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1 Introduction

1.1 Motivation

Material science, investigating the relationship between the structure of materials at atomic or molecular scales and their macroscopic properties, has driven the development of modern science and technology. Due to the difficulty of observing material phenomena in very small scale (generally nano-scale), it may be impossible to study them through physical experiments. Instead, computational material science comes out by employing numerical simulation to predict the properties of materials. Traditional computational framework in material simulation has been the continuum physical model, where the behaviour or structure of materials is usually characterized by solutions of partial differential equations (PDEs).

However, materials are ultimately comprised of discrete particles, this is an essential feature that had to be included in the material description. For example, crystal defects (see Figure 1) such as grain boundaries, cracks or dislocations requires that the atomistic structure of the defects to be correctly modeled. The fact that real materials are not perfect crystals is critical to materials engineering. If materials were perfect crystals then their properties would be dictated by their composition and crystal structure alone, and would be very restricted in their values and their variety. Yet, it is the possibility of making imperfectly crystalline materials that permits materials scientists to tailor material properties into the diverse combinations that modern engineering devices require. The most important features of the microstructure of an engineering material are the crystalline defects that are manipulated to control its behavior.

![Different defects](image)

(a) Point defects  (b) Edge dislocations  (c) Crack

Figure 1: Different defects

The primary step to simulation of crystal defects is to model the physical process in mathematics. It is impossible, however, to use only atomistic models to simulate all material properties because of the sheer number of atoms that would be required for such a simulation. Fortunately, since defects occupy only a small proportion of bulk crystals, it is more advisable to model the elastic field using more efficient continuum models wherever they are reasonable to apply. Much research has already occurred in the field of coupling the atomistic model around a defect to a continuum model further away (so called ‘a/c coupling’). We however notice an important distinction in this field: the continuum elasticity models, according to the strength of deformation, can be divided into two classes: nonlinear elasticity model and linear elasticity model.

This project is devoted to propose an optimized coupling mechanism between not only atomistic and continuum, but rather between the (now distinct) atomistic and nonlinear continuum, or atomistic and linear elastic continuum. We also may further consider even a full atomistic/nonlinear/linear coupling. The distinction should provide many benefits in accuracy and efficiency as linear theories are prolific areas of research and a there are often many strong methods that may only be applied to linear elastic
equations (many more so than the nonlinear field), so our crystal defects may be simulated more effectively. Also, computationally we are of course seeking more efficient models, and linear models are the least computationally complex models you could consider, thus coupling should provide a more efficient implementation.

1.2 Mathematical Modeling

Many mathematicians and engineers are researching the development of atomistic-to-continuum coupling (a/c coupling) mechanisms to gain insight to material science problems accurately and efficiently. In this subsection, we firstly provide a brief overview of atomistic models and its continuum approximations.

1.2.1 Atomistic Model

We begin by defining some notation. Consider a two dimensional Bravais lattice given by \( \Lambda = AZ^2 \). For simplicity we take the square lattice, so that \( A = Id \). We then add a defect, an alteration of \( \mathbb{Z}^2 \). This generates a reference lattice and the lattice interactions—how atoms in the lattice will affect each other. Centered on 0 where possible. To fully specify an atomistic system we need both the lattice structure, types of defects. A simple example is a homogeneous deformation of \( \Lambda \), given by

\[
\begin{align*}
\phi : & \Lambda \\
\phi : & \Lambda \\
\end{align*}
\]

We denote the set of differences \( \{ \ell' \in \Lambda : |\ell' - \ell| \leq \text{rcut} \} \). We allow the atoms inside some cut-off radius \( \text{rcut} \) to interact, and denote an atom’s interaction set by \( \mathcal{N}_\ell := \mathcal{N}_\ell \setminus \{ \ell \} \).

We denote the set of differences \( \mathcal{R}_\ell := \{ \ell - \ell' \in \mathcal{N}_\ell \} \). With this, given \( v : \Lambda \to \mathbb{R}^m, \ell \in \Lambda, \rho \in \mathcal{R}_\ell := (\Lambda - \ell) \setminus 0 \), we define the fine difference operators and finite difference stencil

\[
D_\rho v(\ell) := v(\ell + \rho) - v(\ell) \quad \text{and} \quad D v(\ell) := (D_\rho v(\ell))_{\rho \in \mathcal{R}_\ell}.
\]

Using this notation we will show how to model defects in a later section. We now give examples of atomistic interactions. To describe these we assume each lattice site \( \ell \) is given a potential \( V_\ell \). As our goal is for the atoms to move off their reference positions into a lower energy configuration, our potential must take values from a different set. More precisely, we take \( \text{dom}(V_\ell) \to \mathbb{R} \) with \( \text{dom}(V_\ell) \subset (\mathbb{R}^m)^{\mathcal{R}_\ell} \). Then for a given deformation \( y \), we can define the site energy the deformation possesses by \( \Phi_\ell(y) := V_\ell(Dy(\ell)) \). The explicit form of \( \Phi_\ell \) is usually chosen by physical considerations.

We must endow the space of displacements with a norm in order to do our analysis. We choose the following, as in [14]. The discrete energy norm of \( u \) is defined by

\[
\| u \|_{\psi^1,2} := \| D u \|_{\ell^2} := \left( \sum_{\ell \in \Lambda} \sum_{\rho \in \mathcal{R}_\ell} \frac{|D_\rho u(\ell)|^2}{|\rho|^2} \right)^{1/2}
\]

which is actually a discrete \( H^1 \) semi-norm. The associated discrete function space is give by

\[
\psi^{1,2} := \{ u : \Lambda \to \mathbb{R}^2 : \| u \|_{\psi^1,2} < +\infty \}.
\]

Moreover, we assume that there is a regular partition \( T_\Lambda \) of \( \mathbb{R}^2 \) into triangles whose nodes lie on reference lattice sites. Moreover assume it is homogeneous in \( \mathbb{R}^2 \setminus \Lambda_{\text{def}}, \) i.e. if \( T \in T_\Lambda \) and \( \rho \in \mathbb{Z}^2 \) with \( T + \rho \in \mathbb{R}^2 \setminus \Lambda_{\text{def}} \), then \( \rho + T \in T_\Lambda \). For \( u : \Lambda \to \mathbb{R}^m \) we denote its piecewise interpolant with respect to \( T_\Lambda \) by \( Iu \). Then the gradient can be defined piecewise as \( \nabla u := \nabla Iu \), and we may use the \( L^2 \) gradient norm on this triangulation. The discrete norm above and the norm \( \nabla_{L^2} \) are equivalent under the above assumptions.

3
Now the above is in place we may state our problem. For a deformation $y$ and a far-field configuration $z$ such that $y - z \in W^{1,2}$ and $Dy, Dz \in \text{dom}(V_\ell)$, our goal is to find the atomistic configuration that minimises the total energy of the system. As such a problem is ill-posed on an infinite lattice, taking the energy difference functional
\[ E(y, z) := \sum_{\ell \in \Lambda} (\Phi_\ell(y) - \Phi_\ell(z)) \]
instead leads to a well defined object [14]. Given a proper deformation $y_0$ (the precise conditions can be found in [14]), prescribing the far field boundary condition (or a predictor), we define an energy difference functional of displacement $u$
\[ E^a(u) := E(y_0 + u; y_0) \]
for $u$ lies in the admissible deformations set
\[ \text{dom}(E^a) := \{ u \in W^{1,2} : Dy_0(\ell) + Du(\ell) \in \text{dom}(V_\ell) \text{ for all } \ell \in \Lambda \} \]
In general, $y_0$ is an asymptotic equilibrium (i.e. the internal forces acting on $y_0$ tend to zero sufficiently rapidly at infinity). For example, for point defects, $y_0(x) = Bx$ with $B \in \text{SL}(2)$. The predictor for other defects will be presented later in the proposal.

The atomistic problem can be formulated as the following variational problem
\[ \text{Find } u^a \in \arg \min \{ E^a(u) \mid u \in \text{dom}(E^a) \} \tag{1} \]
where ‘arg min’ means to find local minimizers.

### 1.2.2 Atomistic-to-Continuum Model

Due to the large number of atoms, it is computationally inefficient to solve the atomistic problem (1). However, since the defects only occupy a small part of the lattice, the deformation is relatively ‘smooth’ outside the defect region. Because of this, most of the lattice can be more efficiently modelled by using continuum elasticity, and then be coupled to the atomistic part of the system. The key constituent is the Cauchy-Born model [2]. This is a way to approximate the atomistic potential in terms of nonlinear elasticity theory. Consider the lattice $\mathbb{Z}^2$ with site potential $V : (\mathbb{R}^2)^\text{hom} \to \mathbb{R} \cup \{+\infty\}$. Take a homogeneous deformation $\mathbb{R}^2 \ni y : \mathbb{R}^2 \to \mathbb{R}^m$, $y(x) = Fx$ for some $F \in \mathbb{R}^{m \times 2}$. That is we take a macroscopic, continuum deformation.

If we now consider $y$ as describing an atomistic configuration, then the energy per unit undeformed volume in the deformed configuration $y$ is by the Cauchy-Born rule
\[ W(F) := V(F \cdot \text{Rhom}). \]
That is, the stored energy per unit volume under a macroscopically homogeneous deformation equals the energy per unit volume in the corresponding homogeneous crystal. This is exactly the atomistic energy for a homogeneous lattice deformation.

We then use this idea to give an approximation for heterogeneous deformations. Of course this requires justification, and a much more detailed exposition is found in [26]. Roughly speaking, if $y, y_0 : \mathbb{R}^2 \to \mathbb{R}^m$ are both ‘smooth’ (i.e. $|\nabla^2 y(x)|, |\nabla^2 y_0(x)| \ll 1$), then
\[ \int_{\mathbb{R}^2} (W(\nabla y) - W(\nabla y_0)) \, dx \]
is a good approximation to the atomistic energy difference $E(y; y_0)$. Since the deformation is not smooth near the defects, one can not apply the Cauchy-Born approximation in the whole lattice at. This further demonstrates the necessity of needing atomistic simulation to acquire sensible results. In fact the Cauchy Born rule is often obtained in a limiting procedure of the discrete lattice [26] that destroys the characteristic
spacing of atoms the atomistic model possesses. This is the source of many spurious results if it is not applied carefully (see [2]).

The idea of atomistic-continuum coupling is to decompose the (bounded) computational domain $\Omega = \Omega^a \cup \Omega^c$ (see Figure 2), with atomistic region $\Omega^a$ containing defects $\Lambda_{\text{def}}$ where the atomistic model is applied and continuum region $\Omega^c$ where we can employ Cauchy-Born model as the elastic field varies slowly.

![Figure 2: Atomistic-to-continuum coupling for point defect](image)

Let $T_h$ be a regular partition of $\Omega$ and $I_h$ be the associated nodal interpolation operator. We decompose the set $\Lambda^{a,i} := \Lambda \cap \Omega^a = \Lambda^a \cup \Lambda^i$ into a core atomistic region $\Lambda^a$ and an interface region $\Lambda^i$. Define the space of coarse-grained displacement maps for a/c coupling

$$\mathcal{W}_{ac}^h := \{ u_h : T_h \to \mathbb{R} | u_h \text{ is continuous and p.w. affine w.r.t } T_h, \text{ and } u_h = 0 \text{ on } \partial \Omega \}.$$ 

Here we impose an artificial Dirichlet boundary condition on $\partial \Omega$ to cut the infinite lattice into a bounded computational domain, and we shall see how to avoid this truncation in the next section.

We define the Cauchy-Born strain energy function

$$W(F) := |\text{vol}(\ell)|^{-1} \Phi \ell(F : \mathcal{R}(\ell))$$

where $\text{vol}(\ell)$ denotes the Voronoi cell associated with lattice site $\ell$.

The final ingredient in this coupling method is known as GRAC (geometric reconstruction atomistic continuum) introduced in [15]. This method is based on the interface between the continuum and atomistic regions because the nearest neighbour interaction difference stencil limits the communication between the atomistic and continuum regions down to modifying the potentials on the interface boundary. Further field interactions require more modifications to ‘near boundary’ layers of atoms in $\Lambda^a$.

The method is required due to the imbalance of forces that is demonstrated in Figure 3, known as Ghost forces these are one of the primary sources of error in energy based atomistic-continuum coupling methods. The solution proposed with GRAC is to modify the potential on the interface nodes $\Lambda^i$. Firstly the atoms are given a effective volume, this is based on the proportion of the atomistic energy contribution relative to the continuum energy contribution outside the atomistic domain in the voronoï cell of the atom. In a square domain for example this will have value $\frac{1}{2}$ on and edge, $\frac{1}{4}$ for a corner.

Secondly we modify the site energy functional on $\Lambda^i$ (recall our atomistic domain $\Lambda^{a,i} = \Lambda^a \cup \Lambda^i$ interior and interface subdomains of our lattice), such that it gives a natural value to the ‘missing’ gray differences seen in Figure 3

$$\Phi^i_\ell(y) := V(\tilde{D}_1 y(\ell), \tilde{D}_2 y(\ell), \tilde{D}_3 y(\ell), \tilde{D}_4 y(\ell))$$
where \( \tilde{D}_i \) depends on the edge or corner that \( \ell \) lies on. For example, for the northeast corner, \( \tilde{D}_1 = -D_3, \tilde{D}_2 = -D_4, \tilde{D}_3 = D_3, \tilde{D}_4 = D_4 \) and for sites on the upper inner edge, \( \tilde{D}_1 = D_1, \tilde{D}_2 = -D_4, \tilde{D}_3 = D_3, \tilde{D}_4 = D_4 \). Thus we define the GRAC energy:

\[
E_{\text{GRAC}}(y; z) = \sum_{\ell \in \Lambda} w^i_\ell (\Phi_\ell^i(y) - \Phi_\ell^i(z))
\]

where \( w^i_\ell = \begin{cases} 
\frac{1}{2} & \text{if } \ell \text{ is an edge atom} \\
\frac{1}{4} & \text{if } \ell \text{ is a corner atom}
\end{cases} \)

and for convenience, with a predictor \( y_0 \) we define \( E_{\text{GRAC}}(u) := E_{\text{GRAC}}(y_0 + u; y_0) \). Overall we have the a/c energy difference functional:

\[
E_{\text{ac}}(y_0) := E_{\text{ac}}(y_0; y_0) = E^a(y_0; y_0) + E_{\text{GRAC}}(y_0; y_0) + E^c(y_0; y_0)
\]

with

\[
E^a(y_0) := \sum_{\ell \in \Lambda^a} \Phi_\ell(y) - \sum_{\ell \in \Lambda^c} \Phi_\ell(y_0)
\]

\[
E^c(y_0) := \int_{\Omega^c \cap T_h} (W(\nabla(I_h y)) - W(\nabla(I_h y_0))) \, dx
\]

\[
= \sum_{\ell \in \Omega^c} \sum_{T \in T_h} |\text{vol}(\ell) \cap T| (W(\nabla(I_h y)|T)) - \sum_{\ell \in \Omega^c} \sum_{T \in T_h} |\text{vol}(\ell) \cap T| (W(\nabla(I_h y_0)|T))
\]

Then the a/c coupling problem seeks to find

\[
u^{ac} \in \arg \min \{ E_{\text{ac}}(u) \mid u \in \mathcal{H}^{ac}_h \}\]

### 1.2.3 Linear Elasticity Model

We can further simplify our model by linearizing elasticity in an appropriate region. The idea is that far enough away from a defect, the elastic response of a crystal is effectively linear and we may then employ classical linear elasticity as a valid approximation. The linear elasticity model itself is only valid under small deformation, and is ruled out as a model that can be directly coupled to atomistics. A way to obtain the desired form of linear elasticity is as follows, from [14]. As what follows requires many indices, we employ the indicial summation convention. Let \( F_0 \in \mathbb{R}^{m \times 2} \) be a reference strain, then we linearise the Cauchy Born energy

\[
W(F_0 + G) \approx W(F_0) + \partial_{F_{i\alpha}} W(F_0) G_{i\alpha} + \frac{1}{2} \partial_{F_{i\alpha}} F_{j\beta} W(F_0) G_{i\alpha} G_{j\beta}
\]

If denote the fourth order tensor \( A^{i\beta}_{i\alpha} := \partial_{F_{i\alpha}} F_{j\beta} W(F_0) \), then for a small displacement \( u \), we obtain the linearised energy difference functional:

\[
E^l(u) = \frac{1}{2} \int_{\mathbb{R}^2} A^{j\beta}_{i\alpha} \nabla_i u_i \nabla_\beta u_j \, dx
\]
In particular, in this paper we are concerned with 1D motion in an antiplane fashion, (i.e displacements occur perpendicular to the atomistic lattice). Under this assumption, which implies $F_0 = 0$ here, and the homogeneous potential $V$ uses nearest neighbour interactions, the linearised energy difference functional becomes

$$E_l(u) = \frac{\mu}{2} \int_{\mathbb{R}^2} |\nabla u|^2 \, dx,$$

whose minimizer $u$ satisfies the simple Laplace equation. The constant $\mu$ is the standard shear modulus of the bulk material.

1.2.4 Atom-Nonlinear-Linear Coupling Model

As the continuum models are fundamentally defined on local regions, there is no issue with coupling linear continuum domains to nonlinear continuum domain. We mark the distinction nonlinear continuum and linear continuum domains by $\Omega^c = \Omega^n \cup \Omega^l$. Similarly we naturally define the restriction $E^n(u) := E^c(u)$ where $u \in \mathcal{W}_{an}^m$

$$\mathcal{W}_{an}^m := \{ u_h : \mathcal{T}_h \to \mathbb{R} \mid u_h \text{ is continuous and p.w. affine w.r.t } \mathcal{T}_h, \text{ and } u_h = 0 \text{ on } \partial(\Omega^n \cup \Omega^a) \}.$$ analogously we may define $\mathcal{W}_{an}^l$, then the a/n/l energy difference functional is given by:

$$E^{anl}(u) = E^a(u) + E^{GRAC}(u) + E^n(u) + E^l(u)$$

And the a/n/l/ coupling problem is

$$u^{anl} \in \arg \min \{ E^{anl}(u) \mid u \in \mathcal{W}_{anl}^m \}$$

2 Error Analysis

Once a mathematical framework for a problem has been developed, many further steps must be taken to accurately and consistently link it to the “real world”: a way to study models and produce concrete results using computational methods. In doing so, practical considerations must be taken into account.

In this project, we have implemented a model problem derived from the mathematical framework found in [14]. As mentioned in the introduction, to make these problems numerically tractable approximations must be used. We now detail the various errors incurred when attempting to learn about the exact solution to the problem, and how these errors can be balanced so that one error is not significantly larger than the others. For obvious reasons, this ensures the model produces a consistent approximation.

2.1 Variational Problem

Recall our problem is to find minimisers for the energy functional in the closure of $\mathcal{W}^{1,2}$ under the appropriate energy norm. That is, we wish to find

$$u^a \in \arg \min \{ E^a(u) \mid u \in \mathcal{W}^{1,2} \}$$

The variational form of this problem is extremely useful. To make this precise we define the first and second variation of the energy functional by

$$\langle \delta E^a(u), v \rangle := \frac{d}{dt} E^a(u + tv)|_{t=0} \quad \text{and} \quad \langle \delta^2 E^a(u)v, w \rangle := \frac{d}{dt} \langle \delta E^a(u + tv), w \rangle|_{t=0}$$

We require that a minimiser satisfies the following two conditions:

$$\langle \delta E^a(u), v \rangle = 0 \quad \text{and} \quad \exists \gamma > 0, \text{ s.t. } \langle \delta^2 E^a(u)v, v \rangle \geq \gamma \|v\|^2 \quad \forall v \in \mathcal{W}^{1,2} \quad (2)$$
The first term comes directly from the Euler Lagrange equation. The second condition is called stability of the solution: In this project we assume that this condition is satisfied.

\[ u : \langle \delta E(u), v \rangle = \langle f, v \rangle \quad \forall v \in H^{1,2} \]

Note that in general we will only find local minimisers.

For complicated problems it is impossible to calculate a minimiser analytically, and infeasible to apply naïve computational tools to approximate it to a reasonable accuracy. To deal with these issues, we introduce and analyse the following models to overcome this.

### 2.2 Error Framework

Our problem is now to find

\[
\text{Find } u \in \arg \min \{ E_{\text{model}}(v) \mid v \in H^1_{\text{model}} \}
\]

with appropriate functions spaces and in an appropriate norm. In order for a model to be a “good” approximation it must be both stable and consistent. Here the consistency condition is expressed by

\[ \langle E^a(u) - E^{ac}(u), v \rangle \leq \gamma_{\text{cons}} \| v \|, \]

where \( \gamma_{\text{cons}} \) is a small constant. Coupled with the (assumed) stability of a model, this will yield an a priori error estimate.

#### 2.2.1 A Priori Error Estimate

If we assume that \( I_h u_a \) and \( u_{ac} \) are close in the infinity norm, then looking at the error \( e_h = I_h u_a - u_{ac} \) and the second variation yields by stability

\[ \gamma_{\text{stab}} \| e_h \|^2 \leq \langle \delta^2 E^{ac}(u_{ac}) e_h, e_h \rangle \approx \int_0^1 \delta^2 E^{ac}(u_{ac} + t e_h) e_h dt, e_h \rangle
\]

\[ = \int_0^1 \delta E^{ac}(I_h u) - \delta E^{ac}(u_{ac}), e_h \rangle \leq \gamma_{\text{cons}} \| e_h \|, \]

and so

\[ \| e_h \| \leq \frac{\gamma_{\text{cons}}}{\gamma_{\text{stab}}} + \delta \]

where this \( \delta \) comes from the first approximation, and can be sufficiently controlled by applying the Inverse Function Theorem as in [23]. With the above derived (at least formally), we wish specifically to determine rates of the convergence - we will find consistency errors in terms of the differences of \( u \) in an appropriate norm as follows:

Show \( \exists C > 0, k > 0 \ s.t \ \langle \delta E^a(u) - \delta E_{\text{model}}(u), v \rangle \leq C \| \nabla^{k_1} u \|^{k_2} \)

where \( k_1, k_2 \) will describe the rate of convergence if the strong stability given by (2) is assumed of the system.

We will now introduce and analyse a series of models, and later provide numerical tests to demonstrate the rates obtained.
2.2.2 Error Estimates and Decay Rates: Pure Atomistic

Our first step will be to acquire error estimates between an energy minimiser \( \bar{u} \) and a Galerkin approximation, again following [14]. Defining the space

\[
\mathcal{W}_0(\Omega) = \{ u : \Omega \to \mathbb{R} | u(\ell) = 0 \forall \ell \in \Omega^c \}
\]

then \( \mathcal{W}_0 = \mathcal{W}^{1,2} \), with the closure taken under the norm defined in the introduction. We have the following result from [14]:

Let \( \bar{u} \) be the exact solution to the problem formulated above. Then denoting \( \bar{u}_c \) as the solution to the problem

\[
\bar{u}_c \in \text{argmin}\{ E(u) : u \in \mathcal{W}_0(\Omega) \} \tag{3}
\]

We have the following:

**Theorem 2.1.** Let \((\Omega)_R\) be a sequence of computational domains such that \( \Lambda \cap B(0, R) \subseteq \Omega_R \). If \( \bar{u} \) is a strongly stable solution, then for all sufficiently large \( R \) there exists a strongly stable solution to (3) such that

\[
\| \bar{u} - \bar{u}_c \| \leq CR^{-1}, \quad 0 \leq E(\bar{u}) - E(\bar{u}_c) \leq CR^{-2}.
\]

We may use this to find approximations to the exact solution. Our goal is to reduce computational complexity by introducing a continuum analogue of (3), and coupling it to an atomistic description to improve its accuracy. In doing so, we must ensure the error still has the same or better asymptotic behaviour (or else we have chosen a poor model).

3 Consistency Analysis

We now introduce the framework for different consistent coupling schemes, and demonstrate the errors incurred in doing so.

The idea is that in a small region where forces are large, we will use an atomistic description. Further out (at a radius chosen by considering the analysis) we will replace the atoms with a continuum, with the atomistic part of the problem providing boundary conditions. Once this is done, we will demonstrate how to optimise the coupling: that is, determine the sizes of the regions of the lattice that will be subject to different models so that each model contributes the same order of error. One difficulty is that the potential given to each atom relies on atomistic positions of its neighbours, and of course on the interface with the continuum region an atom will have no neighbours on one “side”. Many methods have been introduced to surmount this difficulty. We describe a particular method which achieves the desired consistency.

In our atomistic continuum coupling, if we investigate a defect with no bulk forces, we can confine these to the atomistic interior to make the implementation and analysis less involved. We can decompose \( \mathbb{R}^2 \) into two open sets \( \Omega^a \) and \( \Omega^c \). This will yield convergence rates for the error. We now introduce the framework for different consistent coupling schemes, and demonstrate the errors incurred in doing so.

To model the continuum we will employ the Cauchy Born rule or its linearised variant, and implement this using the finite element method. We will firstly analyse the atomistic part of our coupled problem.

3.1 Atomistic and GRAC Variations

We wish to inspect the variations of the the coupling firstly between atomistic and (possibly nonlinear) continuum (linearisation discussed in §3.4.2). The variation of the atomistic-continuum energy is given by:

\[
\langle \delta \mathcal{E}_{ac}(u), v \rangle = \langle \delta \mathcal{E}_a(u), v \rangle + \langle \delta \mathcal{E}_{GRAC}(u), v \rangle + \langle \delta \mathcal{E}_c(u), v \rangle, \quad \forall v \in \mathcal{W}_h^{ac}
\]
Firstly, we wish to write these variations all in the same form, we choose this to be formulated as bond densities, hence we define the set of edges in the atomistic lattice $\Lambda$ as $\mathcal{E}$. Then, we calculate for suitable test function $v$: (recalling the symmetry of our potential defined as $V(\{D_i u\}_{i=1}^4) = \sum_{i=1}^4 f(D_i u)$)

$$
\langle \delta E^a(u), v \rangle = \frac{d}{dt} E^a(u + tv) |_{t=0} = \sum_{\ell \in \Lambda^a} \frac{d}{dt} \Phi_\ell(u + tv) |_{t=0}
= \sum_{\ell \in \Lambda^a} V'(D_u) \cdot D v = 2 \sum_{e \in \mathcal{E}} f'(D_e u) \cdot D v
$$

where the final summation now takes place over the set of edges in the atomistic lattice $\mathcal{E}$, thus we have written this variation as a sum over bond weights.

For the boundary atoms (thus boundary bonds), we have two different cases due to the modified potential and weights.

- **Edge atom - Example: $p_4$ is imaginary atom**

  We show that the weighting of the variation on the boundary edges are a half that of the interior edges, and that the weighting to the interior bond is the same as in the interior atomistic case (i.e these bonds remain unaffected by the GRAC coupling. (Notation: $D_i$ represents the finite difference from the centre atom to $p_i$)

  $$
u^i_{\text{edge}} \langle \delta \Phi^i_{\text{edge}}(u), v \rangle = \frac{1}{2} \langle \delta V(D_1 u, D_2 u, D_3 u, -D_2 u), v \rangle
= \frac{1}{2} \left( \sum_{k=3}^3 f'(D_k u)D_k v - f'(D_2 u)D_2 v \right)
= \frac{1}{2} f'(D_1 u)D_1 v + \frac{1}{2} f'(D_3 u)D_3 v + f'(D_2 u)D_2 v
$$

Thus we can see that the contribution for bonds either side of an edge atom in the energy variation will only alter the weight of bonds on the boundary.

- **Corner atom - Example: $p_1, p_4$ are imaginary atoms**

  Now we know that the edge atoms have the same contributions to the variation, we wish to confirm that the corner atoms with two reflections are still consistent with this.

  $$u^i_{\text{vert}} \langle \delta \Phi^i_{\text{vert}}(u), v \rangle = \frac{1}{4} \langle \delta V(-D_3 u, D_2 u, D_3 u, -D_2 u), v \rangle
= \frac{1}{4} \left( \sum_{k=3}^3 f'(D_k u)D_k v - f'(-D_3 u)D_3 v - f'(-D_2 u)D_2 v \right)
= \frac{1}{2} f'(D_2 u)D_2 v + \frac{1}{2} f'(D_3 u)D_3 v
$$

Hence we have the correct weights that correspond to the diagram.

We now may write this over all bonds, we obtain the form ($\mathcal{E}^i$ the set of all bonds in the boundary layer):

$$
\langle \delta E^{\text{GRAC}}(u), v \rangle = \sum_{e \in \mathcal{E}^i} f'(D_e u) \cdot D v,
$$

where we multiply by two due to undercounting.
3.2 Nonlinear Continuum

We begin considering if or how we can write the continuum variation in the following form:

\[ \langle \delta \mathcal{E}^{ac}(u), v \rangle = \sum_{e \in \Omega^c} \eta^e_{ac} D_e v \]

To accomplish this, we use \( Q^1 \) finite elements. We assume the radius of the atomistic region is approximately \( R \). We then write out the above for the continuum region:

\[
\int_{\Omega^c} \nabla W(\nabla u) \cdot \nabla v = \sum_{Q \in \Omega^c} \int_Q \nabla W(\nabla u) \cdot \nabla v - \sum_{Q \in \Omega^c} [\nabla W(F_Q)] \cdot \nabla v + \sum_{Q \in \Omega^c} [\nabla W(F_Q)] \cdot \nabla v
\]

\[
= \sum_{Q \in \Omega^c} \int_Q (\nabla W(\nabla u) - \nabla W(F_Q)) \cdot \nabla v + \sum_{Q} \nabla W(F_Q) \int_Q \cdot \nabla v
\]

\[
\leq R^{-3} ||\nabla v||_{L^2} + \sum_{Q \in \Omega^c} \int_Q \nabla W(F_Q) \cdot \nabla v,
\]

Here \( F_Q \) is chosen by taking the average gradient on each element. This allows us to use Poincaré’s inequality on the left hand term, and use the right hand term in calculating the consistency error. We have that

\[
||\nabla W(\nabla u) - \nabla W(\langle \nabla u \rangle)||_{L^2(\Omega^c)} \lesssim \sum_{Q} ||\nabla u - \langle \nabla u \rangle||_{L^2(Q)} + ||\nabla u - \langle \nabla u \rangle||^2_{L^2(Q)} \lesssim R^{-3}.
\]

Proceeding with writing the continuum variation in terms of edges, we begin by noting that

\[
\int_Q \nabla W(F) \cdot \nabla v = \int_{\partial Q} (\nabla W(F)) \cdot n v \, dl,
\]

where \( n \) denotes the outward normal on \( \partial Q \), and \( dl \) denotes the integral over the edges. We have that

\[
\nabla W(F) = (\partial_1 W(F_1, F_2), \partial_2 W(F_1, F_2)),
\]

and recalling the Cauchy Born rule, this is just given by

\[
\partial_1 W = 2\partial_1 V(F_1, F_2, -F_1, -F_2) = 2f'(F_1),
\]

and similarly for the other component. We now take the inner product with the outward normal to each edge- this allows us to write (the subscripts refer to the normal on edge \( i \))

\[
\nabla W(F) \cdot n_1 = 2f'(F_2), \quad \nabla W(F) \cdot n_3 = -2f'(F_2),
\]

and similarly for the other two parallel edges. Collecting all this, we can write the variation as a sum over all edges

\[
- f'(F_2) \int_{\partial Q} v \, dl_1 + f'(F_2) \int_{\partial Q} v \, dl_3 = f'(F_2)(v(x_3) - v(x_4)) + v(x_2) - v(x_1))
\]

as the trapezoidal rule is exact for affine functions. A similar calculation is applied to the other edges. Combining the above we have

\[
\sum_{e \in \Omega^c} \eta^e_{ac} D_e v = \sum_{e \in \Omega^c} (f'(F_e^{Q^-}) + f'(F_e^{Q})) D_e v, \quad F \text{ defined on each } Q.
\]
This shows a reference edge calculation. The edge considered in the derivation below is \( \{ u_3 - u_4 \} \). The second term appears because each edge has two contributions: the third part of the line integral in the element below it, and the first part of the line integral in the element above.

### 3.3 Modelling Consistency Errors

Now, recall that the atomistic variation is given by

\[
0 = \langle \delta \mathcal{E}^a(u), v \rangle = \sum_{e \in \Lambda} \partial_e V D_e v,
\]

and we will now use this to generate our consistency errors. We begin by looking at the simplest case: the edges inside the atomistic region.

#### 3.3.1 Atomistic Consistency Error

This is 0 everywhere in the interior of the atomistic region: \( \mathcal{E}^{ac} = \mathcal{E}^a + \ldots \) so inside the atomistic region there is no contribution to the variation. We must deal with the interface, however. Firstly we calculate the error inside the continuum region, which will enable us to evaluate the interface errors.

#### 3.3.2 Interior Continuum Consistency Error

We now consider consistency errors in the interior of the continuum region. By this we mean that no edge of a Q1 element touches the atomistic boundary \( \Lambda^i \)- this will be dealt with later. Recall that

\[
\langle \mathcal{E}^{ac}(u)|_{\text{int}(\Omega_c)} - \mathcal{E}^{(a)}(u)|_{\text{int}(\Omega_c)}, v \rangle = CR^{-3} + \sum_{e \in \text{int}(\Omega_c)} (\eta^{ac}_e(u) - \eta^a(u)) D_e v.
\]

Applying the Cauchy Schwarz inequality to the above, we need only bound the \( \ell^2 \) difference of these coefficients:

\[
|\langle \mathcal{E}^{ac}(u) - \mathcal{E}^{(a)}(u), v \rangle_{\text{int}(\Omega_c)}| \leq ||Dv||_{\ell^2} \left( \sum_{e \in \text{int}(\Omega_c)} (\eta^{ac}_e(u) - \eta^a(u))^2 \right)^{\frac{1}{2}}.
\]

Now, we consider

\[
\sum_{e \in \text{int}(\Omega_c)} (\eta^{ac}_e(u) - \eta^a(u))^2 = \sum_{e \in \text{int}(\Omega_c)} |2f'(D_e u) - f'(F^{Q^-}_e) - f'(F_e)|^2
\]

\[
= \sum_{e \in \text{int}(\Omega_c)} |f''(0)| \cdot |(2D_e u - F^{Q^-}_e) - F_e|^2 + \sum_{e \in \text{int}(\Omega_c)} |O((D_e u)^2)|^2
\]

by Jensen’s inequality. As \( Du \sim \ell^{-2} \) this error will be much smaller than the other terms, and we henceforth neglect it in our calculations. We now recall the definition of forward differences: here \( v_i \) is a single atom spacing in direction \( i \).
\[ D_e u(\ell) = u(\ell + v_i) - u(\ell), \]

and the 2nd forward difference operator

\[ D_e^2 u(\ell) = \frac{1}{2} (u(\ell + 2v_i) - 2u(\ell + v_i) + u(\ell)), \]

we will show the consistency error be written in terms of second differences of \( u \). For a particular edge we have that

\[ F_2^- = \frac{u_3 - u_4}{2} + \frac{u_3 - u_4}{2}, \]

\[ F_2 = \frac{u_3 - u_4}{2} + \frac{u_2 - u_1}{2}, \]

and that

\[ F_2^- + F_2 = \frac{u_3 - u_4 + u_3 - u_4 + u_3 - u_4 + u_2 - u_1}{2} = \frac{u_3 + 2u_3 + u_2 - u_4 - 2u_4 - u_1}{2} \]

and so

\[ (\eta_{ec} - \eta^a)^2 \leq C((4u_3 - 4u_4 - u_3 + 2u_3 + u_2 - u_4 - 2u_4 - u_1)^2 = (D_e^2 u_3 - D_e^2 u_4)^2, \]

which are 3rd order difference terms. It follows that we can bound the consistency errors in the following way:

\[ \left( \sum_{e \in \text{int}(\Omega^c)} (\eta_{ec} - \eta^a)^2 \right)^{1/2} \leq 4C \left( \sum_{\ell \in \text{int}(\Omega^c)} |D_e^3 u(\ell)|^2 \right)^{1/2} \leq C \left( \sum_{\ell \in \text{int}(\Omega^c)} |\ell|^{-8} \right)^{1/2} \]

\[ \approx C \left( \int_R r \cdot r^{-8} \, dr \right)^{1/2} = \frac{C}{R^{5/2}} = \frac{C}{R^3}. \]

To get an explicit error rate we treat the lattice sum as a Riemann sum to yield an approximate integral form.

### 3.4 Coupling Consistency Errors

#### 3.4.1 Atomistic-Continuum Coupling

For the tiles touching the boundary, instead of the tile above and tile below contributing to the continuum bond weights \( \eta_{ec} \), only one tile contributes. However, the grac weight is one half on this interface: we must now consider

\[ \sum_{e \in \mathcal{E}^t} (\eta_{ec} - \eta^a)^2 = \sum_{e \in \mathcal{E}^t} \left| f'(D_e u) - f'(F_e^Q) \right|^2 \]

due to the weighting of a half that GRAC gives to the \( \eta^a \) and a second tile not contributing, an analogous calculation yields

\[ f'(D_e u) - f'(F_e^Q) \approx \frac{C}{2} \left( (u_4 - u_1) - \frac{(u_3 - u_2) + (u_4 - u_1)}{2} \right) = \frac{C}{2} \left( (u_4 - u_1) - (u_3 - u_2) \right) \]

\[ \lesssim \frac{1}{\ell^2} - \frac{1}{(\ell + 1)^2} \approx \frac{2\ell + 1}{\ell^4} \lesssim \frac{1}{\ell^{-3}} \]
and as before, we approximate with a boundary integral on which we assume $R$ is constant: $R$ in fact varies by a factor of up to $\sqrt{2}$. This gives the estimate

$$\sum_{c \in E_i} (\eta_{ac}^e(u) - \eta^e(u))^2 \lesssim \left( \int \frac{1}{R^6} \, dl \right)^{\frac{1}{2}} \lesssim \left( \frac{R}{R^6} \right)^{\frac{1}{2}} \lesssim R^{-\frac{5}{2}}.$$  

3.4.2 Atomistic-Nonlinear-Linear Coupling

We wish to also couple the nonlinear continuum to a linear continuum which is also calculated using finite element method (contrary to using boundary elements). We recall that the full continuum domain $\Omega^c$ is written as $\Omega^c = \Omega^n \cup \Omega^l$, the nonlinear and linear domains respectively. The consistency analysis is straightforward as we are able to split up the consistency difference into two parts:

$$\langle \delta \mathcal{E}^a(u) - \delta \mathcal{E}^{anl}(u), v \rangle = \langle \delta \mathcal{E}^a(u) - \delta \mathcal{E}^{ac}(u), v \rangle + \langle \delta \mathcal{E}^{ac}(u) - \delta \mathcal{E}^{anl}(u), v \rangle \quad \text{for } v \in \mathcal{W}_h^{ac}$$

the first of these is the **modelling error** that we have already considered in the previous subsection. The second is called the **linearisation error** and will be considered here. For any test function $v$, and shear modulus $\mu := \nabla^2 W(\nabla y_0)$, recalling that $y_0 = 0$ is our homogeneous **predictor**:

$$\langle \delta \mathcal{E}^{anl}(u), v \rangle = \frac{d}{dt} \int_{\Omega^l} \mu \nabla (u + tv) \cdot \nabla v \, dx \bigg|_{t=0} = \int_{\Omega^l} \mu \nabla u \cdot \nabla v \, dx$$

We may then write our consistency as the difference (for $N$ the total number of lattice sites and continuum nodes):

$$\langle \delta \mathcal{E}^{ac}(u) - \delta \mathcal{E}^{anl}(u), v \rangle = \int_{\Omega^l} (\nabla W(\nabla u) - \mu \nabla u) \cdot \nabla v \, dx = \sum_{i=1}^{N} \int_{\Omega^l} (\partial_i W(\nabla u) - \mu \partial_i u) \partial_i v \, dx$$

An application of Taylor’s theorem about the homogeneous strain yields $\forall i \in \{1 \ldots, N\} \exists \theta \in (0, 1)$ s.t:

$$\int_{\Omega^l} (\partial_i W(\nabla u) - \mu \partial_i u) \partial_i v \, dx = \int_{\Omega^l} \left( \frac{\partial_\theta W(0)}{\theta \mu} + \frac{\partial^2_\theta W(0)(\nabla u)}{\theta^2 \mu} + \frac{\partial^3_\theta W(\theta e_i)(\nabla u)^2}{\theta^3 \mu} - \mu \nabla u \right) \cdot \nabla v \, dx$$

$$= \int_{\Omega^l} \left( \frac{\partial^3_\theta W(\theta e_i)(\nabla u)^2}{\theta^3 \mu} \right) \cdot \nabla v \, dx \leq C_i \| (\nabla u)^2 \|_{L^2} \| \nabla v \|_{L^2} \quad (*)$$

where $e_i$ is the $i^{th}$ standard orthonormal basis vector of $\mathbb{R}^N$ and the $\{C_i\}_{i=1}^N$ are uniformly bounded, then

$$(*) \implies \langle \delta \mathcal{E}^{ac}(u) - \delta \mathcal{E}^{anl}(u), v \rangle \leq \tilde{C} \| (\nabla u)^2 \|_{L^2} \| \nabla v \|_{L^2}$$

Thus we have for the atomistic-FEM radius $R$ for the and using the decay rate $\nabla u \lesssim R^{-2}$ (in the case of point defects) we have

$$\| (\nabla u)^2 \|_{L^2} \lesssim \left( \int_R^{\infty} r^{-7} \, dr \right)^{\frac{1}{2}} = \left( \int_R^{\infty} r^{-7} \, dr \right)^{\frac{1}{2}} = \frac{C}{R^5}$$

which yields our convergence rate.
3.4.3 Atomistic-Linearisation Coupling

We have seen in last subsection that the nonlinear elasticity model can be approximated by a linear elasticity model, but the problem is still defined in an infinite domain. In this subsubsection, we consider how to couple the atomistic model directly with the linear elasticity model, which allows us to reduce the problem into a bounded domain. Assume that the whole space $\mathbb{R}^2 = \Omega^a \cup \Omega^l$ with $\Gamma = \Omega^a \cap \Omega^l$, and $\Lambda = \Lambda^a \cup \Lambda^l \cup \Lambda^i$. For displacements $u$ in $\Omega^a$ and $v$ in $\Omega^l$ satisfying $v|_{\Gamma} = I_h u|_{\Gamma}$, we define a new energy functional $E^{al}(u,v) = E^a(u) + E^{GRAC}(u) + E^l(v)$ with $E^l(v) = \frac{\mu}{2} \int_{\Omega^l} |\nabla v|^2$ and $\mu \text{ Id} = \partial^2 W(\nabla(I_h u_0))$ in $\Omega^l$. Then it is obvious that

$$\min_{v|_{\Gamma} = I_h u|_{\Gamma}} E^{al}(u,v) = \min E^r(u)$$

where the reduced energy $E^r(u)$ is defined as

$$E^r(u) := E^a(u) + E^{GRAC}(u) + \min_{v|_{\Gamma} = I_h u|_{\Gamma}} E^l(v)$$

Since $E^l(v)$ is the linear elasticity energy, recalling that $v$ satisfying far field condition, then minimizing $E^l(v)$ is equivalent to finding solution to the following exterior Laplacian problem

$$-\mu \Delta v = 0 \text{ in } \Omega^l$$

$$v|_{\Gamma} = I_h u|_{\Gamma}$$

$$v(x) \sim O\left(\frac{1}{|x|}\right) \text{ as } |x| \to \infty$$

(4)

Since $v$ is defined in infinite domain, it is unrealistic to apply the finite element method to solve the problem numerically. Instead, one can use boundary integral methods to solve it. The Galerkin boundary element method can be employed to discretise the boundary integral equation. In [28], it has been proved that the above exterior problem has a unique solution. Furthermore, the solution $v$ has the following integral representation in $\Omega^l$

$$v(x) = \int_{\Gamma} v(y) \frac{\partial G(x,y)}{\partial n(y)} - \frac{\partial v}{\partial n}(y) G(x,y) \, ds(y), \quad x \in \Omega^l$$

(5)

with $G(x,y) := -\frac{1}{2\pi} \ln(|x-y|)$ being the fundamental solution of Laplace equation in two dimensions. Given density $\varphi \in C(\Gamma)$, if we define single-layer potential

$$S\varphi(x) := \int_{\Gamma} G(x,y)\varphi(y) \, ds(y), \quad x \in \mathbb{R}^2 \setminus \Gamma$$

and double-layer potential

$$D\varphi(x) := \int_{\Gamma} \frac{\partial G(x,y)}{\partial n(y)} \varphi(y) \, ds(y), \quad x \in \mathbb{R}^2 \setminus \Gamma$$

then

$$v(x) = D\left(v|_{\Gamma}\right) - S\left(\frac{\partial v}{\partial n}|_{\Gamma}\right), \quad x \in \Omega^l$$

(6)

To study boundary integral equations, we also introduce the following integral operators

$$(V\varphi)(x) := \int_{\Gamma} G(x,y)\varphi(y) \, ds(y), \quad x \in \Gamma$$

$$(K\varphi)(x) := \int_{\Gamma} \frac{\partial G(x,y)}{\partial n(y)} \varphi(y) \, ds(y), \quad x \in \Gamma$$
and
\[ (K'\varphi)(x) := \int_{\Gamma} \frac{\partial G(x,y)}{\partial n(x)} \varphi(y) \, ds(y), \quad x \in \Gamma \]
where \( S \) is called the single-layer operator, \( K \) is called the double-layer operator and \( K' \) is its adjoint. Here we assume that \( \Gamma \) is Lipschitz and piece-wise smooth, then we collect some mapping properties of layer operators in the following (see [16])

(i) \( S : H^{-1/2}(\Gamma) \to H^1_{\text{loc}}(\mathbb{R}^2) \)
(ii) \( D : H^{1/2}(\Gamma) \to H^1_{\text{loc}}(\mathbb{R}^2 \setminus \Gamma) \)
(iii) \( V : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma) \)
(iv) \( K : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma) \)
(v) \( K' : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma) \)

Since \( v \) has the representation (5), the Dirichlet boundary condition in (4) gives us the following first kind boundary integral equation on \( \Gamma \)
\[ V\varphi = f \] (7)
with unknown density \( \varphi := \frac{\partial v}{\partial n} \) and right hand side \( f := (K - \frac{1}{2} I)u \).

**Theorem 3.1.** Given \( f \in H^{1/2}(\Gamma) \), the boundary integral equation (7) has a unique solution \( \varphi \in H^{-1/2}_s(\Gamma) \) where \( H^{-1/2}_s(\Gamma) = \{ \varphi \in H^{-1/2}(\Gamma) : \int_\Gamma \varphi = 0 \} \).

**Proof.** Since \( H^{-1/2}_s(\Gamma) \subset H^{-1/2}(\Gamma) \), then \( f \in H^{1/2}(\Gamma) = (H^{-1/2}(\Gamma))^* \subset (H^{-1/2}_s(\Gamma))^* \). For \( \varphi, \psi \in H^{-1/2}_s(\Gamma) \), define a bilinear form \( b(\varphi, \psi) := \langle V\varphi, \psi \rangle_{H^{-1/2} \times H^{1/2}} \). By Theorem 6.22 in [29], \( b(\cdot, \cdot) \) is coercive in \( H^{-1/2}_s(\Gamma) \), i.e.
\[ \langle V\varphi, \varphi \rangle \geq c\|\varphi\|_{H^{-1/2}(\Gamma)} \quad \text{for} \quad \varphi \in H^{-1/2}_s(\Gamma) \]
Hence it follows from the Lax-Milgram Theorem that (7) has a unique solution \( \varphi \in H^{-1/2}_s(\Gamma) \).

Once we have found the solution \( \varphi \) of (7), the solution of the exterior Laplacian problem \( v \) is given by integral equation (5) with \( \frac{\partial v}{\partial n} = \varphi \). Now we consider the numerical discretization of (7). Let \( \Gamma \) is decomposed by boundary elements \( \tau_i \), i.e. \( \Gamma = \bigcup_{i=1}^{M} \tau_i \), and define \( S^0_\Gamma(\Gamma) := \text{span}\{ \varphi^0_k \}_{k=1}^{M} \) as the space of functions which are piece-wise constant with respect to the boundary decomposition \( \{ \tau_i \}_{i=1}^{M} \). The basis functions \( \varphi^0_k \) are given by
\[ \varphi^0_k(x) = \begin{cases} 1 & \text{for } x \in \tau_k, \\ 0 & \text{otherwise} \end{cases} \]
In addition to \( S^0_\Gamma \), one can also define piece-wise linear basis function space \( S^1_\Gamma(\Gamma) := \text{span}\{ \varphi^1_i \}_{i=1}^{M} \) with basis
\[ \varphi^1_i(x) = \begin{cases} 1 & \text{for } x = x_i, \\ 0 & \text{for } x = x_j \neq x_i, \\ \text{linear} & \text{otherwise} \end{cases} \]
Since \( S^0_\Gamma(\Gamma) \) is densely included in \( H^{-1/2}(\Gamma) \), by using \( \varphi_h(x) = \sum_{k=1}^{M} a_k \varphi^0_k(x) \in S^0_\Gamma(\Gamma) \), the Galerkin variational formulation of (7) seeks \( \varphi_h \in S^0_\Gamma(\Gamma) \) such that
\[ \langle V\varphi_h, \psi_h \rangle = \langle f, \psi_h \rangle = \langle (K - \frac{1}{2} I)u, \psi_h \rangle, \quad \text{for} \ \psi_h \in S^0_\Gamma(\Gamma) \]
Since \( V \) is only coercive in \( H^{\frac{1}{2}}(\Gamma) \), to ensure the approximate solution \( \varphi_h \in H^{1}(\Gamma) \), we need to supply an additional condition \( \sum_{k=1}^{M} a_k = 0 \). So we define

\[
S_{s,h}^{0}(\Gamma) := \{ \varphi_h(x) \in S_{h}^{0}(\Gamma) : \varphi_h(x) = \sum_{k=1}^{M} a_k \varphi_k(x) \text{ with } \sum_{k=1}^{M} a_k = 0 \}
\]

and find solution \( \varphi_h \in S_{s,h}^{0}(\Gamma) \) such that

\[
\langle V \varphi_h, \psi_h \rangle = \langle f, \psi_h \rangle = \langle (K - \frac{1}{2} I)u, \psi_h \rangle, \quad \text{for } \psi_h \in S_{s,h}^{0}(\Gamma)
\]  (8)

And then the approximated solution in the exterior domain is given by

\[
v_h = D(u_{1|\Gamma}) - S(\varphi_h)
\]  (9)

Applying Theorem 12.7 in [29], we can obtain the convergence result in the following theorem.

**Theorem 3.2.** Let \( \varphi \in H^{1}(\Gamma) \) be the unique solution of (7) with right hand side \( u \in H^{2}(\Gamma) \), and \( \varphi_h \in S_{s,h}^{0}(\Gamma) \) be the solution to (8), then there holds the error estimate

\[
\| \varphi - \varphi_h \|_{H^{-\frac{1}{2}}(\Gamma)} \leq ch^{\frac{3}{2}} \| \varphi \|_{H^{1}(\Gamma)}
\]

and

\[
\| \nabla v - \nabla v_h \|_{L^{2}(\Omega')} \leq ch^{\frac{3}{2}} \| u \|_{H^{\frac{1}{2}}(\Gamma)} \| \varphi \|_{H^{1}(\Gamma)}
\]

Now we turn to the consistency analysis for a/l coupling methods. We begin with the consistency of the BEM discretization. Assume that \( v \) and \( v_h \) are given by (6) and (9) respectively, for any test function \( w \in H^{1}(\Omega') \), by using Theorem 3.2, we have

\[
|\langle \delta E'(v), w \rangle - \langle \delta E'(v_h), w \rangle | = \mu |\langle (\frac{\partial v}{\partial n} - \frac{\partial v_h}{\partial n}), w \rangle | = \mu |\langle (\varphi - \varphi_h), w \rangle | \leq \mu \| w \|_{H^{\frac{1}{2}}(\Gamma)} \| \varphi - \varphi_h \|_{H^{-\frac{1}{2}}(\Gamma)}
\]

\[
\leq ch^{\frac{3}{2}} \| w \|_{H^{\frac{1}{2}}(\Gamma)} \| \varphi \|_{H^{1}(\Gamma)} = ch^{\frac{3}{2}} \| w \|_{H^{\frac{1}{2}}(\Gamma)} \| \frac{\partial v}{\partial n} \|_{H^{1}(\Gamma)} \leq cR^{-\frac{3}{2}} h^{\frac{3}{2}} \| w \|_{H^{\frac{1}{2}}(\Gamma)}
\]

with \( R \) sufficiently large and the last inequality follows from the far field condition that \( v^{(j)}(x) \sim O(|x|^{-j-1}) \) at infinity. Recalling the consistency error for the GRAC energy in a/n/l coupling method is of \( O(R^{-\frac{5}{2}}) \), we obtain the consistency error for a/l coupling method

\[
|\langle E^a(u) - E^{al}(u), w \rangle | \leq CR^{-\frac{3}{2}} \| w \|_{H^{1}}
\]

Under the assumption of stability, we obtain the following error estimate

\[
|u^a - u^{al}|_{H^{1}} \leq CR^{-\frac{3}{2}}, \quad E^a(u^a) - E^{al}(u^{al}) \leq CR^{-5}
\]  (10)

### 3.5 Remark on Other Defects

In this report the primary focus for the analysis is on the point defect. However given some rates of decay that are ‘known’ (see [14], [30]), we may then deduce some heuristics about the linearisation procedure.

<table>
<thead>
<tr>
<th>Defect Classification</th>
<th>Decay Rate of ( \nabla u )</th>
<th>Decay of CB ( \lesssim | \nabla^2 u |_{L^2} )</th>
<th>Decay of linear CB ( \lesssim | (\nabla u)^2 |_{L^2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point Defect</td>
<td>( R^{-\frac{5}{2}} )</td>
<td>( R^{-\frac{5}{2}} )</td>
<td>( R^{-\frac{7}{2}} )</td>
</tr>
<tr>
<td>Dislocation</td>
<td>( R^{-1} )</td>
<td>( R^{-1} )</td>
<td>( R^{-1} )</td>
</tr>
<tr>
<td>Crack</td>
<td>( R^{-\frac{5}{2}} )</td>
<td>( R^{-\frac{5}{2}} )</td>
<td>( \int_{R}^{N} r (\nabla u^2)^2 \sim (\ln(N))^\frac{1}{2} \rightarrow \infty )</td>
</tr>
</tbody>
</table>
These decay estimates have been proven for point defects here and dislocations in [14] but obtaining rigorous decay rates for the crack is still open (the decay of $\nabla u$ is based on continuum predictions). However these results show heuristically that for point defects the linearised model FEM should prove more effective than the Cauchy Born model FEM in coupling. In dislocation it also appears as effective and linearised models are less computationally complex hence could prove beneficial. Unfortunately linearisation is unlikely to be possible for the crack due to the highly nonlocal nonlinearities of these phenomena, which gives rise to such a slow ($R^{-\frac{1}{2}}$) decay of the gradient of the solution, which leads to the linearisation gradient actually diverging!

4 Implementation

This section is dedicated to the essential steps and calculations that were performed for the implementation of the models and the coupling methods. To begin we create a template algorithm that will be used throughout the implementation process - this will be adapted and shown in more detail in § 4.2 for model coupling.

Stepest descent algorithm

1. Begin with reference defect displacements $u_0$, the initial displacement $u^{(0)}$, and a tolerance $T$.
2. On the $i$th step, calculate the gradient of the energy functional which is being minimized: $\nabla E_{\text{model}}(u^{(i)} + u_0)$
3. Adjust this gradient according to $u_0$ and imposed boundary conditions to obtain $\nabla E_{\text{model}}(u^{(i)} + u_0)$.
4. Pick a step size $\alpha$ and step $u^{(i+1)} = u^{(i)} - \alpha \nabla E_{\text{model}}(u^{(i)} + u_0)$
5. If $|\nabla E_{\text{model}}(u^{(i+1)} + u_0)| < T$ then the solution is $u = u^{(i+1)}$, otherwise, repeat algorithm from step 2.

$E_{\text{model}}$ represents which energy the model coupling will require minimisation in the more specific frameworks further on. We now move onto the implementation of the three models that we wish to couple together.

4.1 Implementing the Models

For this section we consider a particular atomistic potential $V(\{Du_i\}_{i=1}^4) = \sum_{i=1}^4 (Du_i)^2 + (Du_i)^4$

4.1.1 Atomistic Model

The first model that is considered is the atomistic model. With regards to computation we must calculate everything directly from the atomistic potential $\Phi$. For a reference deformation $u_0 : \mathbb{R}^2 \to \mathbb{R}$ and displacement $u : \mathbb{R}^2 \to \mathbb{R}$, with the atomistic energy $E^a(u)$. Consider taking $u_0 = 0$ for simplicity and then we look at $E^a(u) = \sum_{\ell \in \Lambda^a} \Phi_\ell(u)$ with

$$\Phi_\ell(y) = V(D_1 y(\ell), D_2 y(\ell), D_3 y(\ell), D_4 y(\ell))$$
where $V$ is a potential function of the finite stencil $D_i y(\ell) = y(\ell + v_i) - y(\ell), D_{i+2} y(\ell) = y(\ell - v_i) - y(\ell)$, $i = 1, 2$. In our project, $V : \mathbb{R}^4 \to \mathbb{R}$ is given by

$$V(F_1, F_2, F_3, F_4) = \sum_{i=1}^{4} f(F_i), \quad \text{with} \quad f(t) := t^2 + t^4.$$  

We wish to calculate the gradient of the energy on the interior of $\Lambda^a$, (if for example using Dirichlet boundary conditions), hence consider $\nabla E^a(u) = \{ \partial_{u_k} E^a(u) \}_{k=1}^{N}$ (N represents the size of the interior atomistic domain, $u_k$ interior atom displacements).

$$\partial_{u_k} \nabla E^a(u) = \sum_{\ell \in \Lambda^a} \partial_{u_k} \Phi_{\ell}(u) = \sum_{\ell \in \Lambda^a} \partial_{u_k} V(D_1 u(\ell), D_2 u(\ell), D_3 u(\ell), D_4 u(\ell))$$

$$= \partial_{u_k} V(u_{k_1} - u_k, u_{k_2} - u_k, u_{k_3} - u_k, u_{k_4} - u_k)$$

$$+ (-1) \partial_{u_k} V(u_k - u_{k_1}, \cdots, \cdots, \cdots) + (-1) \partial_{u_k} V(\cdots, u_k - u_{k_2}, \cdots, \cdots)$$

$$+ (-1) \partial_{u_k} V(\cdots, \cdots, u_k - u_{k_3}, \cdots) + (-1) \partial_{u_k} V(\cdots, \cdots, \cdots, u_k - u_{k_4})$$

$$= 2 \sum_{i=1}^{4} \partial_{u_k} f(u_{k_i} - u_k)$$

4.1.2 Cauchy Born Model

In general, the Cauchy Born Energy (at a site) $\ell$, $W : \mathbb{R}^N \to \mathbb{R}$ is given by

$$W(F) = \frac{1}{|\text{Vor}(\ell)|} V(F \cdot R_{\ell}),$$

where $\text{Vor}(\ell)$ is the Voronoi cell of $\ell$ and $R_{\ell}$ is the matrix representation of the interaction range at the site $\ell$. The crystal is a regular square lattice of length 1 (atom spacing), thus we have $\forall \ell \text{Vor}(\ell) = 1$ and nearest neighbour interactions yields $R_{\ell} = \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$ representing our interaction stencil.

We obtain:

$$W(F_1, F_2) = V \left( F_1 F_2 \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \right) = V(F_1, F_2, -F_1, -F_2)$$

We wish to calculate the discrete function $u$, the derivative of the energy $E^{ac}(u) = E^a(u) + \int_{\Omega^c} W(\nabla(u)) \, dx \tag{*}$

where $I$ is a linear interpolant of $u$. We consider

$$E^c = \sum_{T \in T} \int_T W(\nabla(Iu|_T)) \, dx = \sum_{T \in T} \int_T W \left( \sum_{i=1}^{3} u_i \nabla \phi_i \right) \, dx$$

Where $\phi_i$ are the local basis functions, $u_i$ evaluation at int vertex of element $T$. In our specific case, $t \in \mathbb{R}^4$ the site potential is given by $V(t) = \sum_{i=1}^{4} t_i^2 + t_i^4$. Denoting $S_j = \sum_{i=1}^{3} u_i \partial_j \phi_i$ (for each local basis of elements $T$)

$$\sum_{T \in T} \int_T W(S_1, S_2) \, dx = \sum_{T \in T} \int_T V(S_1, S_2, -S_1, -S_2) \, dx$$

$$= 2 \sum_{T \in T} \int_T \sum_{j=1}^{2} ((S_j)^2 + (S_j)^4) \, dx$$
There is another important quantity we must calculate with the Cauchy Born approximation, which is the derivative of the energy - as this will be used to calculate direction of step in the steepest descent argument. We proceed viewing the Cauchy Born approximate entirely from a finite element standpoint, then it is straightforward application of the chain rule. We denote the number of degrees of freedom (finite element nodes) by \( N \):

\[
\nabla \mathcal{E}^c(u) = (\partial_{u_k} \mathcal{E}^c(u))_{k=1}^{N}
\]

\[
\partial_{u_k} \mathcal{E}^c(u) = \partial_{u_k} \int_{\Omega} W(\nabla (Iu)) \, dx = \sum_{T \in \mathcal{T}} \int_{T} \partial_{u_k} W \left( \sum_{i=1}^{3} u_i \nabla \phi_i \right) \, dx = \sum_{T \in \mathcal{T}} \int_{T} W' \left( \sum_{i=1}^{3} u_i \nabla \phi_i \right) \cdot \nabla \phi_k \, dx
\]

where \( W'(F) = V'(F_1, F_2, -F_1, -F_2) = \partial_1 V + \partial_2 V - (-\partial_1 V) - (-\partial_2 V) = 2 \sum_{j=1}^{2} \partial_j V \). Thus we may implement the following equation

\[
\partial_{u_k} \mathcal{E}^c(u) = \sum_{T \in \mathcal{T}} \sum_{j=1}^{2} \partial_j V \left( \sum_{i=1}^{3} u_i \nabla \phi_i \right) \cdot \nabla \phi_k \, dx
\]

where the derivative of our site potential of a 4-vector \( t \), is given by \( \partial_{j} V(t) = 2 t_j + 4 t_j^3 \).

### 4.1.3 Linearisation of the Cauchy Born Model

As we consider antiplanar motion and do not prescribe an overall shear to the crystal, our identity map is \((x, y, 0) \rightarrow (x, y, 0)\) so the atoms’ movement in the z-direction is the 0 map. We therefore expand the Cauchy-Born energy as follows:

\[
W(F_0 + G) \approx W(F_0) + \nabla W(F_0)(G - F_0) + \frac{1}{2} (G - F_0)^T \nabla^2 W(F_0)(G - F_0).
\]

Noting \( W(F_0) = W(0) = 0 \) and using the symmetry of \( V \),

\[
\nabla W(F) = \begin{pmatrix} \partial_{F_1} W \\ \partial_{F_2} W \end{pmatrix} = \begin{pmatrix} \partial_1 V - \partial_3 V \\ \partial_2 V - \partial_4 V \end{pmatrix} = 0
\]

Thus, the linearisation is given by the second order term only:

\[
\nabla^2 W = \begin{pmatrix} \partial_1^2 V - 2 \partial_{13} V + \partial_3^2 V & \partial_{12} V - \partial_{14} V - \partial_{23} V + \partial_{34} V \\ \partial_{12} V - \partial_{14} V - \partial_{23} V + \partial_{34} V & \partial_2^2 V - 2 \partial_{24} V + \partial_4^2 V \end{pmatrix}
\]

\[
= \begin{pmatrix} \partial_1^2 V - 2 \partial_{13} V + \partial_3^2 V & 0 \\ 0 & \partial_2^2 V - 2 \partial_{24} V + \partial_4^2 V \end{pmatrix}
\]

because the cross-derivatives are 0 from the linear composition of \( \Phi \) in our case. Denoting \( \Phi(t) = \sum_{i=1}^{4} f(t_i) \) we obtain that, from inputting the form \( f(t_3) = f(-t_1) \)

\[
\partial_1^2 V(0) - 2 \partial_{13} V(0) + \partial_3^2 V(0) = 2 f''(s)|_{s=0} = 2(2 + 12 s^2)|_{s=0} = 4,
\]

with the other nonzero entry having this value. It follows that \( \nabla^2 W(0) = \mu I, \mu := 4 \).

Our linearised energy term looks as follows:

\[
\mathcal{E}'(v) = \int_{\Omega} \frac{\mu}{2} |\nabla v|^2 \, dx = 2 \int_{\Omega} |\nabla v|^2 \, dx
\]

Finding out the value of the shear modulus \( \mu \) is important in the coupling of the linear model as seen in the following subsection.
4.2 Implementing the Coupling Methods

4.2.1 Atom-FEM

With these preliminaries and the definition of the Atomistic and Cauchy Born energies as given in subsections 4.1.1 and 4.1.2, we may implement the atomistic continuum energy.

During the steepest descent we must calculate the gradient of $\mathcal{E}^{\text{GRAC}}$, the case of the interface atoms is less trivial that for the nearest neighbour atomistic potential but follows with a similar method as found in 4.1.1. We consider as an example the case of an atom $u_k$, positioned on the ‘left hand edge’:

$$
\partial u_k \nabla \mathcal{E}^{\text{GRAC}}(u) = \sum_{\ell \in \Lambda^i} w^i_{\ell} \partial u_k \Phi^i_{\ell}(u) = \sum_{\ell \in \Lambda^i} w^i_{\ell} \partial u_k V(D_1 u(\ell), D_2 u(\ell), -D_1 u(\ell), D_4 u(\ell))
$$

$$
\begin{align*}
&= \frac{1}{2} \partial u_k V(u_{k_1} - u_k, u_{k_2} - u_k, u_k - u_{k_1}, u_{k_4} - u_k) \\
&\quad + \frac{1}{2} (-1) \partial u_k V(u_k - u_{k_1}, \ldots, \ldots, \ldots) + \frac{1}{2} (-1) \partial u_k V(\ldots, u_k - u_{k_2}, \ldots, \ldots) \\
&\quad + \frac{1}{2} \partial u_k V(\ldots, \ldots, u_k - u_{k_1}, \ldots) + \frac{1}{2} (-1) \partial u_k V(\ldots, \ldots, \ldots, u_k - u_{k_4}) \\
&= 2 \cdot \frac{1}{2} \sum_{i=1}^4 \partial u_k f(u_{k_i} - u_k)
\end{align*}
$$

One can check that for corners we arrive at the above expression with factor $2 \cdot \frac{1}{4}$ and for the outermost interior layer of atoms, despite the new introduced non locality we still arrive with factor 2 as with the atomistic energy gradient.

We may now implement the above gradient with the Cauchy Born and atomistic gradients to update the atom positions in our steepest descent method. Note that Step 3. does not effect the atomistic-continuum interface.

4.2.2 Atom-BEM

To minimize the a/l energy functional $\mathcal{E}^{\text{al}}(u)$ by the steepest decent method, we need to evaluate the energy and its gradient, both involving the computation of exterior problem (4) or its equivalent integral equation (7).

Since the discrete function $u$ can be viewed as a vector $u$, we decompose the vector as $u = [u^A, u^I]$ according to whether the site lies on the boundary. Suppose we seek approximated density $\varphi_h = \sum_{k=1}^{M} a_k \varphi_k^0(x) \in H^{-\frac{1}{2}}(\Gamma)$ with $\sum_{k=1}^{M} a_k = 0$. If $u|_{\Gamma}$ is replaced by its linear interpolation $u_h = \sum_{i=1}^{M} u^I_i \varphi_i^1 \in S_h^1(\Gamma)$, then the load vector $\mathbf{f} = (f_\ell)_{\ell=1}^{M}$ can be evaluated as

$$
f_\ell = \sum_{i=1}^{M} u^I_i \langle (K - \frac{1}{2} I) \varphi_i^1, \varphi^0_\ell \rangle
$$

i.e.

$$
\mathbf{f} = (K_h - M_h/2) \mathbf{u}^I
$$

where $\mathbf{u}^I = (u^I_i)_{i=1}^{M}$ and

$$
M_h[\ell, i] = \langle \varphi_i^1, \varphi^0_\ell \rangle, \quad K_h[\ell, i] = \langle K \varphi_i^1, \varphi^0_\ell \rangle
$$

If we denote $\mathbf{V}_h := \{(V \varphi_i^0, \varphi^0_\ell)\}_{i,\ell=1}^{M}$, then the solution vector $\mathbf{a}$ satisfies the following linear system

$$
\mathbf{V}_h \mathbf{a} = (K_h - M_h/2) \mathbf{u}^I
$$
and the linearisation energy

\[ \mathcal{E}^l(v) = -\frac{\mu}{2} \int_{\Gamma} \frac{\partial v}{\partial n} v \approx -\frac{\mu}{2} \int_{\Gamma} \varphi_h u_h = -\frac{\mu}{2} \sum_{i=1}^{M} a_i u_i^l \langle \varphi_i^1, \varphi_i^0 \rangle = -\frac{\mu}{2} a^T M_h u^I \]

Furthermore, its gradient can be evaluated as

\[ \nabla_u \mathcal{E}^l(v[u]) = \left( \nabla_u a^T M_h \right) = -\mu \left( \begin{array}{c} 0 \\ M_h a \end{array} \right) \]

Those above together with the evaluations on atomistic energy allows us to carry out the steepest decent method to minimize the ATOM-BEM energy.

5 Numerical Results

Test Example: Let \( \Phi_\ell(u) = V(D_1 y(\ell), D_2 y(\ell), D_3 y(\ell), D_4 y(\ell)) \) with \( y = u + u_0 \). Here \( V : \mathbb{R}^4 \rightarrow \mathbb{R} \) is define as \( V(t_1, t_2, t_3, t_4) = \sum_{i=1}^{4} f(t_i) \) with \( f(t) = t^2 + t^4 \). Consider the reference displacement \( u_0 \) shown below

![Graph showing the displacement field with a reference point marked at (50, 50)]
5.1 Atom-FEM Couplings

To test the atomistic continuum couplings, we used the defect described above. We chose a sequence of atomistic radii [3, 4, 6, 8]. We then scaled the start of the continuum region as $R^{3/2}$. An atomistic simulation of radius $2 \times (8 + 8^{3/2}) \approx 62$ was used to approximate the exact solution. The following results were produced:

![Figure showing the EOC for atom-nonlinear FEM using a log-log plot.](image1)

![Figure showing the EOC for atom-linear FEM using a log-log plot.](image2)

in line with expectations, as scaling the continuum region as $R^{3/2}$ should allow us to see this rate.

We also ran simulations for the linear FEM with a continuum region scaled as $R^2$: however for this to run due to time constraints the gradient tolerance was increased from $1e^{-6}$ to $1e^{-5}$. The reference solution was produced on a correspondingly larger grid. This produced the following results: again as expected according to theory.
5.2 Atom-BEM Coupling

To test the convergence rate of a/l coupling method, we firstly compute a reference solution $u^{al}_{e}$ which is regarded as the 'exact' solution by our Atom-Bem solver with a large domain (101×101 in the experiment). Then we compare the error between energy of the Atom-Bem solution in a series of small domain and the reference energy in Figure 4. It is shown that the computational rate is $O(R^{-4})$ which seems contradicting with the theoretical rate. However, we are not clear whether the constant in the error estimate (10) depends on $R$, so the theoretical rate might be $O(R^{-4})$ in that case.

Figure 4: Convergence rate for Atom-Bem Energy
6 Further Work

There are numerous avenues for to pursue in any future work. Some examples include:

- Implement many body nearest neighbour potentials, with EAM model [1]
- Include coarse graining of FEM regions to allow for larger simulations
- Include preconditioning for drastically larger simulations
- Extend analysis to cover these cases
- Expand to more complicated defects. Nonlinear elasticity (formally) seem to be the better choice there.

Incorporating EAM potentials would yield more realistic simulations- and preconditioning/coarse graining would allow simulations to be run on much larger scales. However, of course, the accompanying analysis must be generalised to verify any convergence rates obtained through further implementation.

In our work thus far there is no qualitative difference between nonlinear and linear elasticity. Coarse graining and including more elaborate defects would require a balancing of errors incurred: where to place different regimes so that the error from each does not overwhelm the others.
References


[27] H. Föll, online notes on crystal defects, relevant section
http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_2_2.html.

