259 The following lemma in [36] characterizes the discrete divergence-free tensor field.

260 LEMMA 2.3. A tensor field $\sigma \in \mathbf{P}_0(\mathcal{T})^{2 \times 2}$ is divergence free if and only if there exists a constant
 261 $\sigma_0 \in \mathbb{R}^{2 \times 2}$ and a function $c \in N_1(\mathcal{T})^2$ such that

$$262 \quad \sigma = \sigma_0 + \nabla c \mathbf{J}, \quad \text{where } \mathbf{J} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \in \text{SO}(2).$$

263

264 The immediate corollary provides a representation of the stress tensor.

265 COROLLARY 2.4. The stress tensors in the definitions (16)-(18) are not unique. Given any stress
 266 tensor $\sigma \in \mathbf{P}_0(\mathcal{T})^{2 \times 2}$ satisfies one of the definitions (16)-(18), where \mathcal{T} is the corresponding triangulation.
 267 Define the admissible set as $\text{Adm}(\sigma) := \{\sigma + \nabla c \mathbf{J}, c \in N_1(\mathcal{T})^2\}$, then any $\sigma' \in \text{Adm}(\sigma)$ satisfies
 268 the definition of stress tensor.

269 **2.4.4. A Priori Error Estimates.** In the analytical framework proposed in [20, 11], the numerical
 270 error can be split into 3 parts: the *modeling error* due to the discrepancy between the atomistic
 271 model and the continuum model at the interface and the finite element edges, the *coarsening error* due
 272 to finite element discretization of the solution space in the continuum region, and the *truncation error*
 273 due to the finite size of the computational domain. It is proven in [11] that there exists a strongly
 274 stable solution $y_{h,R}$ to (10) and a constant $C^{\text{a-priori}}$ for GRAC method such that,

$$275 \quad (22) \quad \|\nabla u_{h,R} - \nabla u\|_{L^2} \leq C^{\text{a-priori}} (\|hD^2u\|_{\ell^2(\Lambda \cap (\Omega_R^c))} + \|Du\|_{\ell^2(\Lambda \setminus B_{R/2})})$$

276 where $u_{h,R} = y_{h,R} - y^B$.

277 With the generic decay property (8), and the following quasi-optimal conditions:

278 • the radius of the atomistic region $\mathcal{T}_{h,R}^a$ satisfies,

$$279 \quad (23) \quad \underline{C}R_a^{1+2/d} \leq R \leq \overline{C}R_a^{1+2/d},$$

280 • $\mathcal{T}_{h,R}^c$ is a graded mesh so that the mesh size function $h(x) = \text{diam}(T)$ for $x \in T \in \mathcal{T}_{h,R}^c$ satisfies,

$$281 \quad (24) \quad |h(x)| \leq C^{\text{mesh}} \left(\frac{|x|}{R_a}\right)^\beta, \quad \text{with } 1 < \beta < \frac{d+2}{2}.$$

282 It holds that there exists a constant $C_0 > 0$, depending on $C^{\text{a-priori}}$, \underline{C} , \overline{C} , C^{mesh} , and β such that
 283 for R sufficiently large,

$$284 \quad (25) \quad \|\nabla u_{h,R} - \nabla u\|_{L^2} \leq C_0 R^{-d/2-1}.$$

285 In particular, when $d = 2$, and when P1 finite elements are used in the continuum region, we have,

$$286 \quad (26) \quad \|\nabla u_{h,R} - \nabla u\|_{L^2} \leq C_0 N^{-1},$$

287 where N is the overall degrees of freedom.

288 **3. Error Analysis.** We present the a posteriori error analysis in this section. In § 3.1, we derive
 289 the residual estimate for the consistent GRAC a/c coupling scheme introduced in § 2.4. Then, we give
 290 a lower bound for the stability constant which is computable from the a/c solution u_h in § 3.2. Finally,
 291 we put forward the main results Theorem 3.7 and Theorem 3.9 in § 3.3.

292 **3.1. Residual Estimate.** To be more precise, we restrict ourselves to the case of nearest neigh-
 293 bour multibody interactions, namely, we use the so-called "grac23" method introduced in [36] as the
 294 a/c coupling mechanism. We will extend the formulation to general short-range multibody interactions
 295 in a future work and discuss it briefly in § 5.

296 For lattice function $u : \Lambda \rightarrow \mathbb{R}^m$, we denote its continuous and piecewise affine interpolant with
 297 respect to the micro-triangulation \mathcal{T}_a by $I_a u$. Notice that Λ is a lattice with defect, we can construct the

298 piecewise interpolant with respect to Λ^{hom} by extending u to vacancy sites, which will be introduced
 299 in § Appendix A. Identifying $u = I_a u$, we can define the (piecewise constant) gradient $\nabla u = \nabla I_a u : \mathbb{R}^m \rightarrow \mathbb{R}^{m \times d}$ and the spaces of compact and finite energy displacements, respectively, by

$$300 \quad \mathcal{U}^c := \{u : \Lambda \rightarrow \mathbb{R}^m \mid \text{supp}(\nabla u) \text{ is compact}\}.$$

302 It can be shown that that \mathcal{U}^c is dense in $\mathcal{U}^{1,2}$ [11].

303 The first variation of the atomistic variational problem (7) is to find $y - y^B \in \mathcal{U}^{1,2}$ such that

$$304 \quad (27) \quad \langle \delta \mathcal{E}^a(y), v \rangle = 0, \quad \forall v \in \mathcal{U}^{1,2}.$$

305 The first variation of the a/c coupling variational problem (10) is to find $y_h - y^B \in \mathcal{U}_{h,R}$ such that

$$306 \quad (28) \quad \langle \delta \mathcal{E}^h(y_h), v_h \rangle = 0, \quad \forall v_h \in \mathcal{U}_{h,R}.$$

307 We introduce the truncation operator T_R as in [11] by first choosing a C^1 cut-off function $\eta(x) = 1$
 308 for $|x| \leq 4/6$ and $\eta(x) = 0$ for $|x| \geq 5/6$. Define $T_R : \mathcal{U}^{1,2} \rightarrow \mathcal{U}_R$ for $R > 0$ by

$$309 \quad T_R u(\ell) := \eta(\ell/R)(u(\ell) - a_R), \quad \text{where } a_R := \int_{B_{5R/6} \setminus B_{4R/6}} I_a u(x) \, dx,$$

310 where \mathcal{U}_R is defined by

$$311 \quad \mathcal{U}_R := \{u \in \mathcal{U}^c \mid u(x) = 0 \, \forall x \in \Lambda \setminus \Omega_R\}.$$

312 The residual R is defined as an operator on $\mathcal{U}^{1,2}$ which is given by

$$313 \quad (29) \quad R[v] = \langle \delta \mathcal{E}^a(I_a y_h), v \rangle, \quad \forall v \in \mathcal{U}^{1,2}.$$

314 By (28), denote $v_R = T_R v$, and take $v_h = C_h T_R v : \mathcal{U}^{1,2} \rightarrow \mathcal{U}_{h,R}$, where $C_h : \mathcal{U}_R \rightarrow \mathcal{U}_{h,R}$ is the
 315 modified Clément operator [5, 49] whose definition will be made clear in the following subsections. By
 316 (28) we can separate the residual into three groups,

$$\begin{aligned} 317 \quad R[v] &= \langle \delta \mathcal{E}^a(I_a y_h), v \rangle = \langle \delta \mathcal{E}^a(I_a y_h), v \rangle - \langle \delta \mathcal{E}^h(y_h), v_h \rangle \\ 318 &= \langle \delta \mathcal{E}^a(I_a y_h), v \rangle - \langle \delta \mathcal{E}^a(I_a y_h), v_R \rangle \\ 319 &\quad + \langle \delta \mathcal{E}^a(I_a y_h), v_R \rangle - [\delta \mathcal{E}^h(y_h), v_R] \\ 320 &\quad + [\delta \mathcal{E}^h(y_h), v_R] - \langle \delta \mathcal{E}^h(y_h), v_h \rangle. \end{aligned}$$

322 Notice that $v_R \notin \mathcal{U}_{h,R}$, therefore we cannot use the pairing $\langle \delta \mathcal{E}^h(y_h), v_R \rangle$. Instead, we define operation
 323 $[\cdot, \cdot]$ as,

$$\begin{aligned} 324 \quad [\delta \mathcal{E}^h(y_h), v_R] &:= \sum_{T \in \mathcal{T}_h} \int_T \sigma^h(y_h, T) \nabla v_R \, dx \\ 325 &= \sum_{T \in \mathcal{T}_h} \sigma^h(y_h, T) \left(\sum_{T' \in \mathcal{T}_a, T' \cap T \neq \emptyset} |T \cap T'| \nabla v_R \right) \\ 326 \quad (30) &= \sum_{T \in \mathcal{T}_a} |T| \left(\sum_{T' \in \mathcal{T}_h, T' \cap T \neq \emptyset} \frac{|T' \cap T|}{|T|} \sigma^h(y_h, T') \right) \nabla v_R \\ 327 & \end{aligned}$$

328 In the above decomposition of the residual $R[v]$, the first group $R_1 := \langle \delta \mathcal{E}^a(I_a y_h), v \rangle - \langle \delta \mathcal{E}^a(I_a y_h), v_R \rangle$
 329 represents the *truncation error*, the second group $R_2 := \langle \delta \mathcal{E}^a(I_a y_h), v_R \rangle - [\delta \mathcal{E}^h(y_h), v_R]$ represents the
 330 *modeling error*, and the third group $R_3 := [\delta \mathcal{E}^h(y_h), v_R] - \langle \delta \mathcal{E}^h(y_h), v_h \rangle$ represents the *coarsening error*.
 331 We will deal with the contributions from those three groups separately in the following subsections.

332 *Remark 3.1.* Those residual estimators R_1 , R_2 and R_3 are based on first variation of the energies,
 333 and can be in turn represented by stress formulation. By Lemma 2.3 and Corollary 2.4, the stresses
 334 are unique up to a divergence-free tensor field. Therefore, we need to minimize those estimators with
 335 respect to divergence-free tensor field, which will be introduced in § 4.1.1.

336 **3.1.1. Truncation error.** To analyze the truncation error R_1 , we need the Lemma 7.3 for the
 337 truncation operator T_R in [11], namely, if the radius of the computational domain R is sufficiently
 338 large (in the nearest neighbour case, we only need $R > 6$), the following estimates hold

$$339 \quad \|Dv_R - Dv\|_{\ell^2} \leq C^{\text{Tr}} \|Dv\|_{\ell^2(\Lambda \setminus B_{R/2})} \quad \forall v \in \mathcal{U}^{1,2},$$

$$340 \quad \|Dv_R\|_{\ell^2} \leq C^{\text{Tr}} \|Dv\|_{\ell^2(\Lambda \cap B_R)} \quad \forall v \in \mathcal{U}^{1,2},$$

342 where $v_R = T_R v$, and C^{Tr} is independent of R .

343 For any $v \in \mathcal{U}^{1,2}$, the stress-based formulation of the first variation (31), the fact that $v_R(\ell) = v(\ell)$
 344 for $|\ell/R| \leq 4/6$, the equivalence of $\|Dv\|_{\ell^2}$ and $\|\nabla v\|_{L^2}$, and Cauchy-Schwarz inequality lead to,

$$345 \quad |\mathbf{R}_1| = |\langle \delta \mathcal{E}^a(I_a y_h), v \rangle - \langle \delta \mathcal{E}^a(I_a y_h), v_R \rangle|$$

$$346 \quad (31) \quad = \left| \sum_{T \in \mathcal{T}_a} \sigma^a(I_a y_h, T) (\nabla v - \nabla v_R) - \sum_{T \in \mathcal{T}_a} \sigma^0(\nabla v - \nabla v_R) \right|$$

$$347 \quad \leq \int_{\Omega_R \setminus B_{R/2}} |(\sigma^a(I_a y_h) - \sigma^0)(\nabla v - \nabla v_R)| \, dx$$

$$348 \quad \leq \|\sigma^a(I_a y_h) - \sigma^0\|_{L^2(\Omega_R \setminus B_{R/2})} \|\nabla v - \nabla v_R\|_{L^2}$$

$$349 \quad (32) \quad \leq C^{\text{Tr}} \|\sigma^a(I_a y_h) - \sigma^0\|_{L^2(\Omega_R \setminus B_{R/2})} \|\nabla v\|_{L^2}$$

351 where σ^0 is divergence-free, i.e. $\sum_{T \in \mathcal{T}_a} \sigma^0(\nabla v - \nabla v_R) = 0$. In this paper, we assume a macroscopic
 352 applied strain $B \in \mathbb{R}^{d \times d}$, hence we can specify $\sigma^0 = \partial W(y^B)$. If we do not have uniform deformation
 353 at far field, for example in the case of nano-indentation, σ^0 can be computed from surface deformation.
 354 Thus, the truncation error estimator η_T is given by

$$355 \quad (33) \quad \eta_T(u_h) := C^{\text{Tr}} \|\sigma^a(I_a u_h) - \sigma^0\|_{L^2(\Omega_R \setminus B_{R/2})}.$$

356 *Remark 3.2.* The numbers $4/6$, $5/6$ in the definition of truncation operator T_R , and consequently
 357 $R/2$ in the estimator η_T are not essential. We can choose different numbers to define an estimator on
 358 a smaller outer domain, but the constant C^{Tr} will increase correspondingly. In practice, since \mathcal{T}_h is a
 359 graded mesh, we can choose the boundary layer of triangles to evaluate η_T .

360 **3.1.2. Modeling error.** In the analysis of the modeling error R_2 , the stress based formulation
 361 of $\langle \delta \mathcal{E}^a(I_a y_h), v_R \rangle$ and the definition of $[\delta \mathcal{E}^h(y_h), v_R]$ (30) lead to,

$$362 \quad |\mathbf{R}_2| := |\langle \delta \mathcal{E}^a(I_a y_h), v_R \rangle - [\delta \mathcal{E}^h(y_h), v_R]|$$

$$363 \quad = \left| \sum_{T \in \mathcal{T}_a} |T| \sigma^a(I_a y_h, T) \nabla v_R - \sum_{T \in \mathcal{T}_a} |T| \left(\sum_{T' \in \mathcal{T}_h, T' \cap T \neq \emptyset} \frac{|T' \cap T|}{|T|} \sigma^h(y_h, T') \right) \nabla v_R \right|$$

$$364 \quad (34) \quad \leq C^{\text{Tr}} \left\{ \sum_{T \in \mathcal{T}_a} |T| \left[\sigma^a(I_a y_h, T) - \sum_{T' \in \mathcal{T}_h, T' \cap T \neq \emptyset} \frac{|T' \cap T|}{|T|} \sigma^h(y_h, T') \right]^2 \right\}^{\frac{1}{2}} \|\nabla v\|_{L^2}.$$

366 As a result, we define the modeling error estimator η_M by,

$$367 \quad (35) \quad \eta_M(y_h) := C^{\text{Tr}} \left\{ \sum_{T \in \mathcal{T}_a} |T| \left[\sigma^a(I_a y_h, T) - \sum_{T' \in \mathcal{T}_h, T' \cap T \neq \emptyset} \frac{|T' \cap T|}{|T|} \sigma^h(y_h, T') \right]^2 \right\}^{\frac{1}{2}}.$$

368 With the canonical choice of σ^a and in (19) and (20), we can see that only those $T \in \mathcal{T}_a$ intersects
 369 with the interface and edges in \mathcal{T}_h^c have nontrivial contributions to η_M .

370 **3.1.3. Coarsening error.** For the coarsening error R_3 , we first observe that

$$371 \quad \mathbf{R}_3 := [\delta \mathcal{E}^h(y_h), v_R] - \langle \delta \mathcal{E}^h(y_h), v_h \rangle,$$

$$372 \quad (36) \quad = \sum_{T \in \mathcal{T}_h} \int_T \sigma^h(y_h, T) (\nabla v_R - \nabla v_h) \, dx.$$

374 Here, we take $v_h = \mathcal{C}_h v_R$, where \mathcal{C}_h is the modified Clément interpolation operator [5, 49]. For
 375 any node $x \in \mathcal{N}_h$ in the triangulation \mathcal{T}_h , let ϕ_x be the nodal basis with respect to x on \mathcal{T}_h , and
 376 $\omega_x = \text{supp}(\phi_x)$ be the support of ϕ_x . The interpolation operator $\mathcal{C}_h : L^1(\Omega_{h,R}) \rightarrow V_h$ can be defined
 377 by,

$$378 \quad \mathcal{C}_h w = \sum_{x \in \mathcal{N}_h \cap \text{Int}(\Omega_h)} w_x \phi_x, \quad \text{where } w_x = \frac{\int_{\omega_x} w \phi_x \, dx}{\int_{\omega_x} \phi_x \, dx}, \forall x \in \mathcal{N}_h.$$

379 By definition, $\mathcal{C}_h w$ satisfies the Dirichlet boundary condition. The Clement interpolation enjoys
 380 the following properties [4, 49], for any element $T \in \mathcal{T}_h$, and any interior edge $f \in \mathcal{F}_h \cap \text{int}(\Omega_{h,R})$,

$$381 \quad (37) \quad \|w - \mathcal{C}_h w\|_{L^2(T)} \leq C_{\mathcal{T}_h} h_T \|\nabla w\|_{L^2(\omega(T))},$$

$$382 \quad (38) \quad \|w - \mathcal{C}_h w\|_{L^2(f)} \leq C'_{\mathcal{T}_h} h_f^{\frac{1}{2}} \|\nabla w\|_{L^2(\omega(f))},$$

384 where h_T is the diameter of T , and h_f is the length of f . The element patch is $\omega(T) := \bigcup_{x \in \mathcal{N}_h \cap T} \omega_x$,
 385 and the edge patch is $\omega(f) := \bigcup_{x \in \mathcal{N}_h \cap f} \omega_x$. The constants $C_{\mathcal{T}_h}$ and $C'_{\mathcal{T}_h}$ depend only on the shape
 386 regularity of \mathcal{T}_h .

387 For notational convenience, we assume that each interior edge $f \in \mathcal{F}_h \cap \text{int}(\Omega_h)$ has a prescribed
 388 orientation. T_f^+ and T_f^- are the triangles on the left hand side and right hand side of the edge f , ν^+
 389 and ν^- are the corresponding outward unit norm vector. The integration by parts of (36) leads to,

$$390 \quad \begin{aligned} \mathbf{R}_3 &= \sum_{T \in \mathcal{T}_h} \int_T \sigma^h(y_h, T) (\nabla v_R - \nabla v_h) \, dx \\ 391 &= \sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} \int_f (\sigma^h(y_h, T_f^+) \nu^+ + \sigma^h(y_h, T_f^-) \nu^-) \cdot (v_R - v_h) \, ds \\ 392 &= \sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} \llbracket \sigma^h \rrbracket_f \cdot \int_{f \in \mathcal{F}_h} (v_R - v_h) \, ds, \end{aligned}$$

395 where $\llbracket \sigma^h \rrbracket_f := \sigma^h(y_h, T_f^+) \nu^+ + \sigma^h(y_h, T_f^-) \nu^-$ denotes the jump of σ^h across the edge f . Cauchy-
 396 Schwarz inequality and the property of Clement interpolation (38) give rise to,

$$397 \quad \begin{aligned} |\mathbf{R}_3| &\leq \sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} \llbracket \sigma^h \rrbracket_f |h_f^{\frac{1}{2}}| \|v_R - v_h\|_{L^2(f)} \\ 398 &\leq C'_{\mathcal{T}_h} \sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} \llbracket \sigma^h \rrbracket_f |h_f| \|\nabla v_R - \nabla v_h\|_{L^2(\omega_f)} \\ 399 &\leq C'_{\mathcal{T}_h} \left(\sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} (h_f \llbracket \sigma^h \rrbracket_f)^2 \right)^{\frac{1}{2}} \left(\sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} \|\nabla v_R - \nabla v_h\|_{L^2(\omega_f)}^2 \right)^{\frac{1}{2}} \\ 400 &\leq \sqrt{3} C'_{\mathcal{T}_h} \left(\sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} (h_f \llbracket \sigma^h \rrbracket_f)^2 \right)^{\frac{1}{2}} \|\nabla v_R - \nabla v_h\|_{L^2(\Omega)} \\ 401 &\leq \sqrt{3} C^{\text{Tr}} C'_{\mathcal{T}_h} \left(\sum_{f \in \mathcal{F}_h \cap \text{int}(\Omega_R)} (h_f \llbracket \sigma^h \rrbracket_f)^2 \right)^{\frac{1}{2}} \|\nabla v\|_{L^2(\Omega)}. \end{aligned}$$

403 The coarse-graining error estimator is then defined as,

$$404 \quad (39) \quad \eta_C(u_h) := \sqrt{3} C^{\text{Tr}} C'_{\mathcal{T}_h} \left(\sum_{f \in \mathcal{F}_h} (h_f \llbracket \sigma^h \rrbracket_f)^2 \right)^{\frac{1}{2}}$$

405 **3.1.4. Residual Estimate.** Combining the above estimates, we have the following theorem for
 406 the residual.

407 **THEOREM 3.3.** For $\forall v \in \mathcal{U}^{1,2}$, let y_h be the a/c solution of variational problem (10), the residual
 408 $R[v] = \langle \delta \mathcal{E}^a(I_a y_h), v \rangle$ can be bounded by the sum of the truncation error (the L^2 norm of the atomistic
 409 stress tensor close to the outer boundary), modeling error (the difference of a/c stress tensor and
 410 atomistic stress tensor), and the coarsening error (jump of a/c stress tensor across interior edges),
 411 namely,

$$412 \quad (40) \quad \langle \delta \mathcal{E}^a(I_a y_h), v \rangle \leq (\eta_T(y_h) + \eta_M(y_h) + \eta_C(y_h)) \|\nabla v\|_{L^2},$$

413 where $\eta_T(y_h)$, $\eta_M(y_h)$ and $\eta_C(y_h)$ are given in (33), (35) and (39) respectively.

414 *Remark 3.4.* All the estimators η_T , η_M and η_C depend on the a/c solution y_h , through their
 415 dependence on the discrete stress tensor $\sigma^h(y_h)$ and $\sigma^a(I_a y_h)$. We can therefore write,

$$416 \quad (41) \quad \eta(y_h) := \tilde{\eta}(\sigma^a(I_a y_h), \sigma^h(y_h)) = \eta_T(y_h) + \eta_M(y_h) + \eta_C(y_h).$$

417 By Remark 3.1 we denote $\text{Adm}(\sigma^h)$, $\text{Adm}(\sigma^a)$ the sets of all possible stress tensors. Therefore, the
 418 desired estimate of the residual is

$$419 \quad (42) \quad \langle \delta \mathcal{E}^a(I_a y_h), v \rangle \leq \min_{\text{Adm}(\sigma^h(y_h)), \text{Adm}(\sigma^a(I_a y_h))} \tilde{\eta}(\sigma^a(I_a y_h), \sigma^h(y_h)) \|\nabla v\|_{L^2}.$$

420 We refer to the exact or approximate minimization of the residual with respect to the admissible
 421 tensor field as “stress tensor correction”, and we will discuss the implementation of stress tensor
 422 correction in detail in § 4.1.1.

423 **3.2. Stability.** In this subsection, we will deduce a computable estimate of the a posteriori sta-
 424 bility constant. Similar as the residual estimate, we restrict ourselves to the case of nearest-neighbour
 425 interaction with vacancies. We follow the stability analysis in [31]. The main difference is: first, we
 426 derive the stability results for the many-body potentials of generic pair functional form (4), while in
 427 [31] only pair interaction potentials are considered; second, in the a posteriori analysis the stability
 428 constant depends on the atomistic Hessian $\delta^2 \mathcal{E}^a$ and the a/c solution u_h , and therefore it is com-
 429 putable, as opposed to the a priori analysis in [31], the stability constant is related to the a/c Hessian
 430 $\delta^2 \mathcal{E}^h$ and the unknown atomistic solution u where certain assumptions for u have to be made.

431 **THEOREM 3.5.** Suppose that the multi-body interaction potential is of the generic pair functional
 432 form (4), we have the following results,

$$433 \quad (43) \quad \langle \delta^2 \mathcal{E}^a(I_a y_h) v, v \rangle \geq \gamma(y_h) \|\nabla v\|_{L^2(\Omega_R)}^2 \quad \forall v \in \mathcal{U},$$

434 where the precise definition of $\gamma(y_h)$ will be given as the analysis proceeds.

435 The proof of Theorem 3.5 can be divided into the following steps:

- 436 1. Write $\delta^2 \mathcal{E}^a(I_a y_h)$ as a quadratic form with nonuniform coefficients defined on the interaction
- 437 bonds;
- 438 2. Use the perturbation arguments (49), (50) to bound $\delta^2 \mathcal{E}^a$ by quantities from a uniform defor-
- 439 mation;
- 440 3. Define the so-called vacancy stability index (53) to further bound $\delta^2 \mathcal{E}^a$ for lattice with defects
- 441 by the stability constant for a uniformly deformed homogeneous lattice;
- 442 4. The stability constant can be obtained through an optimization procedure.

443 Recall that by (2), \mathcal{B} is the collection of all the nearest neighbour bonds in the reference lattice Λ .
 444 Here we define

$$445 \quad (44) \quad \mathbb{B} := \{(\ell, \ell + \rho) : \ell \in \Lambda^{\text{hom}}, \rho \in \mathcal{R}_\ell\}$$

446 to be the collection of all the nearest neighbour bonds in the homogeneous reference lattice Λ^{hom} . To
 447 simplify notation, we use y to denote $I_a y_h$, and Ω to denote Ω_R in the following analysis of this section.

448 **3.2.1. Second variation of the energy.** Using the generic pair functional form multi-body
 449 interaction potential (4) and Remark 2.1, we write out the second variation of the atomistic energy
 450 $\mathcal{E}^a(y) = \sum_{\ell \in \Lambda} V(|Dy(\ell)|)$ as

$$\begin{aligned}
 451 \quad \langle \delta^2 \mathcal{E}^a(y)v, v \rangle &= \sum_{\ell \in \Lambda} \sum_{\rho, \varsigma \in \mathcal{R}_\ell} \partial_{\rho\varsigma} V(|Dy(\ell)|) (D_\rho v(\ell))^T \left(\frac{D_\rho y(\ell)}{|D_\rho y(\ell)|} \otimes \frac{D_\varsigma y(\ell)}{|D_\varsigma y(\ell)|} \right) (D_\varsigma v(\ell)) \\
 452 \quad &+ \sum_{\ell \in \Lambda} \sum_{\rho \in \mathcal{R}_\ell} \frac{\partial_\rho V(|Dy(\ell)|)}{|D_\rho y(\ell)|} (D_\rho v(\ell))^T \left(1 - \frac{D_\rho y(\ell)}{|D_\rho y(\ell)|} \otimes \frac{D_\rho y(\ell)}{|D_\rho y(\ell)|} \right) D_\rho v(\ell) \\
 453 \quad &= \sum_{\ell \in \Lambda} \sum_{\rho \in \mathcal{R}_\ell} \frac{\partial_{\rho\rho} V(|Dy(\ell)|)}{|D_\rho y(\ell)|^2} (D_\rho y(\ell) \cdot D_\rho v(\ell))^2 \\
 454 \quad &+ \sum_{\ell \in \Lambda} \sum_{\rho, \varsigma \in \mathcal{R}_\ell, \rho \neq \varsigma} \frac{\partial_{\rho\varsigma} V(|Dy(\ell)|)}{|D_\rho y(\ell)| |D_\varsigma y(\ell)|} (D_\rho y(\ell) \cdot D_\rho v(\ell)) (D_\varsigma y(\ell) \cdot D_\varsigma v(\ell)) \\
 455 \quad (45) \quad &+ \sum_{\ell \in \Lambda} \sum_{\rho \in \mathcal{R}_\ell} \frac{\partial_\rho V(|Dy(\ell)|)}{|D_\rho y(\ell)|^3} |D_\rho y(\ell) \times D_\rho v(\ell)|^2, \\
 456
 \end{aligned}$$

457 where $\partial_\rho V(|Dy(\ell)|)$ represents the first order partial derivatives of $V(|Dy(\ell)|)$ with respect to $|D_\rho y(x)|$,
 458 and $\partial_{\rho\varsigma} V(|Dy(\ell)|)$ represents the second order partial derivatives with respect to $|D_\rho y(\ell)|$ and $|D_\varsigma y(\ell)|$,
 459 I is the identity matrix, and $a \times b = a_1 b_2 - a_2 b_1$. We have also used the identity

$$\begin{aligned}
 460 \quad &h_1^T \left(\frac{r_1}{|r_1|} \otimes \frac{r_2}{|r_2|} \right) h_2 = \left(h_1 \cdot \frac{r_1}{|r_1|} \right) \left(h_2 \cdot \frac{r_2}{|r_2|} \right), \\
 461 \quad (46) \quad &\text{and } h^T \left(1 - \frac{r}{|r|} \otimes \frac{r}{|r|} \right) h = |h \times \frac{r}{|r|}|^2. \\
 462
 \end{aligned}$$

463 For nearest neighbour interactions, $|\mathcal{R}(\ell)| \leq 6$, we define

$$\begin{aligned}
 464 \quad C_{\ell, \rho}^1 &= \frac{\partial_{\rho\rho} V(Dy(\ell))}{|D_\rho y(\ell)|^2}, \quad C_{\ell, \rho}^2 = 0 \wedge \min_{\varsigma, \varsigma \neq \rho} \frac{\partial_{\rho\varsigma} V(Dy(\ell))}{|D_\rho y(\ell)| |D_\varsigma y(\ell)|}, \\
 465 \quad C_{\ell, \rho} &= \min_{\ell} (C_{\ell, \rho}^1 - 5C_{\ell, \rho}^2), \quad C_{\ell, \rho}^\perp = \frac{\partial_\rho V(Dy(\ell))}{|D_\rho y(\ell)|^3}. \\
 466
 \end{aligned}$$

467 Applying Cauchy-Schwarz inequality to (45), we obtain the following estimate,

$$\begin{aligned}
 468 \quad \langle \delta^2 \mathcal{E}^a(y)v, v \rangle &\geq \sum_{\ell \in \Lambda} \sum_{\rho \in \mathcal{R}_\ell} C_{\ell, \rho} |D_\rho y(\ell) \cdot D_\rho v(\ell)|^2 + \sum_{\ell \in \Lambda} \sum_{\rho \in \mathcal{R}_\ell} C_{\ell, \rho}^\perp |D_\rho y(\ell) \times D_\rho v(\ell)|^2 \\
 469 \quad &= \sum_{b \in \mathcal{B}} C_b |D_b y(\ell) \cdot D_b v(\ell)|^2 + \sum_{b \in \mathcal{B}} C_b^\perp |D_b y(\ell) \times D_b v(\ell)|^2 \\
 470 \quad &\geq C \sum_{b \in \mathcal{B}} |D_b y(\ell) \cdot D_b v(\ell)|^2 + C^\perp \sum_{b \in \mathcal{B}} |D_b y(\ell) \times D_b v(\ell)|^2 \\
 471 \quad (47) \quad &= C \sum_{b \in \mathcal{B}} \int_b |D_b y \cdot \nabla_b v|^2 \, db + C^\perp \sum_{b \in \mathcal{B}} \int_b |D_b y \times \nabla_b v|^2 \, db. \\
 472
 \end{aligned}$$

473 where $C_b := C_{\ell, \rho}$ and $C_b^\perp := C_{\ell, \rho}^\perp$ for $b = (\ell, \ell + \rho)$, $C^{(\perp)} := \min_{b \in \mathcal{B}} C_b^{(\perp)}$ (here we use $C^{(\perp)}$ to denote
 474 both C and C^\perp for brevity). We have also used the fact that for nearest neighbour interactions,
 475 $D_b v = \nabla_b v(x)$, $\forall x \in \text{int}(b)$, and $D_b y = D_b y(\ell)$ is a constant for each $b = (\ell, \ell + \rho) \in \mathcal{B}$.

476 **3.2.2. The perturbation argument.** Our next task is to obtain the estimates,

$$477 \quad (48) \quad C \sum_{b \in \mathcal{B}} \int_b |D_b y \cdot \nabla_b v|^2 \, db \geq c \|\nabla v\|_{L^2(\Omega)}^2, \quad \text{and } C^\perp \sum_{b \in \mathcal{B}} \int_b |D_b y \times \nabla_b v|^2 \, db \geq c^\perp \|\nabla v\|_{L^2(\Omega)}^2,$$

478 for some $c > 0$ and c^\perp (which could be negative).

479 (48) is not straightforward since $D_b y$ varies on each $b \in \mathcal{B}$. To tackle this issue, we use the following
480 perturbation results from Lemma 6.3 of [31]. For $g \in \mathbb{R}^2$, $b \in \mathcal{B}$, and $\alpha > 0$, we have

$$481 \quad (49) \quad \left| |D_b y \cdot g|^2 - |\mathbf{B}\rho_b \cdot g|^2 \right| \leq \alpha |\mathbf{B}\rho_b \cdot g|^2 + \left(1 + \frac{1}{\alpha}\right) \Delta^2 |\rho_b|^2 |\mathbf{B}^T g|^2,$$

$$482 \quad (50) \quad \text{and} \quad \left| |D_b y \times g|^2 - |\mathbf{B}\rho_b \times g|^2 \right| \leq \alpha^\perp |\mathbf{B}\rho_b \times g|^2 + \left(1 + \frac{1}{\alpha^\perp}\right) \Delta^2 |\rho_b|^2 |\mathbf{B}^T g^\perp|^2.$$

484 where ρ_b is the direction vector of b , $\mathbf{B} \in \mathbb{R}^{2 \times 2}$ is fixed, $\alpha^{(\perp)}$ are unknowns to be determined, and
485 $\Delta = \max_{T \in \mathcal{T}} \|\mathbf{B}^{-1} \nabla y|_T - \mathbf{I}\|$, g^\perp is obtained by $\pi/2$ counterclockwise rotation of g .

486 Given y , Δ and \mathbf{B} can be solved from the convex optimization problem $\Delta = \max_{T \in \mathcal{T}} \|\mathbf{B}^{-1} \nabla y|_T - \mathbf{I}\|$.
487 We will choose free parameters α and α^\perp in the subsequent analysis to keep the estimate of the stability
488 constant sharp. Applying (49) and (50) to (47), taking the same α and α^\perp for each bond $b \in \mathcal{B}$ and
489 using the fact that $|\rho_b| = 1$, we obtain

$$\begin{aligned} 490 & C \sum_{b \in \mathcal{B}} \int_b |D_b y \cdot \nabla_b v|^2 \, db + C^\perp \sum_{b \in \mathcal{B}} \int_b |D_b y \times \nabla_b v|^2 \, db \\ 491 & \geq C \sum_{b \in \mathcal{B}} \int_b |\mathbf{B}\rho_b \cdot \nabla_b v|^2 \, db + C^\perp \sum_{b \in \mathcal{B}} \int_b |\mathbf{B}\rho_b \times \nabla_b v|^2 \, db \\ 492 & \quad - \left(\alpha |C| \sum_{b \in \mathcal{B}} \int_b |\mathbf{B}\rho_b \cdot \nabla_b v|^2 \, db + \alpha^\perp |C^\perp| \sum_{b \in \mathcal{B}} \int_b |\mathbf{B}\rho_b \times \nabla_b v|^2 \, db \right. \\ 493 & \quad \left. + \Delta^2 C \left(1 + \frac{1}{\alpha}\right) \sum_{b \in \mathbb{B}} \int_b |\mathbf{B}^T \nabla_b v|^2 \, db + \Delta^2 C^\perp \left(1 + \frac{1}{\alpha^\perp}\right) \sum_{b \in \mathbb{B}} \int_b |\mathbf{B}^T \nabla_b v^\perp|^2 \, db \right) \\ 494 & = \tilde{C} \sum_{b \in \mathcal{B}} \int_b |\rho_b \cdot \nabla_b v_{\mathbf{B}}|^2 \, db + \tilde{C}^\perp \sum_{b \in \mathcal{B}} \int_b |\rho_b \times \nabla_b v_{\mathbf{B}}|^2 \, db \\ 495 & \quad - \left(\Delta^2 C \left(1 + \frac{1}{\alpha}\right) \sum_{b \in \mathbb{B}} \int_b |\mathbf{B}^T \nabla_b E v|^2 \, db + \Delta^2 C^\perp \left(1 + \frac{1}{\alpha^\perp}\right) \sum_{b \in \mathbb{B}} \int_b |\mathbf{B}^T \nabla_b E v^\perp|^2 \, db \right) \end{aligned}$$

497 where $\tilde{C}^{(\perp)} := C^{(\perp)} - \alpha |C^{(\perp)}|$, we have used $\mathbf{B}^T \nabla_b v = \nabla_b \mathbf{B}^T v$, $\mathbf{B}\rho_b \cdot \nabla_b v = \rho_b \cdot \mathbf{B}^T \nabla_b v$, and $v_{\mathbf{B}} := \mathbf{B}^T v$.
498 $E v$ is the extension of v from Λ to the vacancy sites defined in the Appendix § A, it is clear that
499 $E v^\perp = (E v)^\perp$.

500 Let

$$501 \quad \langle \tilde{H} v, v \rangle := \tilde{C} \sum_{b \in \mathcal{B}} \int_b |\rho_b \cdot \nabla_b v_{\mathbf{B}}|^2 \, db + \tilde{C}^\perp \sum_{b \in \mathcal{B}} \int_b |\rho_b \times \nabla_b v_{\mathbf{B}}|^2 \, db$$

502 and

$$\begin{aligned} 503 \quad \langle \tilde{\mathcal{L}}^{(\perp)} v, v \rangle & := C^{(\perp)} \left(1 + \frac{1}{\alpha^{(\perp)}}\right) \sum_{b \in \mathbb{B}} \int_b |\mathbf{B}^T \nabla_b E v^{(\perp)}|^2 \, db \\ 504 \quad (51) \quad & = \tilde{L}^{(\perp)} \|\nabla(\mathbf{B}^T E v^{(\perp)})\|_{L^2(\Omega)}^2. \end{aligned}$$

506 where $\tilde{L}^{(\perp)} = \frac{3}{\det \mathbf{A}_6} \left(1 + \frac{1}{\alpha^{(\perp)}}\right) C^{(\perp)}$. (51) is due to the application of the so-called bond-density lemma
507 with respect to Dirichlet boundary conditions [41, Lemma 4.5]. Combining the above results, we have
508 the following estimate,

$$509 \quad (52) \quad \langle \delta^2 \mathcal{E}^a(y) v, v \rangle \geq \langle \tilde{H}(y) v, v \rangle - \Delta^2 (\tilde{L} \|\nabla(\mathbf{B}^T E v)\|_{L^2(\Omega)}^2 + \tilde{L}^\perp \|\nabla(\mathbf{B}^T E v^\perp)\|_{L^2(\Omega)}^2)$$

510 **3.2.3. Vacancy stability index.** We introduce the vacancy stability index κ as

$$511 \quad (53) \quad \kappa(\mathbb{V}) = \max \left\{ k > 0 : \Phi_{\mathcal{B}}(u) \geq k \Phi_{\mathbb{B}}(Eu), \forall u \in \mathcal{U} \right\}.$$

512 Since $\tilde{C} > 0$ and \tilde{C}^\perp might be negative, we define the constants

$$513 \quad (54) \quad \bar{C}^{(\perp)} := \min(\tilde{C}^{(\perp)}, \kappa \tilde{C}^{(\perp)}).$$

514 We can further estimate (52) by

$$515 \quad \langle \delta^2 \mathcal{E}^a(y)v, v \rangle \geq \bar{C} \sum_{b \in \mathbb{B}} \int_b |\rho_b \cdot \nabla_b(EB^T v)|^2 db + \bar{C}^\perp \sum_{b \in \mathbb{B}} \int_b |\rho_b \times \nabla_b(EB^T v)|^2 db$$

$$516 \quad (55) \quad - \Delta^2(\tilde{L} \|\nabla(\mathbf{B}^T E v)\|_{L^2(\Omega)}^2 + \tilde{L}^\perp \|\nabla(\mathbf{B}^T E v^\perp)\|_{L^2(\Omega)}^2).$$

517 **3.2.4. Stability of the homogenous lattice.** Now we need the stability estimates for the
519 homogeneous lattice. Let

$$520 \quad (56) \quad \langle \bar{\mathcal{H}}v, v \rangle = \bar{C} \sum_{b \in \mathbb{B}} \int_b |\rho_b \cdot \nabla_b(EB^T v)|^2 db + \bar{C}^\perp \sum_{b \in \mathbb{B}} \int_b |\rho_b \times \nabla_b(EB^T v)|^2 db.$$

521 By Lemma 6.4 of [31], we have

$$522 \quad (57) \quad \langle \bar{\mathcal{H}}v, v \rangle \geq \bar{\gamma} \|\nabla EB^T v\|_{L^2(\Omega)}^2.$$

523 where $\bar{\gamma} := \min(\frac{3}{4}\bar{c} + \frac{9}{4}\bar{c}^\perp, \frac{9}{4}\bar{c} + \frac{3}{4}\bar{c}^\perp)$, and $\bar{c}^{(\perp)} = \frac{3}{\det \mathbf{A}} \bar{C}^{(\perp)}$.

524 Furthermore, by the inequality (79) for the extension operator E in the appendix, we can estimate
525 the stability of atomistic Hessian (55) by,

$$526 \quad (58) \quad \langle \delta^2 \mathcal{E}^a(y)v, v \rangle \geq \gamma(y) \|\nabla v\|_{L^2(\Omega)}^2.$$

527 where

$$528 \quad (59) \quad \gamma(y) = \frac{1}{3} \|\mathbf{B}^{-T}\|_F^{-1} \bar{\gamma} - \Delta^2 \|\mathbf{B}\|_F^2 (\tilde{L} + \tilde{L}^\perp).$$

529 **3.2.5. Numerical Justification.** Tracing back the derivation of the stability constant γ , the
530 only free parameters are α , α^\perp . Consequently, we can find the optimal γ by maximization with
531 respect to α and α^\perp .

532 We justify our a posteriori estimate for the stability constant of the atomistic Hessian numerically.
533 We apply the same EAM potential as in § 4.2 and take isotropic stretch S and shear loading γ_{II} by
534 setting

$$535 \quad \mathbf{B} = \begin{pmatrix} 1 + S & \gamma_{II} \\ 0 & 1 + S \end{pmatrix} \cdot \mathbf{F}_0.$$

536 where $\mathbf{F}_0 \propto \mathbf{I}$ minimizing the corresponding Cauchy-Born energy density $W(F)$. The numerical results
537 are listed in the following tables, where λ stands for the smallest eigenvalue of atomistic Hessian, and
538 γ represents the optimal estimate of the stability constant.

539 From the numerical results, our estimates indeed give lower bound of the minimal eigenvalue of
540 atomistic Hessian, however, the estimate may become negative when the deformation and number of
541 vacancy sites increase.

542 **3.3. Main results.** We present the main theorems for the a posteriori errors in H^1 norm and
543 energy in this section.

number of vacancies	0	1	2
λ	17.436	14.107	12.905
γ	5.284	2.206	1.451

Table 1: In this example, we test the stability for the reference configuration, namely, $S = \gamma_{II} = 0$. The degrees of freedom of the atomistic model is about 3×10^4 .

number of vacancies	0	1	2
λ	11.125	9.809	8.946
γ	3.159	0.468	-0.258

Table 2: In this example, we test the stability for the deformed configuration with $S = \gamma_{II} = 0.03$. The degrees of freedom of the atomistic model is about 3×10^4 .

544 **3.3.1. A Posteriori Error Estimates in H^1 norm.** We will need the following quantitative
545 version of the inverse function theorem in [20].

546 **LEMMA 3.6.** *Let X be a Hilbert space, $w_0 \in X$, $R, M > 0$, and $E \in C^2(B_R^X(w_0))$ with Lipschitz
547 continuous Hessian, $\|\delta^2 E(x) - \delta^2 E(y)\|_{L(X, X^*)} \leq M\|x - y\|_X$ for $x, y \in B_R^X(w_0)$. Suppose, moreover,
548 that there exists constants $c, r > 0$, such that*

$$549 \quad (60) \quad \langle \delta^2 E(w_0)v, v \rangle \geq c\|v\|_X^2, \quad \|\delta E(w_0)\|_{X^*} \leq r, \quad \text{and } 2Mrc^{-2} < 1.$$

550 *Then there exists a unique $\bar{w} \in B_{2rc^{-1}}^X(w_0)$ with $\delta E(\bar{w}) = 0$ and*

$$551 \quad \langle \delta^2 E(\bar{w})v, v \rangle \geq (1 - 2Mrc^{-2})c\|v\|_X^2.$$

552 Take $X = \mathcal{U}_h$, w_0 as the a/c solution y_h of (28), and M as the Lipschitz constant of $\delta^2 \mathcal{E}^a$. Combine
553 the residual estimate in Theorem 3.3, stability estimate in Theorem 3.5, and Lemma 3.6, we have the
554 following theorem for the a posteriori existence and error estimate.

555 **THEOREM 3.7.** *Let y_h be the a/c solution of (28), $\eta(y_h)$ be the residual defined in (41), $\gamma(y_h)$ be
556 the stability constant defined in (59), and M be the Lipschitz constant of $\delta^2 \mathcal{E}^a$. Under the assumption
557 that $\gamma(y_h) > 0$ and $2M\eta(y_h) < \gamma(y_h)^2$, there exists a unique y satisfying $y - y^B \in \mathcal{W}^{1,2}$ which solves
558 the atomistic variational problem (27), and satisfies the following error bound,*

$$559 \quad (61) \quad \|\nabla I_a y_h - \nabla y\|_{L^2} \leq 2 \frac{\eta(y_h)}{\gamma(y_h)},$$

560 *and the strong stability condition,*

$$561 \quad (62) \quad \langle \delta^2 E(y)v, v \rangle \geq \left(1 - 2 \frac{M\eta(y_h)}{\gamma(y_h)^2}\right) \gamma(y_h) \|\nabla v\|_{L^2}^2, \quad \forall v \in \mathcal{W}^{1,2}.$$

562 **Remark 3.8.** Alternatively, the a posteriori error estimate can be deduced by the following argu-
563 ment in [35], but we need to assume the existence of the atomistic solution y and the closeness of y to
564 $I_a y_h$ in $W^{1,\infty}$. By mean value theorem, there exists $\theta \in \text{conv}\{y, I_a y_h\}$ such that

$$565 \quad \langle \delta^2 \mathcal{E}^a(\theta)v, v \rangle = \langle \delta \mathcal{E}^a(I_a y_h), v \rangle - \langle \delta \mathcal{E}^a(y), v \rangle \\ 566 \quad = \langle \delta \mathcal{E}^a(I_a y_h), v \rangle \\ 567 \quad (63) \quad \leq \eta(y_h) \|\nabla v\|_{L^2(\Omega)}.$$

568 Combining the coercivity of \mathcal{E}^a at $I_a y_h$,

$$570 \quad \langle \delta^2 \mathcal{E}^a(I_a y_h)v, v \rangle \geq \gamma(y_h) \|\nabla v\|_{L^2}^2,$$

571 and the Lipschitz continuity (Fréchet differentiability) of $\delta^2 \mathcal{E}^a$, we obtain that

$$572 \quad \langle \delta^2 \mathcal{E}^a(\theta)v, v \rangle \geq \langle \delta^2 \mathcal{E}^a(I_a y_h)v, v \rangle - M \|y - I_a y_h\|_{W^{1,\infty}} \|\nabla v\|_{L^2}^2$$

$$573 \quad (64) \quad \geq (\gamma(y_h) - M \|y - I_a y_h\|_{W^{1,\infty}}) \|\nabla v\|_{L^2}^2$$

575 Let $v = y - I_a y_h$ in (64), using (63), we have

$$576 \quad (65) \quad \|\nabla y - \nabla I_a y_h\|_{L^2} \leq \frac{2\eta(y_h)}{\gamma(y_h)}$$

577 if the closeness assumption $\|\nabla y_h - \nabla y\|_{L^\infty} \leq \frac{\gamma(y_h)}{2M}$ holds true.

578 **3.3.2. A Posteriori Error Estimate for the Energy.** Total energy is an important physical
579 quantity to be approximated in applications. In this section, we will derive an estimate for the energy
580 difference $\mathcal{E}^a(y) - \mathcal{E}^h(y_h)$. The energy difference can be split into the sum of $\mathcal{E}^a(y) - \mathcal{E}^a(I_a y_h)$ and
581 $\mathcal{E}^a(I_a y_h) - \mathcal{E}^h(y_h)$, thus,

$$582 \quad (66) \quad |\mathcal{E}^a(y) - \mathcal{E}^h(y_h)| \leq |\mathcal{E}^a(y) - \mathcal{E}^a(I_a y_h)| + |\mathcal{E}^a(I_a y_h) - \mathcal{E}^h(y_h)|$$

583 For the first part, since \mathcal{E}^a is twice differentiable along the segment $\{(1-s)y + sI_a y_h | s \in (0,1)\}$,
584 we obtain,

$$585 \quad |\mathcal{E}^a(y) - \mathcal{E}^a(I_a y_h)| = \left| \int_0^1 \langle \delta \mathcal{E}^a((1-s)y + sI_a y_h), y - y_h \rangle ds \right|$$

$$586 \quad = \left| \int_0^1 \langle \delta \mathcal{E}^a((1-s)y + sI_a y_h) - \delta \mathcal{E}^a(y), y - I_a y_h \rangle ds \right|$$

$$587 \quad \leq M \|Dy - DI_a y_h\|_{\ell^2}^2$$

$$588 \quad (67) \quad \leq M \|\nabla y - \nabla I_a y_h\|_{L^2}^2.$$

590 which can be further estimated by Theorem 3.7, the constant M is the Lipschitz constant of $\delta^2 \mathcal{E}^a$
591 which is independent of y_h .

592 For the second part, let $\mu_E(y_h) := \mathcal{E}^a(I_a y_h) - \mathcal{E}^h(y_h)$. We can rewrite \mathcal{E}^a in the site based form,

$$593 \quad \mathcal{E}^a(I_a y_h) = \sum_{T \in \mathcal{T}_a} \frac{1}{6} \sum_{\ell \in T \cap \Lambda} V_\ell(I_a y_h).$$

594 Moreover, given \mathcal{E}^h of the form (9), assuming for simplicity $\omega_\ell^i = 1$, and \mathcal{T}_h^i is a few layers of atomistic
595 micro-triangulation around the \mathcal{T}_h^a , which is actually the case for the implementation in [36], we can
596 rewrite \mathcal{E}^h as follows,

$$597 \quad \mathcal{E}^h(y_h) = \sum_{T \in \mathcal{T}_h^a} \frac{1}{6} \sum_{\ell \in T \cap \Lambda^a} V_\ell(I_a y_h) + \sum_{T \in \mathcal{T}_h^a} \frac{1}{6} \sum_{\ell \in T \cap \Lambda^i} V_\ell^i(I_a y_h) +$$

$$598 \quad \sum_{T \in \mathcal{T}_h^i \cap \mathcal{T}_h^c} \left\{ \sum_{\ell \in T \cap \Lambda^i} \frac{1}{6} \sum_{\ell \in T} V_\ell^i(I_a y_h) + \left(1 - \frac{\#\{\ell \in T \cap \Lambda^i\}}{3}\right) |T| W(\nabla I_a y_h) \right\} +$$

$$599 \quad \sum_{T \in \mathcal{T}_h^c \setminus \mathcal{T}_h^i} \sum_{T' \in \mathcal{T}_a, T' \cap T \neq \emptyset} |T \cap T'| W(\nabla I_a y_h).$$

600

Hence μ_E can be expanded as,

$$\begin{aligned}
\mu_E(y_h) &= \sum_{T \in \mathcal{T}_h^a} \frac{1}{6} \sum_{\ell \in T \cap \Lambda^i} (V_\ell(I_a y_h) - V_\ell^i(I_a y_h)) + \\
&\sum_{T \in \mathcal{T}_h^i \cap \mathcal{T}_h^c} \left\{ \sum_{\ell \in T \cap \Lambda^i} \frac{1}{6} \sum_{\ell \in T} V_\ell(I_a y_h) - \sum_{\ell \in T \cap \Lambda} \frac{1}{6} \sum_{\ell \in T} V_\ell^i(I_a y_h) + \right. \\
&\left. \left(1 - \frac{\#\{\ell \in T \cap \Lambda^i\}}{3}\right) |T| W(\nabla I_a y_h) \right\} + \\
&\sum_{T \in \mathcal{T}_h^c \setminus \mathcal{T}_h^i} \sum_{T' \in \mathcal{T}_a, T' \cap T \neq \emptyset} \frac{|T \cap T'|}{|T'|} \left(\frac{1}{6} \sum_{\ell \in T'} V_\ell(I_a y_h) - W(\nabla y_h) \right).
\end{aligned}
\tag{68}$$

We note that the summand in the last term, which is summed over $T \in \mathcal{T}_h^c$, is nonzero only if $\omega(T') \cap \partial T \neq \emptyset$, therefore can be rewritten as

$$\sum_{T \in \mathcal{T}_h^c} \sum_{T' \in \mathcal{T}_a, \omega(T') \cap \partial T \neq \emptyset} \frac{|T \cap T'|}{2|T'|} \left(\frac{1}{3} \sum_{\ell \in T'} V(DI_a y_h(\ell)) - V(\nabla I_a y_h \rho) \right),$$

noticing that $V_\ell = V$ when $T \cap \Lambda^a = \emptyset$.

Hence we have the following theorem,

THEOREM 3.9. *Given the same conditions in Theorem 3.7, the difference of the energy can be bounded by the following inequality,*

$$|\mathcal{E}^a(y) - \mathcal{E}^h(y_h)| \leq C^E (\eta(y_h))^2 + |\mu_E(y_h)|.$$

where $C^E = \frac{4M}{\gamma(y_h)^2}$, $\eta(y_h)$ and $\mu_E(y_h)$ are defined in (41) and (68) respectively.

We denote the energy estimator by

$$\eta_E(y_h) := C^E (\eta(y_h))^2 + |\mu_E(y_h)|.
\tag{69}$$

4. Adaptive Algorithms and Numerical Experiments. In this section, we propose an adaptive mesh refinement algorithm based on the a posteriori error estimates in Theorem 3.7 and Theorem 3.9. Numerical experiments show that our algorithm achieves an optimal convergence rate in terms of accuracy vs. the degrees of freedom, which is the same as the a priori error estimates.

4.1. Adaptive mesh refinement algorithm.. Our goal is to design adaptive refinement algorithms by utilizing the residual based error estimators η_M , η_C , η_T in § 3.1 and μ_E in § 3.3.2. The algorithm follows the usual Solve-Estimate-Mark-Refine procedure as in [8, 48]. However, compared to adaptive mesh refinement algorithms for the numerical solution for continuous PDEs, the major differences are trifold, and to address those differences, we need new ingredients for the implementation of the adaptive algorithm.

- The errors η_M , η_C and η_T depend on u_h through stress tensors σ^h and σ^a which are not unique. Therefore, we have to minimize the error estimator with respect to all the admissible stress tensors, and we call this procedure "stress tensor correction". This will be addressed in § 4.1.1.
- The truncation error η_T is introduced by the truncation of an infinite lattice to a finite domain. If the size of the computation domain is fixed, we shall see the saturation of the numerical error when the degrees of freedom N keep increasing. Therefore, when η_T is dominant in the overall error η , we need to enlarge the computational domain in order to achieve the optimal convergence rate. This will be addressed in § 4.3.2.

- 637 • The modeling error η_M results from the inconsistency of the atomistic model and the contin-
 638 uum model at the interface and finite element edges. In particular, when the interface error is
 639 large, we need to enlarge the atomistic domain Ω^a , and adjust the triangulation in the contin-
 640 uum domain such that the mesh in the continuum region aligns with the micro-triangulation
 641 \mathcal{T}_a close to the interface, and the overall triangulation still maintains good quality. This will
 642 be addressed in Remark 4.3.

643 **4.1.1. Stress tensor correction.** By Theorem 3.3 and Remark 3.4, the error estimators η_T , η_M ,
 644 and η_C depend on the stress tensors σ^h and σ^a , which are unique up to divergence free tensor fields.
 645 Therefore, we need to minimize $\eta(y_h) = \eta_T(y_h) + \eta_M(y_h) + \eta_C(y_h)$ with respect to all the admissible
 646 stress tensors. Recall the "stress tensor correction" of the residual estimate (42),

$$647 \quad (70) \quad \langle \delta \mathcal{E}^a(I_a y_h), v \rangle \leq \min_{c_a \in N_1(\mathcal{T}_a)^2, c_h \in N_1(\mathcal{T}_h)^2} \tilde{\eta}(\sigma^a(I_a y_h) + \nabla c_a \mathbf{J}, \sigma^h(y_h) + \nabla c_h \mathbf{J}) \|\nabla v\|_{L^2}.$$

648 In (70), we need to solve a nonlinear minimization problem with respect to c_a and c_h which are
 649 both defined over whole Ω , the dimension of c_a is $2|\mathcal{F}_h|$, and the dimension of c_h is $2|\mathcal{F}_a|$. The cost for
 650 the exact stress tensor correction is proportional to solving the original energy minimisation problem.

651 Here, we introduce an approximate version of stress tensor correction, which is motivated by the
 652 explicit calculation in [36, Lemma 5.2] as well as the analysis of a/c stress tensor in [28, § 6.2.3]: a
 653 "good" a/c stress tensor can be chosen such that it equals to the atomistic stress tensor in the atomistic
 654 domain, and equals to the continuum stress tensor for uniform deformation. To be precise, we only
 655 need to apply the stress tensor correction to the modelling error η_M ; and in addition, we choose $c_a \equiv 0$,
 656 and $c_h(q_f) = 0$, where q_f is the midpoint of $f \in \mathcal{F}_h$, $f \cap \Lambda_i = \emptyset$. Thus the only degrees of freedom to
 657 be determined are those $c_h(q_f)$ such that $f \cap \Lambda_i \neq \emptyset$.

We propose the following algorithm for approximate stress tensor correction:

Algorithm 1 Approximate stress tensor correction

1. Take $\sigma^a(I_a y_h)$ and $\sigma^h(y_h)$ as the canonical forms in (19) and (21) respectively.
2. Denote q_f as the midpoint of $f \in \mathcal{F}_h$. c_h minimizes the following sum

$$658 \quad (71) \quad \sum_{T \in \mathcal{T}^1} |T| [\sigma^a(I_a y_h, T) - (\sigma^h(I_a y_h, T) + \nabla c_h \mathbf{J})]^2$$

subject to the constraint that $c_h(q_f) = 0$, for $f \cap \Lambda_i = \emptyset$.

3. Let $\sigma^h(y_h) = \sigma^h(y_h) + \nabla c^h \mathbf{J}$, compute η_M , η_T and η_C with $\sigma^a(I_a y_h)$ and $\sigma^h(y_h)$.
-

659 Instead of minimizing the total error estimator η with respect to c_a and c_h as in (70), now we
 660 only need to minimize the modeling error η_M with respect to the degrees of freedom of σ^h adjacent
 661 to the interface. This dramatically reduced the computational cost of "stress tensor correction". In
 662 the implementation, the cost of stress tensor correction is only a small fraction of the total cost, but
 663 it greatly improves the accuracy.

664 We numerically demonstrate the effect of the approximate stress tensor correction in Figure 2. We
 665 fix the computational domain in this example, therefore we expect the "optimal" error will follow the
 666 N^{-1} asymptotics as the degrees of freedom N increase, and get saturated at the level of the truncation
 667 error. Figure 2a shows H^1 errors with respect to degrees of freedom N . If the stress tensor correction
 668 is applied, the error follows the optimal N^{-1} asymptotics before the saturation is reached; if the stress
 669 tensor correction is not applied, the error is suboptimal. Figure 2b shows the error estimator η with
 670 respect to degrees of freedom N . The N^{-1} convergence of η is much more significant with correction;
 671 without correction η may even increase with respect to N .

672 **4.1.2. Local error estimator.** We need to assign global estimators to local elements properly,
 673 then mark and subdivide those elements which contribute most to the estimator.

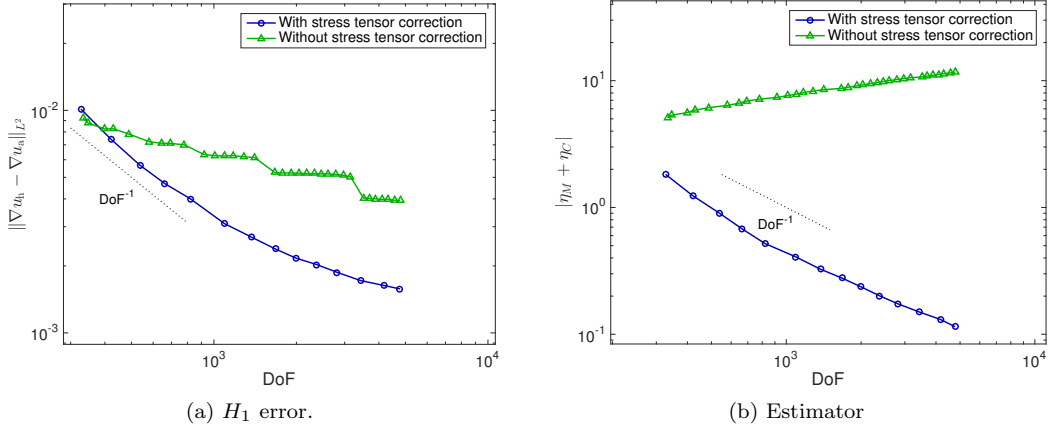


Fig. 2: Effect of approximate stress tensor correction. Divacancy example, $R_c = 1000$, take $\tau_1 = 0.7$ and $\tau_2 = 0.2$ in Algorithm 2. Figure 2a: H_1 error vs. DoF; Figure 2b: $\eta_M + \eta_C$ vs. DoF.

674 Recall the definition of η_M in (35), and after taking the stress tensor correction in Algorithm 1,
 675 we have

$$676 \quad (\eta_M(y_h))^2 := (C^{\text{Tr}})^2 \sum_{T \in \mathcal{T}_a} |T| [\sigma^a(I_a y_h, T) - \sum_{T' \in \mathcal{T}_h, T' \cap T \neq \emptyset} \frac{|T' \cap T|}{|T|} (\sigma^h(y_h, T'))]^2.$$

677 The contribution is 0 for those $T \in \mathcal{T}_a$ located completely inside an element $T' \in \mathcal{T}_h$. As a result, we
 678 need only take care of those $T \in \mathcal{T}_a$ and $T' \in \mathcal{T}_h$ with $T \cap \partial T' \neq \emptyset$. We first define

$$679 \quad \eta_M(T, T') := |T' \cap T| \left[\sigma^a(I_a y_h, T) - \frac{|T' \cap T|}{|T|} (\sigma^h(y_h, T')) \right]^2.$$

680 for $T \in \mathcal{T}_a$, then let $\eta_M(T') = \sum_{T \in \mathcal{T}_a, T \cap T' \neq \emptyset} \eta_M(T, T')$ for $T' \in \mathcal{T}_h$. Notice that $(C^{\text{Tr}})^2 \sum_{T \in \mathcal{T}_h} \eta_M(T) =$
 681 η_M^2 .

682 Analogously, we can define the local contribution of the truncation error $\eta_T(T')$ for $T' \in \mathcal{T}_h$, such
 683 that $\sum_{T' \in \mathcal{T}_h} \eta_T(T') = \eta_T^2$. Please also refer to Remark 3.2.

684 For the coarsening error, recall the definition (39),

$$685 \quad \eta_C(y_h) := \sqrt{3} C^{\text{Tr}} C'_{\mathcal{T}_h} \left(\sum_{f \in \mathcal{F}_h} (h_f \llbracket \sigma \rrbracket)^2 \right)^{\frac{1}{2}},$$

686 we define $\eta_C(T)$ as follows,

$$687 \quad \eta_C(T) = \sqrt{3} C^{\text{Tr}} C'_{\mathcal{T}_h} \sum_{f \in \mathcal{F}_h \cap T \in \mathcal{T}_h} \frac{1}{2} (h_f \llbracket \sigma \rrbracket_f)^2.$$

688 For the energy estimator μ_E from section § 3.3.2, similar to the case of η_M , we can define the local
 689 contributions similarly as $\mu_E(T)$ such that $\sum_{T' \in \mathcal{T}_h} \mu_E^2(T') = \mu_E^2$.

690 Once all the local estimators are assigned, we are ready to define the indicator ρ_T :

$$691 \quad (72) \quad \rho_T = (C^{\text{Tr}})^2 \frac{\eta_M(T)}{\eta_M} + (C^{\text{Tr}})^2 \frac{\eta_T(T)}{\eta_T} + (\sqrt{3} C^{\text{Tr}} C'_{\mathcal{T}_h})^2 \frac{\eta_C(T)}{\eta_C}.$$

692 Notice that the sum of local estimators is equal to the global estimator.

693 Meanwhile, for the energy based estimate, we have,

$$694 \quad (73) \quad \rho_T^E = C^E (C^{\text{Tr}})^2 (\eta_M(T)^2 + \eta_T(T)^2) + C^E (\sqrt{3} C^{\text{Tr}} C'_{\mathcal{T}_h})^2 (\eta_C(T))^2 + |\mu_E(T)|$$

695 The constants C^{Tr} , C^E , $C'_{\mathcal{T}_h}$ in (72) and (73) are not known a priori, instead, we use their empirical
696 estimates in the implementation.

697 Algorithm 2 is the main algorithm for the adaptive mesh refinement, and Dörfler adaptive strategy
698 [8] is used in the algorithm.

Algorithm 2 A posteriori mesh refinement

Step 0 Prescribe Ω_R , \mathcal{T}_h , N_{\max} , ρ_{tol} , τ_1 and τ_2 .

Step 1 *Solve*: Solve the a/c solution y_h of (10) on the current mesh \mathcal{T}_h .

Step 2 *Estimate*: Carry out the stress tensor tensor correction step in Algorithm 1, and compute the error indicator ρ_T for each $T \in \mathcal{T}_h$. For fixed R , we do not need to include the contribution from truncation error η_T in ρ_T . Set $\rho_T = 0$ for $T \in \mathcal{T}_a \cap \mathcal{T}_h$. Compute the degrees of freedom N and total error $\rho = \sum_T \rho_T$. Stop if $N > N_{\max}$ or $\rho < \rho_{\text{tol}}$.

Step 3 Mark:

Step 3.1 : Choose a minimal subset $\mathcal{M} \subset \mathcal{T}_h$ such that

$$\sum_{T \in \mathcal{M}} \rho_T \geq \frac{1}{2} \sum_{T \in \mathcal{T}_h} \rho_T.$$

Step 3.2 : Find the interface elements $\mathcal{M}_i := \{T \in \mathcal{M} : T \cap \Lambda_i \neq \emptyset\}$. Check if

$$(74) \quad \sum_{T \in \mathcal{M}_i} \rho_T \geq \tau_1 \sum_{T \in \mathcal{M}} \rho_T.$$

where tolerance $0 < \tau_1 < 1$. If true, let $\mathcal{M} = \mathcal{M} \setminus \mathcal{M}_i$.

Step 4 *Refine*: If (74) is true, expand interface Λ_i outward by one layer. Then, bisect all elements $T \in \mathcal{M}$. Stop if $\frac{\eta_T}{\eta_M + \eta_C} \geq \tau_2$, otherwise, go to Step 1.

699 *Remark 4.1.* For the calculation with fixed computational domain, the numerical error will saturate
700 at the level of truncation error. The stopping criteria can be modified as:

701 Step 2: ... Compute the convergence rate β of the estimated total error ρ with respect to the
702 degrees of freedom N . Stop if $\beta \leq \tau_2$.

703 *Remark 4.2.* It is possible to use different mark strategies, for example,

704 *Step 3.1*: Choose a minimal subset \mathcal{M} , s.t.

$$705 \quad \rho_T \geq \text{mean}(\rho), \quad \forall T \in \mathcal{M}.$$

706 *Step 3.2* We can find the interface elements which are within k layers of atomistic distance,
707 $\mathcal{M}_i^k := \{T \in \mathcal{M} \cap \mathcal{T}_h^c : \text{dist}(T, \Lambda^i) \leq k\}$. Choose $K \geq 1$, find the first $k \leq K$ such that

$$708 \quad (75) \quad \sum_{T \in \mathcal{M}_i^k} \rho_T \geq \tau_1 \sum_{T \in \mathcal{M}} \rho_T,$$

709 with tolerance $0 < \tau_1 < 1$. If such a k can be found, let $\mathcal{M} = \mathcal{M} \setminus \mathcal{M}_i^k$. Then in step 3, expand interface
710 Λ_i outward by k layers.

711 *Remark 4.3.* After pushing the interface outward in Step 4, we have to 'remove' those triangles in
712 the continuum mesh which overlap with the new atomistic region. It will generate a gap between the
713 atomistic region and the continuum region. We need to triangulate this gap, and adjust the positions
714 of the nodes to improve the quality of the interfacial triangles. In our implementation, we adapted the
715 Matlab package *EasyMesh*, a two-dimensional quality mesh generator to carry out this task [25].

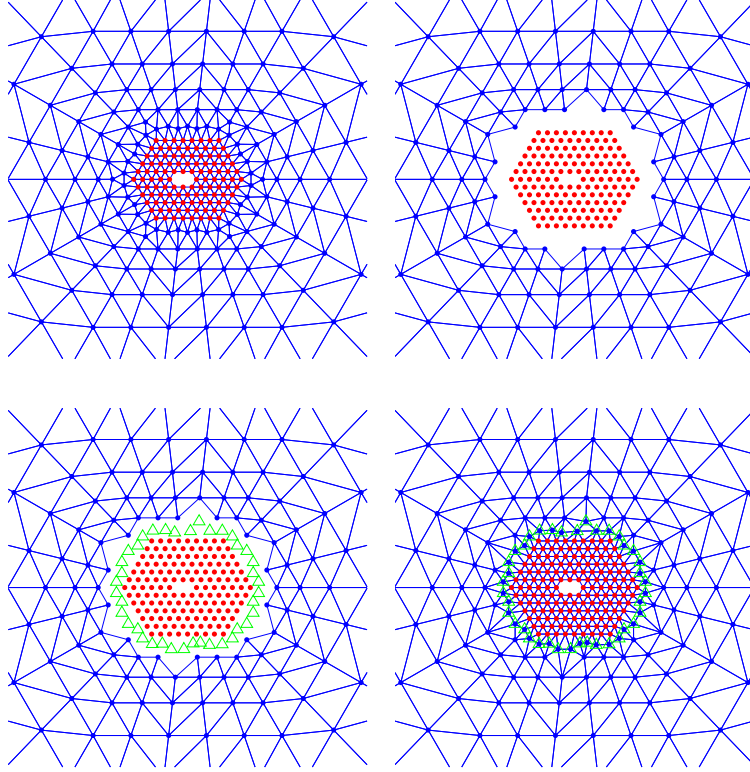


Fig. 3: Snapshots of the expanding interface in Step 4 of Algorithm 2. (Top-left) initial mesh with $R_a = 5$; (Top-right) mesh with $R_a = 6$: after removing the neighboring continuum nodes close to the interface, move the interface outward by 1 layer ; (Bottom-left) generating new continuum nodes (marked with green triangles) and adjusting their positions to maintain the quality of mesh; (Bottom-right) final triangulations.

716 **4.2. Model Problem.** Recall the EAM potential defined in (5). Let

717
$$\phi(r) = \exp(-2a(r-1)) - 2\exp(-a(r-1)), \quad \psi(r) = \exp(-br)$$

718
$$F(\tilde{\rho}) = C [(\tilde{\rho} - \tilde{\rho}_0)^2 + (\tilde{\rho} - \tilde{\rho}_0)^4]$$

719 with parameters $a = 4, b = 3, c = 10$ and $\tilde{\rho}_0 = 6\exp(0.9b)$, which is the same as the numerical
720 experiments in the a priori analysis paper [37].

721 To generate a defect, we remove k atoms from Λ^{hom} ,

722
$$\Lambda_k^{\text{def}} := \{-(k/2)e_1, \dots, (k/2-1)e_1\}, \quad \text{if } k \text{ is even,}$$

723
$$\Lambda_k^{\text{def}} := \{-(k-1)/2e_1, \dots, (k-1)/2e_1\}, \quad \text{if } k \text{ is odd,}$$

724 and $\Lambda = \Lambda^{\text{hom}} \setminus \Lambda_k^{\text{def}}$. See Figure 4 for an illustration.

725 For $\ell \in \Lambda$, consider the nearest neighbour interaction, $\mathcal{N}_\ell := \{\ell' \in \Lambda \mid 0 < |\ell' - \ell| \leq 1\}$, and
726 interaction range $\mathcal{R}_\ell := \{\ell' - \ell \mid \ell' \in \mathcal{N}_\ell\} \subseteq \{a_j, j = 1, \dots, 6\}$. The defect core D^{def} can be defined by
727 $D^{\text{def}} = \{x : \text{dist}(x, \Lambda_k^{\text{def}}) \leq 1\}$, $\Lambda \cap D^{\text{def}}$ is the first layer of atoms around Λ_k^{def} .

728 **4.3. Di-vacancy Example.** In this section, we numerically justify the performance of the pro-
729 posed adaptive mesh refinement algorithm. We take the same di-vacancy example in [37], namely,

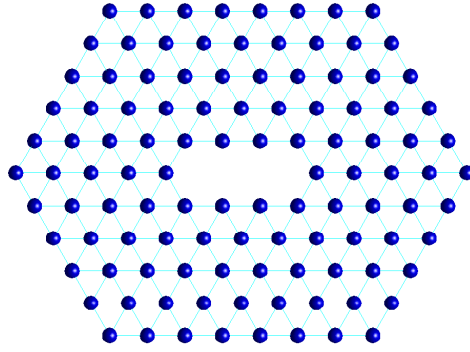


Fig. 4: Illustration of the atomistic lattice Λ with 3 vacancies surrounded by 5 atomistic layers.

732 setting $k = 2$ for Λ_k^{def} . We apply isotropic stretch S and shear γ_{II} by setting

733
$$\mathbf{B} = \begin{pmatrix} 1 + S & \gamma_{II} \\ 0 & 1 + S \end{pmatrix} \cdot \mathbf{F}_0$$

734 where $\mathbf{F}_0 \propto \mathbf{I}$ minimizing the Cauchy-Born energy density W , $S = \gamma_{II} = 0.03$. In our numerical exper-
 735 iments, the reference solution denoted as u_r is solved by GRAC method with a sufficient large mesh
 736 where $R_a = 93$ and $R = 17298$.

737 **4.3.1. Fixed computation domain.** In this subsection, we fix $R = 1000$. The numerical results
 738 are shown in Figure 5 and Figure 6. The red dashed lines in both figures denote the truncation errors
 739 η_T and η_T^2 respectively. The figures show that when N is small, the modelling error and coarsening
 740 error dominates, our results coincide with the optimal a priori convergence rate (N^{-1} for H^1 norm
 741 and N^{-2} for energy, respectively). When N increases, the truncation error becomes dominant, which
 742 results in a suboptimal convergence rate and finally saturates the overall error. These results indicate
 743 that for a fixed computational domain, we can only achieve optimal convergence rate up to a certain
 744 critical degree of freedom. A possible cure is to enlarge the computational domain in order to balance
 745 the truncation error with the modeling and coarsening errors, which motivates the next numerical
 746 experiments.

747 **4.3.2. Adaptive algorithm with automatic control on domain size.** With the estimator
 748 η_T for the truncation error, we can modify the Algorithm 2 to automatically enlarge the computational
 749 domain if the truncation error is dominant in the total error ρ .

750 *Remark 4.4.* In our current implementation, we first generate an initial graded triangulation on
 751 $\Omega_{R_{\max}}$ in a way that it contains the triangulation of a sequence of domains Ω_{R_k} such that $R_0 <$
 752 $R_1 < \dots < R_{\max}$. Therefore, when we need to enlarge the computational domain in Step 4 of the
 753 above algorithm, we simply combine the triangulation for the current domain Ω_{R_k} and the initial
 754 triangulation of $\Omega_{R_{k+1}} \setminus \Omega_{R_k}$ to generate the triangulation for $\Omega_{R_{k+1}}$.

755 From the numerical results in Figures 7 - 8, we can see that with Algorithm 3, it is possible to
 756 change the domain size automatically, and maintain the optimal convergence rate without the error
 757 saturation phenomenon we observed for fixed size computations. The parameter τ_3 can be used to tune
 758 the balance between truncation error and other error contributions. With a smaller τ_3 , the algorithm
 759 tends to enlarge the domain more frequently, while with a larger τ_3 , the algorithm tends to push
 760 outward the atomistic region and refine the coarse mesh more frequently. In the numerical results,
 761 we test two values $\tau_3 = 0.3$ and $\tau_3 = 0.7$. Although there are some small differences, the overall
 762 convergence behaviour looks similar and are comparable to the a priori results.

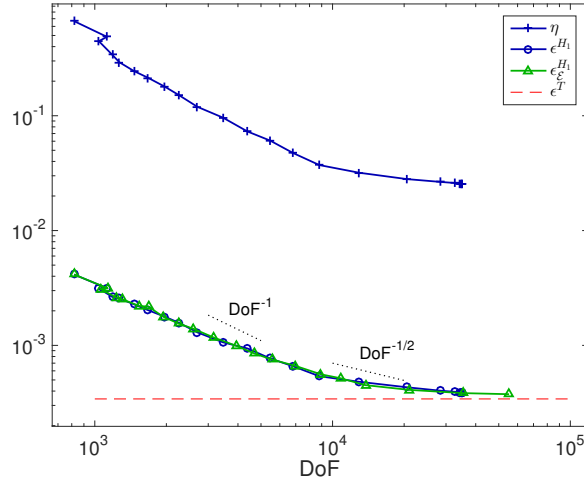


Fig. 5: Numerical results by Algorithm 2 and Remark 4.1 with $R = 1000$, $\tau_1 = 0.7$, $\tau_2 = 0.2$. we denote ϵ^{H_1} as the actual H1 error $\|\nabla u_h - \nabla u_r\|_{L^2}$ with u_h solved by residual estimator driven algorithm, $\epsilon_{\mathcal{E}}^{H_1}$ as the H1 error with solutions solved by energy estimate driven algorithm, ϵ^T the actual residual truncation error.

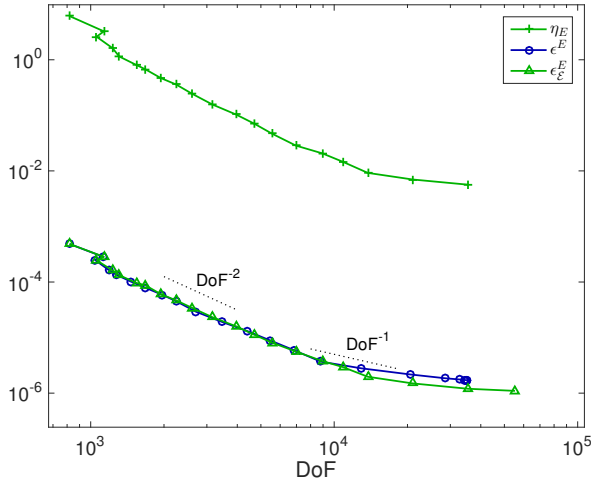


Fig. 6: Numerical results by Algorithm 2 and Remark 4.1 with $R = 1000$, $\tau_1 = 0.7$, $\tau_2 = 0.2$. we denote ϵ^E as the actual energy difference $\|\mathcal{E}^h - \mathcal{E}^r\|_{L^2}$ with u_h solved by residual estimator driven algorithm, $\epsilon_{\mathcal{E}}^E$ as the energy difference with solutions solved by energy estimate driven algorithm, $\epsilon_{\mathcal{E}}^T$ the actual energy truncation error.

Algorithm 3 A posteriori mesh refinement with size control.

Step 0 Prescribe Ω_{R_0} , \mathcal{T}_h , N_{\max} , ρ_{tol} , τ_1 , τ_3 and R_{\max} .

Step 1 *Solve*: Solve the a/c solution $u_{h,R}$ of (10) on the current mesh $\mathcal{T}_{h,R}$.

Step 2 *Estimate*: carry out the stress tensor correction step in Algorithm 1, and compute the error indicator ρ_T for each $T \in \mathcal{T}_h$, including the contribution from truncation error η_T . Set $\rho_T = 0$ for $T \in \mathcal{T}_a \cap \mathcal{T}_h$. Compute the degrees of freedom N , error estimator ρ_T and $\rho = \sum_T \rho_T$. Stop if $N > N_{\max}$ or $\rho < \rho_{\text{tol}}$ or $R > R_{\max}$.

Step 3 Mark:

Step 3.1 : Choose a minimal subset $\mathcal{M} \subset \mathcal{T}_h$ such that

$$\sum_{T \in \mathcal{M}} \rho_T \geq \frac{1}{2} \sum_{T \in \mathcal{T}_h} \rho_T.$$

Step 3.2 : We can find the interface elements which are within k layers of atomistic distance, $\mathcal{M}_i^k := \{T \in \mathcal{M} \cap \mathcal{T}_h^c : \text{list}(T, \Lambda^i) \leq k\}$. Choose $K \geq 1$, find the first $k \leq K$ such that

$$(76) \quad \sum_{T \in \mathcal{M}_i^k} \rho_T \geq \tau_1 \sum_{T \in \mathcal{M}} \rho_T,$$

with tolerance $0 < \tau_1 < 1$. If such a k can be found, let $\mathcal{M} = \mathcal{M} \setminus \mathcal{M}_i^k$. Then in step 3, expand interface Λ_i outward by k layers.

Step 4 *Refine*: If (76) is true, expand interface Λ_i outward by one layer. If $\eta_T \geq \tau_3 \rho$, enlarge the computational domain (details in Remark 4.4) . Bisect all elements $T \in \mathcal{M}$. Go to Step 1.

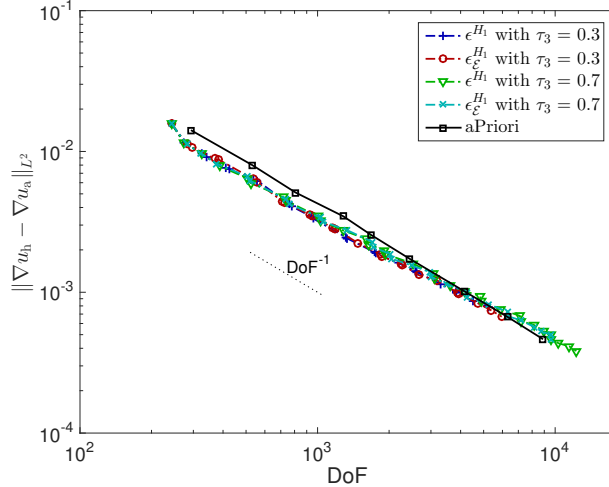


Fig. 7: Numerical results by Algorithm 3 and Remark 4.4: H^1 error vs. Degree of Freedom with $\tau_3 = 0.3$ and $\tau_3 = 0.7$ or both residual estimate driven and energy estimate driven algorithms. The aPriori curve shows the corresponding a priori convergence.

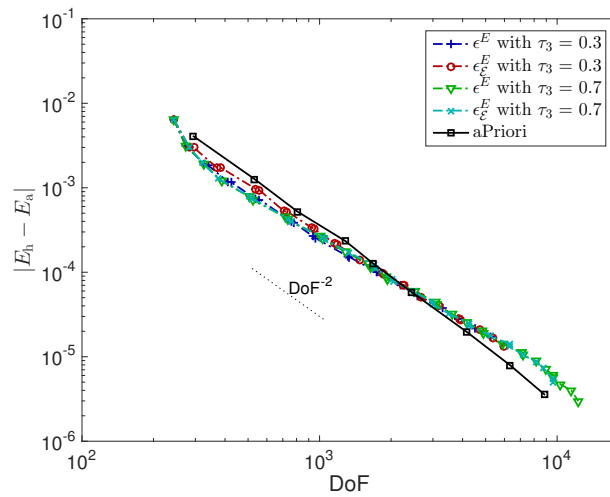


Fig. 8: Numerical results by Algorithm 3 and Remark 4.4: Energy difference vs. Degree of Freedom with $\tau_3 = 0.3$ and $\tau_3 = 0.7$ for both residual estimate driven and energy estimate driven algorithms. The aPriori curve shows the corresponding a priori convergence.

763 **5. Conclusion.** In this paper, we derive rigorous a posteriori error estimates for a class of consist-
 764 tent (ghost force free) atomistic/continuum coupling schemes. Numerical results for the corresponding
 765 adaptive algorithms are comparable to optimal a priori analysis. This opens an avenue for further
 766 mathematical analysis and algorithmic developments for longer range interactions, higher dimensional
 767 problems, and general atomistic/continuum coupling algorithms.

768 For general short range interactions longer than the nearest neighbour, the stress tensor can be
 769 defined using the localization formula and quasi-interplant as in the a priori analysis [28, 30, 33].
 770 The residual estimate can be carried out analogously as in this paper. However, such a stress tensor
 771 is not anymore piecewise constant, and may require complicated geometric operations to evaluate.
 772 Therefore, the numerical implementation is difficult and we are currently pursuing an alternative
 773 approach to define piecewise constant stress tensor field for general short range interactions.

774 The extension to the case of the straight screw dislocation in 2D and point defect case in 3D is
 775 straightforward. More practical problems, for example, the study of dislocation nucleation and dislo-
 776 cation interaction by a/c coupling methods has attracted considerable attention from the early stage
 777 of a/c coupling methods [45, 39]. The difficulty is to deal with boundary condition and complicated
 778 geometry changes of the interface.

779 For general atomistic/continuum coupling schemes, such as BQCE, BQCF and BGFC, the a priori
 780 analysis in [18, 15, 38] provide a general analytical framework and the stress tensor based formulation
 781 plays a key role in the analysis. Therefore, the a posteriori analysis for those coupling schemes can
 782 inherit this analytical framework and the stress tensor formulation. The stress tensor correction method
 783 and other techniques developed in this paper will be essential for the efficient implementation of the
 784 corresponding adaptive algorithms.

785 **Acknowledgement.** The authors thank Christoph Ortner and Huajie Chen for the stimulating
 786 discussions on the adaptive computation of material defects. The authors also thank the referees for
 787 their insightful comments. Their feedback has helped clarify various aspects of our work.

788 Appendix A. Extension to the vacancies.

789 We need to extend v from Λ to Λ^{hom} which includes the vacancy sites. We first define the extension
 790 operator E on \mathcal{U} by

$$791 \quad (77) \quad Eu := \underset{v \in \mathcal{U}, v=u \text{ on } \Lambda}{\operatorname{argmin}} \Phi_{\mathbb{B}}(v) := \operatorname{argmin} \sum_{b \in \mathbb{B}} |\rho_b \cdot D_b v|^2, \quad \forall u \in \mathcal{U},$$

792 where \mathbb{B} defined in (44) is the set of all nearest-neighbour interaction bonds in Λ^{hom} . Notice that for
 793 $v \in \mathcal{U}$, $\|\nabla v\|_{L^2}$ can be properly and uniquely defined by $\|\nabla Ev\|_{L^2}$.

794 It is known from [31, Proposition 4.1] that $\Phi_{\mathbb{B}}(v)$ is equivalent to $\|\nabla v\|_{L^2}^2$ such that,

$$795 \quad (78) \quad \frac{3}{4} \|\nabla v\|_{L^2}^2 \leq \Phi_{\mathbb{B}}(v) \leq \frac{9}{4} \|\nabla v\|_{L^2}^2$$

796 Since $A^{-1}EA v = Ev$ on Λ , by definition of Ev , we have $\Phi_{\mathbb{B}}(A^{-1}EA v) \geq \Phi_{\mathbb{B}}(Ev)$. Combining with
 797 the inequality $\|GH\|_F \leq \|G\|_F \|H\|_F$ for the matrix Frobenius norm and (78), it holds that,

$$\begin{aligned} 798 \quad \|\nabla Ev\|_{L^2}^2 &\leq \frac{4}{3} \Phi_{\mathbb{B}}(Ev) \\ 799 &\leq \frac{4}{3} \Phi_{\mathbb{B}}(A^{-1}EA v) \\ 800 &\leq 3 \|\nabla A^{-1}EA v\|_{L^2}^2 \\ 801 \quad (79) \quad &\leq 3 \|A^{-1}\|_F \|\nabla EA v\|_{L^2}^2. \end{aligned}$$

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