Analysis of a Predictor-Corrector Method for Computationally Efficient Modeling of Surface Effects in 1D *

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Abstract

The regular Cauchy–Born method is a useful and efficient tool for analyzing bulk properties of materials in the absence of defects. However, the method normally fails to capture surface effects, which are essential to determining material properties at small length scales. In this paper, we present a corrector method that improves upon the prediction for material behavior from the Cauchy–Born method over a small boundary layer at the surface of a 1D material by capturing the missed surface effects. We justify the separation of the problem into a bulk response and a localized surface correction by establishing an error estimate, which vanishes in the long wavelength limit.

1 Introduction

Long-range elastic fields dictate the behavior of crystalline materials in the absence of defects. This elastic response in crystalline systems is often studied through the use of the Cauchy–Born method [1, 18]. In the Cauchy–Born method, the non-local interactions in the atomistic system are replaced by a localized continuum approximation, which may then be further approximated using the finite element method (FEM). This sequence of approximations allows for a reduction in the number of degrees of freedom in the model and yields a computationally efficient and accurate approach to studying the material behavior of perfect crystalline materials. However, this approach fails in the presence of defects since they create rapid variations in the atomistic displacement field which can no longer be accurately captured by the Cauchy–Born model. In particular for the present paper, the Cauchy–Born method often struggles with capturing effects due to the inclusion of surfaces in the model [17].

Surfaces can be characterized as defects because atoms near a surface experience a different interaction environment than atoms in an idealized crystal lattice. For large systems, the surface influence is often negligible since the surface region constitutes such a small portion of the entire system. The bulk — or interior — behavior dominates. Surface effects become increasingly significant, though, as the surface area to volume ratio increases, resulting in a size-dependent response in material behavior, which is an active area of research [3, 8, 15, 16].

While surface effects tend to be most relevant in small systems, these small systems may still be large enough to present computational challenges for a fully-atomistic numerical simulation. Further, even in bulk crystals, if effects of interest take place at or near a crystal boundary (e.g.,

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nano-indentation), then accurately capturing the surface physics remains crucial. Thus, a
computationally efficient means to simulate surface-dominated systems is desirable. Various methods
have been proposed that have the potential to meet this need. These methods generally entail a
modification of the continuum model [9, 10, 17] or a concurrent coupling of atomistic and continu-
num models [4, 7, 12, 13, 19]. Yet, while these methods do result in a superior approximation than
that which comes from the regular Cauchy–Born method, the modified continuum models lack a
systematic control over the error in the approximation while the atomistic-to-continuum coupling
methods may encounter difficulties with surface geometries that would result in a much-reduced
computational savings than might be observed with other defects.

In this paper, we introduce a novel approach to efficiently and accurately capturing surface
behavior through the use of a predictor-corrector method that possesses a more controllable error
and an improved approach to handling surface geometries. In this predictor-corrector method,
the Cauchy–Born method serves as the initial predictor for material behavior, allowing for the
usual tools that study bulk behavior to be applied to the surface problem too. As the Cauchy–
Born method works well for the interior, it should serve well for an approximation of the bulk
response of the material. The solution for the Cauchy–Born method is then corrected in the next
step to take into account surface effects by minimizing the energy difference between the atomistic
energy and the Cauchy–Born energy about the Cauchy–Born solution. This correction occurs over
a boundary layer near the surface at atomistic resolution. The size of the boundary layer is a
controllable parameter in this predictor-corrector method and allows for a systematic control over
the accuracy of the approximation. The corrected solution represents the approximation of this
predictor-corrector method to the atomistic behavior. Proving the validity of the decomposition of
the atomistic solution into a bulk response and surface correction will be the primary goal of the
analysis in this paper in addition to assessing the quality of the approximation.

The paper is organized as follows. In §2, we summarize all main results and illustrate them
via numerical tests. Complete proofs are given in §3–§6.

**Notation for derivatives:** We will employ three types of derivatives. (1) If \( u : \{0, 1, \ldots \} \) is
a discrete function, then we define \( u'_\ell = u_{\ell+1} - u_\ell \). (2) If \( u : [0, \infty) \) is a continuous displacement
or deformation function, then \( \nabla u(x) \) is the standard pointwise or weak derivative (if it exists).
(3) Finally, if \( V : \mathbb{R}^n \to \mathbb{R}^p \) is a potential function (or its derivative), then we denote its partial
derivatives by \( \partial_i V \), while its Jacobian matrix is denoted by \( \partial V \).

## 2 Summary of Results

### 2.1 Atomistic Model

We consider a semi-infinite, 1D chain of atoms. We index the atoms in the chain by the set of
non-negative integers, \( \mathbb{Z}_{\geq 0} \), and we denote the individual location of the atom with index \( \ell \) in
the chain by \( y_\ell \in \mathbb{R} \). The reference position of each atom in the chain is chosen to be \( y_\ell = \ell \). We denote
the displacement of atom \( \ell \) from its reference position by \( u_\ell := y_\ell - \ell \in \mathbb{R} \). The strain (gradient)
in the bond between the atoms indexed by \( \ell \) and \( \ell + 1 \) in the chain will be written as

\[
u'_\ell := u_{\ell+1} - u_\ell = y_{\ell+1} - y_\ell - 1.
\]

The surface of the chain is located at the atom with index 0.

The atoms in this semi-infinite chain interact according to a nearest-neighbor site energy (effect-
ively second-neighbour interaction). This is the simplest setting within which we can still observe

\[\text{(1)}\]
the surface effects we are interested in. The energy due to these interactions is given by

\[ E^a(y) := V_{\text{surf}}(y_1 - y_0) + \sum_{\ell=1}^{\infty} V(y_\ell - y_{\ell-1}, y_{\ell+1} - y_\ell), \quad (2) \]

where \( V \) denotes the site energy for atoms in the interior of the system while \( V_{\text{surf}} \) denotes the surface site energy. The surface atom merits a different site energy than the interior atoms because the 0-th atom has only one neighbor while every other atom has two. We will later assume that \( V_{\text{surf}} \) is the limit of \( V \) as one of the bonds is stretched to infinity.

Since \( E^a \) is translation invariant, configurations are not meaningfully distinct if they differ only up to a translation. Hence, we fix the end point so that \( y_0 = 0 \). Under this constraint, knowledge of \( u' \) allows us to recover the full displacement \( y \). Hence, it will often be more convenient to consider the energy in terms of the strain rather than the deformation:

\[ E^a(u) := V_{\text{surf}}(u'_0) + \sum_{\ell=1}^{\infty} V(u'_{\ell-1}, u'_\ell), \quad (3) \]

where we have now also absorbed the reference strain 1 into the definitions of \( V_{\text{surf}} \) and \( V \).

We assume throughout that the site energies satisfy the following properties:

**Site Energy Properties:**

(i) \( V \in C^k(\mathbb{R}^2) \) and \( V_{\text{surf}} \in C^k(\mathbb{R}) \) with \( k \geq 3 \);

(ii) \( V, V_{\text{surf}} \) and all permissible partial derivatives are bounded.

(iii) \( V(0,0) = 0 \);

(iv) \( \partial^2 V(0,0) > 0 \);

(v) \( \inf_{\{|(r,s)|>\varepsilon\}} V(r,s) > 0 \) for any \( \varepsilon > 0 \);

(vi) For any \( s \in \mathbb{R} \), \( \lim_{r \to \infty} V(r,s) = V_{\text{surf}}(s) \);

If the semi-infinite chain were extended infinitely in both directions so that it had no surface and its energy consisted purely of a sum of bulk site energies, then Properties (iii)–(v) would imply that the ground state of this bulk model is the configuration with a uniform strain of 0. Property (iv) would guarantee that the phonon frequencies of such an infinite chain system are positive so that the infinite crystal is stable. For the surface model, these properties will allow us to prove existence of a ground state and to establish properties of the boundary layer. Property (vi) defines the surface site energy in terms of the limiting behavior of the bulk site energy, and as a consequence of properties (v) and (vi), we see that

\[ \inf_{s \in \mathbb{R}} V_{\text{surf}}(s) > 0. \quad (4) \]

Property (ii) is one of convenience and is not strictly necessary. Throughout the paper, derivatives of \( V_{\text{surf}} \) with respect to its argument will be denoted by \( \partial_F V_{\text{surf}} \). Derivatives of \( V \) with respect to its first and second argument will be denoted by \( \partial_1 V \) and \( \partial_2 V \), respectively. Higher-order derivatives for the two site energies will be denoted similarly.
We are concerned with finding the energy-minimizing configuration of the chain in the presence of external forces. To consider the situation where bulk and surface effects are roughly of the same order, we consider only finite-energy displacements, i.e., displacements from the space
\[ \mathcal{U} := \{ u : \mathbb{Z}_{\geq 0} \to \mathbb{R} \mid u(0) = 0 \text{ and } u' \in \ell^2(\mathbb{Z}_{\geq 0}) \}. \] (5)
When \( \mathcal{U} \) is equipped with the \( H^1 \)-seminorm \( |u|_{H^1} = \|u\|_{\ell^2(\mathbb{Z}_{\geq 0})} \) it becomes a Hilbert space due to the constraint \( u(0) = 0 \). It is easy to see \cite{12} that compact displacements are dense in \( \mathcal{U} \).

Applied forces take the form of a lattice function \( f : \mathbb{Z}_{\geq 0} \to \mathbb{R} \), which must be an element of \( \mathcal{U}^* \). We say that \( f \in \mathcal{U}^* \) if and only if there exists a constant \( \|f\|_{\mathcal{U}^*} \) such that
\[ \langle f, u \rangle \leq \|f\|_{\mathcal{U}^*} \|u'\|_{\ell^2(\mathbb{Z}_{\geq 0})} \quad \text{for all } u \in \mathcal{U} \text{ with } \operatorname{supp}(u) \text{ compact}, \] (6)
where \( \langle f, u \rangle := \sum_{\ell=0}^{\infty} f_{\ell} u_{\ell} \). For arbitrary \( u \in \mathcal{U} \), \( \langle f, u \rangle \) is defined by continuity.

Given such a force \( f \in \mathcal{U}^* \), we seek a minimizer
\[ u^g \in \arg \min \{ \mathcal{E}^g(u) - \langle f, u \rangle_{\mathbb{Z}_{\geq 0}} \mid u \in \mathcal{U} \}. \] (7)
This problem may have several or no solutions. We consider the existence of solutions to this problem as well as their decay in the following section.

We conclude the description of the model by mentioning that Properties [1] and [4] guarantee that the first and second variations are globally Lipschitz continuous. We refer to [12] for a proof.

**Remark.** It is easy to see that \( f \in \mathcal{U}^* \) if and only if there exists \( g \in \ell^2(\mathbb{Z}_{\geq 0}) \) such that \( f = -g' \) by considering a discrete summation by parts of \( \langle f, u \rangle \). From this summation by parts, it can also be shown that
\[ g_n = \sum_{\ell=n+1}^{\infty} f_\ell < \infty; \] (8)
see § 4 for a proof that this sum is well-defined. Therefore, \( \langle f, u \rangle = \langle g, u' \rangle \leq \|g\|_{\ell^2} \|u'\|_{\ell^2} \), and in fact, it is clear that \( \|f\|_{\mathcal{U}^*} = \|g\|_{\ell^2} \).

### 2.1.1 Example: EAM Model

To provide a concrete example of the types of systems encompassed by the model described above, we show how the semi-infinite chain satisfying the Embedded Atom Model (EAM) \cite{2,11} with only nearest-neighbor interactions is described in this framework. The energy for such a system is written in terms of the strain as
\[ \mathcal{E}^g(u') = \phi(1 + u'_0) + \psi(\rho(1 + u'_0)) + \sum_{\ell=1}^{\infty} \left[ \phi(1 + u'_\ell) + \psi(\rho(1 + u'_\ell) + \rho(1 + u'_{\ell-1})) \right], \] (9)
where \( \phi \) is a nearest-neighbor pair potential, \( \psi \) is an embedding energy function, and \( \rho \) is an electron density function. In order to write this energy in the form of [3], we define the bulk and surface site energies, respectively, as
\[ V(u'_{\ell-1}, u'_\ell) = \frac{1}{2} \phi(1 + u'_{\ell-1}) + \frac{1}{2} \phi(1 + u'_\ell) + \psi(\rho(1 + u'_{\ell-1}) + \rho(1 + u'_\ell)), \quad \text{and} \]
\[ V_{\text{surf}}(u'_0) = \frac{1}{2} \phi(1 + u'_0) + \psi(\rho(1 + u'_0)). \]

For the analysis, we will consider the generalized framework described by [3], but we will return to the EAM system for the numerical results in § 2.6.
2.2 Existence, Decay and Stability of Atomistic Solutions

Unlike in a bulk model without surfaces, we do not expect that an energy-minimizing configuration for the semi-infinite chain is homogeneous. Therefore, we have to be satisfied with weaker existence proofs and establishing general properties of a minimizer.

**Theorem 2.1.** There exists a minimizer of $E^a : \mathcal{U} \rightarrow \mathbb{R} \cup \{+\infty\}$.

*Proof.* See Section 3.

While for many systems it is reasonable (and natural) to expect a unique ground state, our assumptions do not preclude the existence of multiple states that achieve the same minimal energy. In the following, $u^a_{gr}$ may refer to any ground state.

The key property of $u^a_{gr}$ that motivates our subsequent developments is that the surface effects are highly localized. This is established next.

**Theorem 2.2.** Let $u^a_{gr}$ be a critical point of $E^a$. Then, there exists $0 \leq \mu_a < 1$ such that

$$|\langle u^a_{gr}, v \rangle| \lesssim \mu^\ell_a \quad \text{for all } \ell \in \mathbb{Z}_{\geq 0}. \quad (10)$$

*Proof.* See Section 3.

The exponential decay of the strain due to surface effects normally justifies ignoring surface effects in large systems. However, we will see that when surface effects are the focus of interest, then this boundary layer cannot be ignored.

We now proceed to incorporating external forces into the analysis. To that end, it is convenient to assume that a ground state $u^a_{gr}$ is strongly stable; that is, we suppose that there exists an atomistic stability constant $c_a > 0$ such that

$$\langle \delta^2 E^a(u^a_{gr})v, v \rangle \geq c_a \|v\|^2_{\ell^2(\mathbb{Z}_{\geq 0})} \quad \text{for all } v \in \mathcal{U}. \quad (11)$$

This stability assumption on $u^a_{gr}$ enables us to prove the existence of nearby strongly stable local minimizers of the atomistic problem from (7) with small external forces. For future reference, an element $u^a \in \mathcal{U}$ is a strongly stable solution to the atomistic problem if and only if it satisfies the Euler–Lagrange equation

$$\langle \delta E^a(u^a), v \rangle = \langle f, v \rangle \quad \text{for all } v \in \mathcal{U} \quad (12)$$

as well as the stability condition

$$\langle \delta^2 E^a(u^a)v, v \rangle \geq c\|v\|^2_{\ell^2(\mathbb{Z}_{\geq 0})} \quad \text{for all } v \in \mathcal{U}, \quad (13)$$

for some constant $c > 0$. The exact form of the first and second variations of $E^a$ are provided in Propositions 7.1 and 7.2

**Corollary 2.3.** There exist $\varepsilon, C > 0$ such that, for all $f \in \mathcal{U}^*$ with $\|f\|_{\mathcal{U}^*} < \varepsilon$, the atomistic problem (7) has a unique, strongly-stable solution with $\|(u^a - u^a_{gr})\|_{\ell^2} \leq C\|f\|_{\mathcal{U}^*}$.

*Proof.* This is an immediate consequence of the inverse function theorem (Theorem 7.3).
2.3 Cauchy–Born Model

A common approach to determining the approximate bulk behavior of perfect crystalline materials utilizes the Cauchy–Born model of atomistic interactions, approximates the non-local atomistic interactions with a local approximation. A limiting procedure then turns the discrete problem into a continuum one [1]. The Cauchy–Born energy for the semi-infinite chain model is

\[ E_{cb}(u) := \int_0^\infty W(\nabla u(x)) \, dx \quad \text{for } u \in U_{cb}, \]

where \( W(F) := V(F,F) \) is the Cauchy–Born energy density function and

\[ U_{cb} := \{ u \in H^1_{\text{loc}}(0, \infty) \mid \nabla u \in L^2(0, \infty) \text{ and } u(0) = 0 \}. \]

The Cauchy–Born energy density function \( W \) inherits the smoothness of \( V_{\text{bulk}} \), i.e., \( W \in C^3(\mathbb{R}) \). Derivatives of \( W \) with respect to its argument (as opposed to \( x \)) will be indicated by \( \partial_F W \). We also note that the space \( U \) may be considered a subspace of \( U_{cb} \) if we identify the lattice functions \( u \in U \) with their piecewise continuous interpolants.

For atomistic systems without defects, the Cauchy–Born approximation and the exact model agree under homogeneous deformation. However, in systems containing defects, such as surfaces, this property is lost. In [14], this discrepancy arises as the Cauchy–Born model treats every point in the chain as an interior point. The absence of a surface component to the energy results in an \( O(1) \) error in the consistency estimate for the Cauchy–Born model as compared to the atomistic system, which we can demonstrate when \( f = 0 \).

**Proposition 2.4.** The unique minimizer of \( E_{cb} \) in \( U_{cb} \) is \( u_{cb} = 0 \). Its atomistic residual is bounded by

\[ \sup_{v \in U, \|v\|_{L^2(\mathbb{R} \geq 0)} = 1} |\langle \delta E^a(0), v \rangle| = \|\delta E^a(0)\|_{U^*} = |\partial_F V_{\text{surf}}(0)|. \]

In particular, \( \|u_{gr} - u_{cb}\|_{L^2} \geq M^{-1}|\partial_F V_{\text{surf}}(0)| \), where \( M \) is the global Lipschitz constant of \( \delta E^a \).

**Proof.** See Section 4. \qed

In general, we expect that \( |\partial_F V_{\text{surf}}(0)| \neq 0 \) so that the Cauchy–Born and atomistic energy-minimizing configurations are not in agreement because of surface effects.

This lack of consistency at the surface indicates that the Cauchy–Born model alone will not serve as an accurate approximation of the original system for the purpose of studying surface effects. However, as we have shown in Theorem 2.2, surface effects are a local phenomenon. The Cauchy–Born model may then still serve as an efficient means to computing the behavior of the system in the interior.

We will show that the bulk and surface effects decouple, which means that a complex concurrent coupling scheme is not required. Instead, we can “add” the surface effects in a predictor-corrector type approach, where the predictor is the Cauchy–Born solution. We therefore consider the general Cauchy–Born problem

\[ u_{cb} \in \arg \min \{ E_{cb}(u) - \langle f, u \rangle_{\mathbb{R}^+} \mid u \in U_{cb} \}, \]

where we identify the lattice function \( f \) with its continuous piecewise affine interpolant and \( \langle f, u \rangle_{\mathbb{R}^+} := \int_0^\infty f u \, dx \). It is easy to see that \( f \in U^* \) implies that \( \langle f, \cdot \rangle_{\mathbb{R}^+} \in (U_{cb})^* \); see §4.
Analogously to the atomistic problem, we say \( u^{cb} \) is a strongly stable solution to (17) if it satisfies the first-order and strong second-order optimality conditions:

\[
\langle \delta E^{cb}(u^{cb}), v \rangle = \langle f, v \rangle_{\mathbb{R}_+, \mathcal{U}^{cb}} \quad \text{for all } v \in \mathcal{U}^{cb}
\]

\[
(\delta^2 E^{cb}(u^{cb})v, v) \geq c_{cb} \| \nabla v \|_{L^2([0, \infty)))}^2 \quad \text{for all } v \in \mathcal{U}^{cb}
\]

(18) for some constant \( c_{cb} > 0 \). The exact forms of the first and second variations of the Cauchy–Born energy may be found in Propositions 7.1 and 7.2.

For small enough external forces, we can guarantee the existence of strongly stable solutions to the Cauchy–Born problem and deduce some additional facts concerning their regularity.

**Theorem 2.5.** There exists \( \varepsilon_{cb} > 0 \) such that for all \( f \in \mathcal{U}^* \) with \( \| f \|_{\mathcal{U}^*} < \varepsilon_{cb} \), a strongly stable solution \( u^{cb} \in \mathcal{U}^{cb} \) of the Cauchy–Born problem (17) exists.

Moreover, \( u^{cb} \in H^3_{\text{loc}}, \) and it satisfies the bounds

\[
|\nabla u^{cb}(0)| \lesssim \| f \|_{\mathcal{U}^*}, \quad |\nabla^2 u^{cb}(x)| \lesssim |f(x)| \quad \text{and} \quad |\nabla^3 u^{cb}(x)| \lesssim |\nabla f(x)| + |f(x)|^2.
\]

(19)

**Proof.** See Section 4.

In the next section, we will use the Cauchy–Born solution to approximate the atomistic solution. To that end, we introduce a projection operator \( \Pi_a : \mathcal{U}^{cb} \to \mathcal{U} \) via

\[
(\Pi_a u)_0 = 0 \quad \text{and} \quad (\Pi_a u)_\ell = \int_\ell^{\ell+1} \nabla u(s) \, ds \quad \text{for } \ell \in \mathbb{Z}_{\geq 0}, u \in \mathcal{U}^{cb}.
\]

### 2.4 Predictor-Corrector Method

Proposition 2.4 demonstrates that the Cauchy–Born method commits an \( O(1) \) consistency error at a material surface. However, the Cauchy–Born method is an excellent method for approximating the bulk response of materials, and Theorem 2.2 indicates that the error due to surface effects may be quite localized. We therefore propose a mechanism to correct the Cauchy–Born solution to obtain an approximation of the form

\[
u^a \approx \Pi_a u^{cb} + q_L,
\]

where the parameter \( L \) for the corrector \( q_L \) determines the quality of the approximation.

Given a predictor \( u^{cb} \) solving the Cauchy–Born problem (17), we define the corrector problem via the minimization of a corrector energy, which is given by

\[
\mathcal{E}^\Gamma(q; F_0) = V^{\text{surf}}(F_0 + q_0) - W(F_0) - q_0 \partial_F W(F_0)
\]

\[
+ \sum_{j=1}^{\infty} (V(F_0 + q_{j-1}, F_0 + q_j) - W(F_0) - q_j \partial_F W(F_0))
\]

(21)

where we will normally take \( F_0 := \nabla u^{cb}(0) \).

The idea of the corrector problem is that it should depend only in a local way on the elastic field \( \nabla u^{cb} \). In this case, this dependence is only on \( \nabla u^{cb}(0) \). This choice was made deliberately so that the corrector problem can be understood as a cell problem on a surface element when the Cauchy–Born model is discretized using finite elements.

For \( L \in \mathbb{N} \cup \{ \infty \} \), a corrector strain on the interval \([0, L]\) is found by solving

\[
q_L \in \arg \min_{q \in Q_L} \{ \mathcal{E}^\Gamma(q; F_0) \mid q \in Q_L \},
\]

(22)
where $Q_L$ describes the the boundary layer over which we correct the Cauchy–Born solution and is defined to be

$$Q_L := \{ q \in \mathcal{U} \mid q'_\ell = 0 \text{ for all } \ell \geq L \}. \quad \text{In particular, } Q_\infty = \mathcal{U}. $$

The choice of $L$ affects the computational expense to solve the corrector problem as well as the accuracy of the approximation of the atomistic system’s behavior. Note that the external force $f$ does not enter directly into the corrector problem. The Cauchy–Born method accounts for the external forces on its own, but the influence of the external force is felt through the dependence on $F_0$.

**Theorem 2.6.** There exists $\varepsilon_\Gamma > 0$ such that, for all $F_0 \in \mathbb{R}$ with $|F_0| < \varepsilon_\Gamma$, the corrector problem (22) with $L = \infty$ has a solution $q_\infty \in Q_\infty$. For all $v \in Q_\infty$, this solution $q_\infty$ satisfies

$$\langle \delta^2 E^\Gamma(q_\infty; F_0) v, v \rangle \geq \frac{c_a}{2} ||v'||^2, \quad (23)$$

where $c_a$ is the atomistic stability constant for $u_{gr}$ in (11). In addition, there exists a constant $0 \leq \mu_q < 1$ such that

$$|(q_\infty)'| \lesssim \mu_q^\ell \quad \text{for all } \ell \in \mathbb{Z}_{\geq 0}. \quad (24)$$

**Proof.** See Section 5.

We can now consider the existence of a solution to the corrector problem for a finite boundary layer as an approximation of the infinite case.

**Proposition 2.7.** Under the conditions of Theorem 2.6, there exists $L_0 > 0$ such that the corrector problem (22) with $L \geq L_0$ has a solution $q_L \in Q_L$ satisfying

$$\|q''_\infty - q'_L\|_2 \lesssim \mu_q^L. \quad (25)$$

**Proof.** See Section 5.

If $\|f\|_{\mathcal{U}^*}$ is sufficiently small, then Theorem 2.5 guarantees the existence of a solution $u^{cb} \in \mathcal{U}^{cb}$ with $|\nabla u^{cb}(0)| \leq \varepsilon_\Gamma$. Thus, if we choose a sufficiently large boundary layer for the corrector problem (22), Theorem 2.6 and Proposition 2.7 ensure that the predictor-corrector approximation

$$u^{pc}_L := \Pi_a u^{cb} + q_L$$

is well-defined. Next, to determine the accuracy of this approximation, we show that a solution to the atomistic problem (7) exists in a neighborhood of $u^{pc}_L$, which we quantify.

**Theorem 2.8.** There exists an $\varepsilon > 0$ such that, for all $f \in \mathcal{U}^*$ with $\|f\|_{\mathcal{U}^*} < \varepsilon$, there exists an atomistic solution $u^a \in \mathcal{U}$ to (7) satisfying

$$\|u^a' - (u^{pc}_L)'\|_2 \lesssim \mu_q^L + |\nabla^2 u^{cb}(0)| + ||\nabla^2 u^{cb}||^2_4 + ||\nabla^3 u^{cb}||_2 + \|f\|_2. \quad (25)$$

**Proof.** This result is a consequence of the inverse function theorem (Theorem 7.3) and Theorems 6.2 (Consistency) and 6.3 (Stability).
Remark. The term \(|\nabla^2 u^{cb}(0)|\) is an error due to the fact that, in the corrector problem, we replaced the nonlinear elastic field \(\nabla u^{cb}(x)\) with a homogeneous field \(\nabla u^{cb}(0)\). Identifying this term is the main result of our analysis.

The term \(\mu_q^L\), which arises due to the approximation of the corrector problem, may now be balanced against the (uncontrollable) \(|\nabla^2 u^{cb}(0)|\) contribution by choosing \(L \approx \log |\nabla^2 u^{cb}(0)|\). The remaining terms are the typical error committed by the Cauchy–Born model and the error committed in the approximation of the external forces, which are represented by \(\|\nabla^2 u^{cb}\|_{L^2}^2 + \|\nabla^3 u^{cb}\|_{L^2}\) and \(\|\nabla f\|_{L^2}\), respectively.

In preparation for the next section, we observe that the error estimate can be rewritten, using Theorem 2.5, in terms of \(f\) only:

\[
\left\| (u^a)' - (u^{PC}_L)' \right\|_{\ell^2} \lesssim \mu_q^L + |f(0)| + \|f\|_{L^4} + \|\nabla f\|_{L^2}. \tag{26}
\]

2.5 Rescaling of the External Forces

We now consider a standard scaling of the external force typically employed in the analysis of the Cauchy–Born model [12,14]. For the sake of simplicity, we discuss this only formally.

Let \(\lambda^{-1}\) denote a length-scale over which we expect elastic strains to vary. This suggests that after a rescaling of space through \(x \sim \lambda x\) and \(u \sim \lambda u\), the variation will be on an \(O(1)\) scale.

The corresponding dual scaling for the force is \(f(x) \sim \lambda f(\lambda x)\), which motivates us to consider an external force \(f \equiv f(\lambda)\) given by

\[f_\ell(\lambda) := \lambda \hat{f}(\ell),\]

where \(\hat{f} = -\nabla \hat{g}\) for some \(\hat{g} \in H^2(0, \infty)\) with \(|\hat{g}|_{H^2}\) sufficiently small. We then obtain that

\[|f^{(\lambda)}(0)| = \lambda |\hat{f}(0)|, \quad \|f^{(\lambda)}\|_{L^4}^2 = \lambda^{3/2} \|\hat{f}\|_{L^4}^2, \quad \text{and} \quad \|\nabla f^{(\lambda)}\|_{L^2} = \lambda^{3/2} \|\nabla \hat{f}\|_{L^2}.\]

We remark that, in the following, we do not use rescaled \(x\) and \(u\), but we only mentioned this rescaling to motivate our chosen scaling of the external force.

For \(|\hat{g}|_{H^2}\) sufficiently small and \(L\) sufficiently large, we can deduce the existence of the predictor \(u^{cb}\), the corrector \(q_L\), and the corresponding atomistic solution \(u^a\). We can then arrive at the resulting error estimate

\[\left\| (u^a)' - (u^{PC}_L)' \right\|_{\ell^2} \lesssim \mu_q^L + \lambda + \lambda^{3/2},\]

where we kept the \(O(\lambda^{3/2})\) term to emphasize that the Cauchy–Born contribution to the error is negligible compared to the surface contribution. We may now balance the error again by choosing \(L = \log \lambda / \log \mu_q\) to finally obtain

\[\left\| (u^a)' - (u^{PC}_L)' \right\|_{\ell^2} \lesssim \lambda + \lambda^{3/2}.\]

Remark. If we take \(f_\lambda\) as a smooth function rather than a piecewise affine interpolant, then the Cauchy–Born solution is rescaled due to the force rescaling according to \(\nabla u^{cb}_\lambda(x) = \nabla u^{cb}(\lambda x)\). In particular, \(\nabla u^{cb}_\lambda(0)\) would then be independent of \(\lambda\), and thus the corrector problem is independent of \(\lambda\) as well.

In the setting of our analysis, our choice of interpolating \(f\), means this observation is still approximately true. In particular, it is fairly straightforward to extend our analysis rigorously to the setting of § 2.5.
2.6 Numerical Results

In this section, we provide numerical demonstrations of the predictor-corrector method as well as corroboration of the error estimates we established.

As atomistic model use the EAM site energies described in (9) with \( \phi, \psi, \) and \( \rho \) given by

\[
\phi(r) = \phi_e \exp\left(-\gamma \left(\frac{r}{r_e} - 1\right)\right), \quad \rho(r) = f_e \exp\left(-\beta \left(\frac{r}{r_e} - 1\right)\right),
\]

\[
\psi(\rho) = -E_c \left[ 1 - \frac{\alpha}{\beta} \log \left(\frac{\rho}{\rho_e}\right) \right] \left(\frac{\rho}{\rho_e}\right)^{\alpha/\beta} - \phi_e \left(\frac{\rho}{\rho_e}\right)^{\gamma/\beta},
\]

where \( \phi_e = 10.6, f_e = 1, E_c = 3.54, \alpha = 21, \beta = 6, \rho_e = 2, r_e = 1, \) and \( \gamma = 8. \) These parameters and potentials are taken from [11] and represent an EAM potential describing a system composed of copper atoms. We note that \( r_e \) represents the equilibrium distance in the infinite atomistic model without surfaces. Therefore, the equilibrium spacing in the infinite model is simply 1 and corresponds to a strain of 0 as our reference spacing is also 1.

For the numerical implementation, we seek energy-minimizing configurations of the semi-infinite atomistic chain model in the space \( U_N := Q_N, \) instead of \( U. \) Provided \( N \) is sufficiently large so that \( \supp(f) \subset [0, N/2], \) say, it can be proven using the techniques we employed in our analysis that the additional error committed is exponentially small in \( N. \) Due to the low computational cost in one-dimensional experiments, we can choose \( N = 1000 \) throughout, which guarantees that the additional error committed from replacing \( U \) with \( U_N \) is negligible.

We find approximate solutions of the Cauchy–Born problem (17) by seeking minimizers of a discretized Cauchy–Born energy given by

\[
E_{cb}(u) := \sum_{\ell=0}^{\infty} W(u'_\ell), \quad \text{where} \quad W(F) = \frac{1}{2} \phi(1 + F) + \frac{1}{2} \phi(1 + F) + \psi(2\rho(1 + F)).
\]

Proposition 4.2 can be employed to prove that this discretization does not introduce new terms to the error bound (25).

The energy-minimizing configurations for the above models are found using the steepest-descent method with a backtracking algorithm.

2.6.1 Test 1: Ground State

The ground states \( (f = 0) \) of the atomistic, pure Cauchy–Born, and predictor-corrector method are shown in Figure 1a. The atomistic ground state exhibits the predicted exponential decay, but we also observe an alternating sign behavior common to certain metals such as copper.

The pure Cauchy–Born solution clearly does not capture any surface effects. For the predictor-corrector method, we see that \( u_{pc}^2 \) already yields good accuracy while \( u_{pc}^5 \) is visually indistinguishable from \( u_{gr}^5. \) In Figure 1b, we quantify this by numerically demonstrating the exponential convergence of \( q_L = u_{pc}^L \) to the ground state.
Comparison of Ground States

(a)

Error Due to Increasing Boundary Layer

(b)

Figure 1: Ground states for the atomistic, Cauchy–Born, and predictor-corrector methods along with a demonstration of the exponential convergence of the boundary layer error.

2.6.2 Test 2: Long Wavelength Limit

We next consider the error under the long wavelength limit and rescaling described in §2.5. We define \( f(x) = \cos(3\pi x/8) \chi_{[0,4]}(x) \), where \( \chi_A(x) \) denotes the characteristic function, and \( f_\ell = \lambda f(\lambda \ell) \). For each \( \lambda \), we compute the solution to the predictor-corrector method with the size of the boundary layer set to \( L = 3 + \lceil \log_{10}(\lambda^{-1}) \rceil \). This choice of \( L \) is motivated from the discussion of balancing the boundary layer contribution to the error in §2.5. By choosing a logarithm with a base less than \( \mu_q^{-1} \) in the choice of \( L \), the surface contribution to the error becomes \( \lambda^\eta \) where \( \eta > 1 \) is a constant. Figure 2 shows the first-order convergence that results when the scaling factor \( \lambda \) is taken to zero. The predictor-corrector method behaves precisely as predicted in §2.5.

2.6.3 Test 3: Error with External Forces

We wish to highlight the fact that the error made by the predictor-corrector method’s approximation will not vanish with increasing boundary layer in the case of fixed non-zero external forces. To that end, we consider \( f_\ell = f(\ell) \), where \( f \) is given in §2.6.2. In Figure 3a, we display the energy-minimizing configurations for the atomistic solution, the Cauchy–Born solution, and the predictor-corrector method with \( L = 5 \). We observe that a small error in the boundary layer still persists. Indeed, since the error depends on the magnitude and regularity of \( f \) as demonstrated in (26), it cannot be driven to zero. This is numerically demonstrated by Figure 3b. We emphasize, however, that despite our extremely concentrated and non-smooth choice of \( f \), the predictor-corrector method is able to reduce the error by a factor of 30, which is an excellent improvement given the simplicity of the predictor-corrector scheme.

2.7 Conclusions

We produced a detailed analysis of an atomistic surface in a 1D model problem. Based on this analysis, we showed that, while a regular Cauchy–Born method fails to accurately capture the surface effects, it can be corrected (post-processed) using a computationally cheap surface cell-problem. We gave a sharp error analysis of this new predictor-corrector scheme and, in particular,
Figure 2: Rate of convergence to atomistic solution in the long-wavelength limit.

Figure 3: (a) Energy-minimizing configuration for atomistic and predictor-corrector systems in the presence of external forces. Here, the size of the boundary layer for the predictor-corrector problem is $L = 5$. (b) Demonstration of non-vanishing error in the presence of non-zero external forces and increasing boundary layer.
showed that its error relative to the fully atomistic solution tends to zero in a natural scaling limit. Our numerical results show promising quantitative behavior of the proposed scheme.

While the analysis is one-dimensional, we anticipate that it can shed some light even on the three-dimensional case, when surface behavior dominates edge or corner effects. An important new effect that will have to be taken into account in two and three dimensions are surface stresses that act tangentially.

3 Proofs: Atomistic Model

Proof of Theorem 2.1 We employ the direct method of the calculus of variations. Property (iii) on the site potential energies and the fact that \(|V_{\text{surf}}(0)| < \infty\) implies that \(E^a(u) \geq 0\). We may therefore consider an energy minimizing sequence \(\{u_n\}_{n=1}^\infty \subset \mathcal{U}\) such that

\[
E^a(u_n) \to \inf_{u \in \mathcal{U}} E^a(u) \quad \text{and} \quad E^a(u_n) < \inf_{u \in \mathcal{U}} E^a(u) + 1. \tag{27}
\]

We wish to show that \(|u_n|_{H^1} = \|u_n'\|_{L^2(\mathbb{Z}_{\geq 0})}\) is uniformly bounded. To that end, we will consider separately the contributions to the norm from the small and large strains. Let \(\varepsilon > 0\). For each \(n \in \mathbb{N}\), we denote the set of indices that indicate the locations of \(\varepsilon\)-defects in the chain to be \(D_n^\varepsilon\):

\[
D_n^\varepsilon := \{\ell \in \mathbb{Z}_{\geq 0} \mid |u_n',\ell| > \varepsilon \text{ or } |u_n',\ell+1| > \varepsilon\}.
\]

Property (v) implies that there exists a \(\tau > 0\) such that

\[
V(u_n',\ell, u_n',\ell+1) \geq \tau \quad \text{for all } \ell \in D_n^\varepsilon.
\]

Since \(V \geq 0\), we obtain

\[
E^a(u_n) \geq \sum_{\ell \in D_n^\varepsilon} V(u_n',\ell, u_n',\ell+1) \geq \tau \# D_n^\varepsilon.
\]

Hence, the cardinality of \(D_n^\varepsilon\) is uniformly bounded; that is,

\[
\max_n \# D_n^\varepsilon < \infty. \tag{28}
\]

We now analyze small strains. By Taylor’s Theorem and Property (iv), we may show that for small enough \(\varepsilon\) there exists a constant \(C_\varepsilon > 0\) such that

\[
V(u_{n,\ell}', u_{n,\ell+1}') \geq C_\varepsilon (|u_{n,\ell}'|^2 + |u_{n,\ell+1}'|^2) \quad \text{for all } \ell \notin D_n^\varepsilon.
\]

With this inequality and the positivity of the site energies, we obtain

\[
E^a(u_n) = V_{\text{surf}}(u_{n,0}') + \sum_{\ell \in \mathbb{Z}_{\geq 0}} V(u_n',\ell, u_n',\ell+1)
\]

\[
= V_{\text{surf}}(u_{n,0}') + \sum_{\ell \in D_n^\varepsilon} V(u_n',\ell, u_n',\ell+1) + \sum_{\ell \notin D_n^\varepsilon} V(u_n',\ell, u_n',\ell+1)
\]

\[
\geq C_\varepsilon \sum_{\ell \notin D_n^\varepsilon} (|u_{n,\ell}'|^2 + |u_{n,\ell+1}'|^2).
\]

From (27), we deduce the bound

\[
\sum_{\ell \notin D_n^\varepsilon} |u_{n,\ell}'|^2 \leq C_\varepsilon^{-1} \left( \inf_{u \in \mathcal{U}} E^a(u) + 1 \right) < \infty. \tag{29}
\]
Note that the upper bound \( |u_{n,\ell}'| \leq C \) for all \( n \in \mathbb{N}, \ell \in \mathbb{Z}_{\geq 0} \) (30) then we obtain a uniform bound on \( \|u_n'\|_{L^2} \).

Suppose, for contradiction, that (30) fails. Then, there exists a subsequence \( \{u_{n_k}\}_{k=1}^\infty \) and a sequence of indices \( \{\ell_k\}_{k=1}^\infty \) such that

\[
\lim_{k \to \infty} |u_{n_k,\ell_k}'| \to \infty.
\] (31)

Since \( \max_n \#D_\varepsilon^n \) is finite, we may add the condition on the indices \( \ell_k \) that there exists a constant \( S > 0 \) such that

\[
|u_{n_k,\ell_k+1}'| \leq S \quad \text{for all } k.
\] (32)

We now split the chain into two components,

\[
E_a(u_{n_k}) = V_{\text{surf}}(u_{n_k,0}') + \sum_{\ell=0}^{\ell_k-1} V(u_{n_k,\ell}', u_{n_k,\ell+1}')
+ V(u_{n_k,\ell_k}', u_{n_k,\ell_k+1}') + \sum_{\ell=\ell_k+1}^\infty V(u_{n_k,\ell}', u_{n_k,\ell+1}')
=: E_1 + E_2.
\]

Since \( V \geq 0 \), we obtain

\[
E_1 = V_{\text{surf}}(u_{n_k,0}') + \sum_{\ell=0}^{\ell_k-1} V(u_{n_k,\ell}', u_{n_k,\ell+1}') \geq \inf_{s' \in \mathbb{R}} V_{\text{surf}}(s') > 0.
\]

To bound \( E_2 \), we observe that this group represents a semi-infinite chain that has, up to a small error, decoupled from the first group. Therefore it is bounded below by the infimum of the energy. To make this precise, let \( \varepsilon_1 := \frac{1}{2} \inf_{s' \in \mathbb{R}} V_{\text{surf}}(s') > 0 \). By Properties (vi) and (ii), there exists \( R > 0 \) such that if \( |r| > R \), then \( |V(r, s) - V_{\text{surf}}(s)| < \varepsilon_1 \) for all \( |s| \leq S \). From (31), there exists a \( K > 0 \) such that \( |u_{n_k,\ell_k}'| > R \) for all \( k \geq K \).

Therefore, we can conclude that, for \( k \geq K \),

\[
E_2 = V(u_{n_k,\ell_k}', u_{n_k,\ell_k+1}') + \sum_{\ell=\ell_k+1}^\infty V(u_{n_k,\ell}', u_{n_k,\ell+1}')
\geq V_{\text{surf}}(u_{n_k,\ell_k+1}') - \varepsilon_1 + \sum_{\ell=\ell_k+1}^\infty V(u_{n_k,\ell}', u_{n_k,\ell+1}')
\geq \inf_{u \in \mathcal{A}} E_a(u) - \varepsilon_1
\]

In summary, we have shown that, for \( k \geq K \),

\[
E_a(u_{n_k}) = E_1 + E_2 \geq \frac{1}{2} \inf_{s' \in \mathbb{R}} V_{\text{surf}}(s') + \inf_{u \in \mathcal{A}} E_a(u).
\]

Since \( \frac{1}{2} \inf_{s' \in \mathbb{R}} V_{\text{surf}}(s') > 0 \), this contradicts the fact that \( \{u_{n_k}\} \) is a minimizing sequence.
Therefore, \[30\] holds and together with (28) and (29), and we deduce that \(\|u_n'\|_{\ell^2}\) is uniformly bounded. Upon passing to a subsequence (not relabeled), we may assume that there exists \(u'_\infty \in \ell^2(\mathbb{Z}_{\geq 0})\) such that \(u'_n \rightharpoonup u'_\infty\) weakly in \(\ell^2\). In particular, this implies that
\[
u_n \to u'_\infty, \quad \text{for all } \ell \in \mathbb{Z}_{\geq 0}.
\]
We may now prove that \(u_\infty\) is a minimizer by employing Fatou’s Lemma to estimate
\[
\inf_{u \in U} \mathcal{E}^a(u) = \liminf_{n \to \infty} \mathcal{E}^a(u_n) \\
\geq \liminf_{n \to \infty} V^{\text{surf}}(u'_n,0) + \sum_{\ell = 0}^\infty \liminf_{n \to \infty} V(u'_{n,\ell},u'_{n,\ell+1}) = \mathcal{E}^a(u_\infty).
\]
Thus, \(u_\infty\) is an energy minimizing configuration of the atomistic energy \(\mathcal{E}^a\) in \(U\).

\textbf{Proof of Theorem 2.2} Critical points of \(\mathcal{E}^a\) satisfy the Euler–Lagrange equation
\[
\langle \delta \mathcal{E}^a(u'), v' \rangle = 0 \quad \text{for all } v \in U.
\]
Expanding the first variation \(\delta \mathcal{E}^a(u')\) about \(u' = 0\) yields
\[
\langle \delta \mathcal{E}^a(0) + \delta^2 \mathcal{E}^a(0)u' + \zeta(u'), v' \rangle = 0,
\]
where \(\zeta(u')\) is the remainder term from the expansion which can be readily shown to satisfy the bounds
\[
|\zeta_0| \lesssim |u'_0|^2 + |u'_1|^2 \quad \text{and} \quad |\zeta_\ell| \lesssim |u'_{\ell-1}|^2 + |u'_\ell|^2 + |u'_{\ell+1}|^2 \quad \text{for } \ell \geq 1.
\]
We may explicitly compute the remaining terms in the Taylor series expansion keeping in mind that \(V(F,F)\) achieves its minimum at \((0,0)\):
\[
\langle \delta \mathcal{E}^a(0), v' \rangle = v'_0 \left\{ \partial_F V^{\text{surf}}(0) \right\} \quad \text{and}
\langle \delta^2 \mathcal{E}^a(0)u', v' \rangle = v'_0 u'_0 \left\{ \partial_F^2 V^{\text{surf}}(0) + \partial_{11}^2 V(0,0) \right\} + v'_0 u'_1 \left\{ \partial_{12}^2 V(0,0) \right\}
+ \sum_{\ell = 1}^\infty v'_\ell \left[ u'_{\ell-1} \left\{ \partial_{12}^2 V(0,0) \right\} + u'_\ell \left\{ \partial_{22}^2 V(0,0) + \partial_{11}^2 V(0,0) \right\} + u'_{\ell+1} \left\{ \partial_{12}^2 V(0,0) \right\} \right].
\]
Let
\[
b := \partial_{12}^2 V(0,0), \quad a := \partial_{11}^2 V(0,0) + \partial_{22}^2 V(0,0), \quad \text{and} \quad a_s := \partial_F^2 V^{\text{surf}}(0) + \partial_{11}^2 V(0,0),
\]
then we see that \(u'\) solves the system
\[
a_s u'_0 + bu'_1 = -\zeta_0 - \left( \partial_F V^{\text{surf}}(0) \right) =: \tilde{\zeta}_0, \quad \text{(34)}
b u'_{\ell+1} + au'_\ell + bu'_{\ell-1} = -\zeta_\ell \quad \text{for } \ell \geq 1. \quad \text{(35)}
\]
We now suppose that \(b \neq 0\). The case when \(b = 0\) is analogous. Solving for the homogeneous solution to this system of equations gives
\[
u'_\ell = c_+ \lambda_+^\ell + c_- \lambda_-^\ell, \quad \text{where} \quad \lambda_{\pm} = \frac{-a \pm \sqrt{a^2 - 4b^2}}{2b}.
\]
Positive definiteness of $\nabla^2 V(0,0)$ from Property [iv] implies that $a - 2b > 0$ and $a + 2b > 0$. Hence, the discriminant is always positive, $a^2 - 4b^2 > 0$, and as a result, $\lambda_+ \neq \lambda_-$. The symmetry of $35$ implies that $\lambda_+ = 1/\lambda_-$. This relation combined with the fact that the discriminant is never 0 implies that $\lambda_\pm \neq 1$. Without loss of generality, then, we must have that $0 < |\lambda_+| < 1$ and $|\lambda_-| > 1$. As solutions to the atomistic problem must belong to $\mathcal{U}$, we have that $u'_0 \to 0$ as $\ell \to \infty$. This boundary condition at infinity implies that $c_\ell = 0$ in order to prevent exponential growth in the strain. Thus, letting $\lambda := \lambda_+$, we have that solutions of the homogeneous equation are of the form $u'_\ell = u'_0 \lambda^\ell$. A discrete Green’s function argument provides the solution for the inhomogeneous equation:

$$u'_\ell = C_{BC} \lambda^\ell + D^{-1} \sum_{k=0}^{\infty} \lambda^{\ell-k} |\zeta_k|,$$

where $D := \sqrt{a^2 - 4b^2}$ and $C_{BC}$ can be determined from $u'_0$. Taking the absolute value of both sides, using the triangle inequality, and applying $33$, we can estimate

$$|u'_\ell| \leq C_{BC} \lambda^\ell + D^{-1} \sum_{k=0}^{\infty} |\lambda|^{\ell-k} |\zeta_k| \leq C_{BC} \lambda^\ell + D^{-1} \sum_{k=0}^{\infty} |\lambda|^{\ell-k} |u'_k|^2.$$

Let $\mu$ be a constant such that $|\lambda| < \mu < (1 + |\lambda|)/2$. Then,

$$\sum_{m=0}^{\infty} \mu^{\ell-m} |u'_m| \leq \sum_{m=0}^{\infty} C_{BC} \mu^{\ell-m} |\lambda|^m + D^{-1} \sum_{m,k\geq 0} \mu^{\ell-m} |\lambda|^{m-k} |u'_k|^2.$$

Using the observation that

$$\sum_{m=0}^{\infty} \mu^{\ell-m} |\lambda|^{m-k} \lesssim \mu^{\ell-k},$$

we arrive at

$$\sum_{m=0}^{\infty} \mu^{\ell-m} |u'_m| \lesssim C_{BC} \mu^\ell + D^{-1} \sum_{k=0}^{\infty} \mu^{\ell-k} |u'_k|^2. \tag{36}$$

Ignoring the prefactor $D^{-1}$, the second term on the right-hand side of (36) can be bounded by

$$\sum_{k=0}^{\infty} \mu^{\ell-k} |u'_k|^2 = \sum_{k\leq k_0} \mu^{\ell-k} |u'_k|^2 + \sum_{k > k_0} \mu^{\ell-k} |u'_k|^2 \lesssim \mu^\ell + \sup_{k \geq k_0} |u'_k| \sum_{k \geq k_0} \mu^{\ell-k} |u'_k|.$$

For any $\varepsilon > 0$, we can choose $k_0$ sufficiently large so that $\sup_{k \geq k_0} |u'_k| \leq \varepsilon$. Hence, we arrive at

$$D^{-1} \sum_{k=0}^{\infty} \mu^{\ell-k} |u'_k|^2 \lesssim \mu^\ell + \varepsilon \sum_{k \geq k_0} \mu^{\ell-k} |u'_k|.$$

Substituting this bound into (36) yields

$$(1 - \varepsilon)|u'_\ell| \leq (1 - \varepsilon) \sum_{k=0}^{\infty} \mu^{\ell-k} |u'_k| \lesssim \mu^\ell.$$
4 Proofs: Cauchy–Born Model

Proof of Proposition 2.4. Let \( u = 0 \). Then, Properties (iii)–(v) imply that \( \delta \mathcal{E}^a(u) \) is given by

\[
\langle \delta \mathcal{E}^a(u), v \rangle = v_0' \left\{ \partial_F V^\text{surf}(u_0) + \partial_1 V(u_0, u_1') \right\} + \sum_{\ell=1}^{\infty} v_\ell' \left\{ \partial_2 V(u_{\ell-1}', u_\ell') + \partial_1 V(u_\ell', u_{\ell+1}') \right\}
\]

\[
= v_0' \partial_F V^\text{surf}(0).
\]

This is maximized by taking \( v_0' = \text{sign}(\partial_F V^\text{surf}(0)) \) and \( v_\ell' = 0 \) for \( \ell > 0 \), thus proving the first statement.

To deduce the lower bound on the error, we simply observe that

\[
|\partial_F V^\text{surf}(0)| = \|\delta \mathcal{E}^a(0)\|_{\mathcal{U}^*} = \|\delta \mathcal{E}^a(0) - \delta \mathcal{E}^a(u^a_0)\|_{\mathcal{U}^*} \leq M \|(u^b - u^a_0)\|_{\ell^2}.
\]

Before we state the next result, recall that \( f \in \mathcal{U}^* \) if and only there exists \( g \in \ell^2(\mathbb{Z}_{\geq 0}) \) such that \( \langle f, u \rangle = \langle g, u' \rangle \). Summation by parts, with the convention \( g_{-1} = 0 \), may be used to show that

\[
f_\ell = g_\ell - g_{\ell-1}.
\]

Conversely, if we are given \( f \), we may recover \( g \) via

\[
g_\ell := \sum_{k=\ell+1}^{\infty} f_k := \lim_{K \to \infty} \sum_{k=\ell+1}^{K} f_k.
\]

In the Cauchy–Born model, we identify \( f \) with its piecewise affine interpolant. The continuous analogue of (38) is

\[
\tilde{g}(x) := \int_0^\infty f(s) \, ds := \lim_{K \to \infty} \int_x^K f(s) \, ds.
\]

Lemma 4.1. Let \( f \in \mathcal{U}^* \). Then, \( g \) and \( \tilde{g} \) are well-defined and satisfy the estimates

\[
|g_\ell - \tilde{g}(\ell + 1/2)| \leq \frac{1}{2} |f'_\ell| \quad \text{for all } \ell \in \mathbb{Z}_{\geq 0}, \quad \text{and}
\]

\[
|\tilde{g}(x)| \leq C \ell+1 \sum_{m=\ell-1}^{\ell+1} |g_m| \quad \text{for all } x \in [\ell, \ell + 1].
\]

Proof. Since \( f \in \mathcal{U}^* \) there exists \( g \in \ell^2 \) such that (37) holds. Let \( M > \ell + 1 \). Then,

\[
\sum_{m=\ell+1}^{M} f_m = \sum_{m=\ell+1}^{M} (g_{\ell-1} - g_\ell) = g_\ell - g_M \to g_\ell \quad \text{as } M \to \infty.
\]

Hence, (38) is well-defined.

Similarly, let \( M \in \mathbb{Z} \) and \( M > \ell + 1 \). Then,

\[
\int_{\ell+1/2}^{\ell+1/2} f(s) \, ds - \sum_{m=\ell+1}^{M} f_m = \int_{\ell+1/2}^{\ell+1/2} f(s) \, ds + \int_{\ell+1/2}^{\ell+1} f(s) \, ds - \sum_{m=\ell+1}^{M} f_m
\]

\[
= \frac{1}{2} \left( \frac{1}{3} (f_\ell + f_{\ell+1}) + \frac{1}{2} f_{\ell+1} \right) + \sum_{m=\ell+1}^{M-1} \left[ \frac{1}{2} (f_m + f_{m+1}) - f_m \right] - f_M
\]

\[
= \frac{1}{2} (f_\ell - f_{\ell+1}) - \frac{1}{2} f_M \to \frac{1}{2} (f_\ell - f_{\ell+1}) \quad \text{as } M \to \infty.
\]
Thus, we can conclude that $\tilde{g}(x)$ is well-defined for all $x$, as well as the stated estimate (40).

To prove the second estimate, we simply note that, for $x \in [\ell, \ell + 1]$,
\[
|\tilde{g}(x) - \tilde{g}(\ell + 1/2)| = \left| \int_{\ell + 1/2}^{x} f(s) \, ds \right| \lesssim |f_\ell| + |f_{\ell+1}|,
\]
and then apply (37).

Next, we prove Theorem 2.5. In addition to the bounds stated therein, we will also establish that
\[
|\nabla u_{cb}(x)| \lesssim |\tilde{g}(x)|,
\]
(42)

Proof of Theorem 2.5 and of (42). The Euler–Lagrange equation of the Cauchy–Born problem (17) is
\[
-\nabla \partial F W(\nabla u) = f.
\]
(43)

Formally integrating over $(x, \infty)$ and using the fact that $\partial F W(0) = 0$, we obtain
\[
\partial F W(\nabla u) = \int_{x}^{\infty} f(s) \, ds = \tilde{g}(x).
\]

We will now produce a function $u \in H^3_{loc}$ satisfying this equation.

From Properties [iv] and [ii], there exists $G > 0$ such that $\partial^2 F W(F) > \frac{1}{2} \partial_F^2 W(0) > 0$ on $[-G, G]$. Thus, $\partial F W(F)$ is strictly monotone on this interval. The bound (41) implies that, for $\varepsilon_{cb}$ sufficiently small, $\tilde{g}([0, \infty)) \subset \partial F W([-G, G])$. Hence, we can define
\[
\nabla u(x) = (\partial F W)^{-1}(\tilde{g}(x)),
\]
where $(\partial F W)^{-1}$ is defined to have range in $[-G, G]$. Due to the restriction on the range of the inverse function, $\nabla u(x) \in [-G, G]$, hence it follows that the solution must be stable with a stability constant $c_{cb} \geq \frac{1}{2} \partial_F^2 W(0)$.

It is further easy to show with this that $(\partial F W)^{-1}$ is twice continuously differentiable, and in particular, Lipschitz. Noting that $(\partial F W)^{-1}(0) = 0$, Lipschitz continuity then yields the bound
\[
|\nabla u_{cb}(x)| = |(\partial F W)^{-1}(\tilde{g}(x)) - (\partial F W)^{-1}(0)| \lesssim |\tilde{g}(x)|,
\]
where we have ignored the Lipschitz constant for the inverse function.

The remaining estimates are consequences of the fact that $\tilde{g} \in C^{1,1}(\mathbb{R}_{\geq 0})$ with $\nabla \tilde{g} = -f$ and $\nabla^2 \tilde{g} = -\nabla f$ along with an elementary computation.

Next, we recall an auxiliary result that allows us to reduce the continuous Cauchy–Born model to a discrete model. To that end, we recall that we can identify discrete test functions $v \in \mathcal{U}$ with continuous test functions $v \in \mathcal{U}_{cb}$ via piecewise affine interpolation. Through the same identification, we can also admit $u \in \mathcal{U}$ as arguments for $\delta \mathcal{E}_{cb}$.

Proposition 4.2. Under the conditions of Theorem 2.5, we have
\[
|\langle \delta \mathcal{E}_{cb}(u_{cb}^v) - \delta \mathcal{E}_{cb}(\Pi_u u_{cb}^v), v \rangle| \lesssim \|\nabla^2 u_{cb}^v\|_{L^4} \|\nabla v\|_{L^2} \quad \text{for all} \quad v \in \mathcal{U}.
\]

Proof. This result is a simplified variant of [12, Lemma 5.2].
5 Proofs: Corrector Problem

Proof of Theorem 2.6: Consistency: It is reasonable to expect that, for \(|F_0|\) small, the corrector solution \(q_\infty\) is close to \(u^a_\partial\), so we may find \(q_\infty\) be applying the inverse function theorem in a neighborhood of \(u^a_\partial\). From Proposition 7.1 the first variation of the corrector energy evaluated at \(\tilde{q} = u^a_\partial\) is

\[
\langle \delta \mathcal{E}^\Gamma(\tilde{q}; F_0), v \rangle = v_0' \left\{ \partial_F V^{\text{surf}}(F_0 + \tilde{q}'_0) + \partial_1 V(F_0 + \tilde{q}'_0, F_0 + \tilde{q}'_1) - \partial_F W(F_0) \right\} \\
+ \sum_{\ell=1}^{\infty} v'_\ell \left\{ \partial_2 V(F_0 + \tilde{q}'_{\ell-1}, F_0 + \tilde{q}'_\ell) + \partial_1 V(F_0 + \tilde{q}'_\ell, F_0 + \tilde{q}'_{\ell+1}) - \partial_F W(F_0) \right\},
\]

where \(v \in Q_\infty\). Using the fact that \(\delta \mathcal{E}^a(\tilde{q}) = 0\) and \(\partial_F W(0) = 0\), we obtain

\[
\langle \delta \mathcal{E}^\Gamma(\tilde{q}; F_0), v \rangle = \langle \delta \mathcal{E}^\Gamma(\tilde{q}; F_0) - \delta \mathcal{E}^a(\tilde{q}), v \rangle \\
= v_0' \left\{ \partial_F V^{\text{surf}}(F_0 + \tilde{q}'_0) + \partial_1 V(F_0 + \tilde{q}'_0, F_0 + \tilde{q}'_1) - \partial_F W(F_0) \\
- \partial_F V^{\text{surf}}(\tilde{q}'_0) - \partial_1 V(\tilde{q}'_0, \tilde{q}'_1) + \partial_F W(0) \right\} \\
+ \sum_{\ell=1}^{\infty} v'_\ell \left\{ \partial_2 V(F_0 + \tilde{q}'_{\ell-1}, F_0 + \tilde{q}'_\ell) + \partial_1 V(F_0 + \tilde{q}'_\ell, F_0 + \tilde{q}'_{\ell+1}) - \partial_F W(F_0) \\
- \partial_2 V(\tilde{q}'_{\ell-1}, \tilde{q}'_\ell) - \partial_1 V(\tilde{q}'_\ell, \tilde{q}'_{\ell+1}) + \partial_F W(0) \right\} \\
= \sum_{\ell=0}^{\infty} v'_\ell A_\ell.
\]

Using Lipschitz continuity of all potential derivatives we easily obtain that

\[|A_0| \lesssim |F_0|\]

To estimate \(A_\ell\) for \(\ell \geq 1\), we proceed more carefully. Expanding with respect to \(\tilde{q}_j\) for \(j = \ell - 1, \ell, \ell + 1\), employing the identity \(\partial_F W(F) = \partial_1 V(F, F) + \partial_2 V(F, F)\), and the global Lipschitz continuity of \(\partial^2 V\), we obtain

\[
|A_\ell| = \left| \left\{ \partial_2 V(F_0, F_0) + \partial_1 V(F_0, F_0) - \partial_2 W(F_0) \right\} - \left\{ \partial_2 V(0, 0) + \partial_1 V(0, 0) - \partial_2 W(0) \right\} \right| \\
+ \int_0^1 \left\{ \partial_2 V(F_0 + t\tilde{q}'_{\ell-1}, F_0 + t\tilde{q}'_\ell) - \partial_2 V(t\tilde{q}'_{\ell-1}, t\tilde{q}'_\ell) \right\} \cdot \frac{\tilde{q}'_{\ell-1}}{\tilde{q}'_\ell} \, dt \\
+ \int_0^1 \left\{ \partial_1 V(F_0 + t\tilde{q}'_{\ell}, F_0 + t\tilde{q}'_{\ell+1}) - \partial_1 V(t\tilde{q}'_{\ell}, t\tilde{q}'_{\ell+1}) \right\} \cdot \frac{\tilde{q}'_\ell}{\tilde{q}'_{\ell+1}} \, dt \\
\lesssim |F_0| (|\tilde{q}'_{\ell-1}| + |\tilde{q}'_\ell| + |\tilde{q}'_{\ell+1}|).
\]

An application of the Cauchy–Schwartz inequality yields

\[
\langle \delta \mathcal{E}^\Gamma(\tilde{q}; F_0), v \rangle \leq \|A\|_{L^2} \|v'\|_{L^2} \lesssim |F_0|(1 + \|q'\|_{L^2}) \|v'\|_{L^2}.
\] (44)
Choosing and an application of Theorem 7.3 implies the existence of an equilibrium that
L theorem, Theorem 7.3, using the projected solution Π
Proof of Proposition 2.7. The result is proven by an application of the quantitative inverse function
Thus, Lemma 5.1. Let
First, note that
Employing Lipschitz continuity of
multiplied by a simple factor. Thus, we obtain, for
The consistency estimate (44), the stability estimate (45), Lipschitz continuity of
To analyze the projection of the corrector problem from
Stability: Recall that \( \bar{q} = v_{\gamma}^\infty \) is strongly stable in the atomistic model (11) with stability constant \( c_a > 0 \). To prove stability of \( \delta^2 \mathcal{E}^\Gamma(\bar{q}; F_0) \), we simply bound the error in the Hessians:

\[
\langle \delta^2 \mathcal{E}^\Gamma(\bar{q}) - \delta^2 \mathcal{E}^\Gamma(\bar{q}; F_0) \rangle \leq C |F_0| \left\| v' \right\|_{\ell_2}^2.
\]

where the constant \( C \) is the upper bound on the Lipschitz constants involved in the estimate multiplied by a simple factor. Thus, we obtain, for \( |F_0| \leq \frac{1}{4} c_a / C \):

\[
\langle \delta^2 \mathcal{E}^\Gamma(\bar{q}; F_0) \rangle \geq \frac{3 c_a}{4} \left\| v' \right\|_{\ell_2}^2 \quad \text{for all} \quad v \in \mathcal{Q}_\infty.
\]

(45)

The consistency estimate (44), the stability estimate (45), Lipschitz continuity of \( q \mapsto \delta^2 \mathcal{E}^\Gamma(q; F_0) \), and an application of Theorem 7.3 implies the existence of an equilibrium \( q_\infty \) with \( \| q' - q_\infty' \|_{\ell_2} \lesssim |F_0| \).

Choosing \( F_0 \) sufficiently small and once again using the Lipschitz continuity of \( \delta^2 \mathcal{E}^\Gamma \) implies (23).

The exponential decay in (24) follows from a straightforward modification of Theorem 2.2.

To analyze the projection of the corrector problem from \( \mathcal{Q}_\infty \) to \( \mathcal{Q}_L \), we introduce a projection operator \( \Pi_L : \mathcal{Q}_\infty \to \mathcal{Q}_L \) via

\[
(\Pi_L q_\ell)' := \begin{cases} q_\ell', & \ell = 0, \ldots, L, \\ 0, & \ell > L. \end{cases}
\]

Lemma 5.1. Let \( q \in \mathcal{Q}_\infty \) satisfy \( |q_\ell'| \lesssim \mu^\ell \) for some \( \mu \in [0, 1) \). Then,

\[
\| q' - \Pi_L q' \|_{\ell_2} \lesssim \mu^L.
\]

Proof. First, note that

\[
q_\ell' - (\Pi_L q)'_\ell = \begin{cases} 0, & 0 \leq \ell \leq L - 1, \\ q_\ell', & \ell > L. \end{cases}
\]

Thus,

\[
\| q' - \Pi_L q' \|_{\ell_2}^2 = \sum_{\ell=L}^\infty |q_\ell'|^2 \lesssim \sum_{\ell=L}^\infty \mu^{2\ell} = \frac{\mu^{2L}}{1 - \mu^2}.
\]

Proof of Proposition 2.7. The result is proven by an application of the quantitative inverse function theorem, Theorem 7.3, using the projected solution \( \Pi_L q_\infty \) as an approximate solution. Observe that

\[
\langle \delta \mathcal{E}^\Gamma(q_\infty; F_0), v \rangle = 0 \quad \text{for all} \quad v \in \mathcal{Q}_L \subset \mathcal{Q}_\infty,
\]

where \( q_\infty \) solves the infinite corrector problem. By the Lipschitz continuity of \( \delta \mathcal{E}^\Gamma \),

\[
|\langle \delta \mathcal{E}^\Gamma(\Pi_L q_\infty; F_0), v \rangle | = |\langle \delta \mathcal{E}^\Gamma(\Pi_L q_\infty; F_0) - \delta \mathcal{E}^\Gamma(q_\infty; F_0), v \rangle | \lesssim \| q_\infty' - \Pi_L q_\infty' \|_{\ell_2} \left\| v' \right\|_{\ell_2}.
\]
According to Theorem 2.6, there exists $0 \leq \mu_q < 1$ such that $|\langle q_\infty \rangle^c| \lesssim \mu_q^L$. Hence, Lemma 5.1 may be applied to show that

$$\|\delta E^\Gamma(\Pi_L q_\infty; F_0)\|_{\mathcal{Q}_L} = \sup_{v \in \mathcal{Q}_L, \|v\|_{\ell^2} = 1} |\langle \delta E^\Gamma(\Pi_L q_\infty; F_0), v \rangle| \lesssim \mu_q^L.$$

Stability of $\Pi_L q_\infty$ follows from the stability of $q_\infty$ (Theorem 2.6), the Lipschitz continuity of $\delta^2 E^\Gamma$, and Lemma 5.1.

$$\langle \delta E^\Gamma(\Pi_L q_\infty; F_0), v \rangle = \langle \delta E^\Gamma(q_\infty; F_0), v \rangle - \left[ \langle \delta E^\Gamma(\Pi_L q_\infty; F_0), v \rangle - \langle \delta E^\Gamma(q_\infty; F_0), v \rangle \right]$$

$$\geq \langle \delta E^\Gamma(q_\infty; F_0), v \rangle - M\|q_\infty' - \Pi_L q_\infty\|_{\ell^2}^2 \|v\|_{\ell^2}^2$$

$$\geq \left( \frac{c_a}{2} - CM\mu_q^L \right) \|v\|_{\ell^2},$$

where $M$ is the Lipschitz constant for $E^\Gamma$ and $C$ is the unlisted constant in [5].

For $L$ sufficiently large, all assumptions of Theorem 7.3 are met, and its application completes the proof.

### 6 Proofs: Predictor-Corrector Method

The center-piece of our analysis of the predictor-corrector method is the following consistency error estimate. In its statement, we employ the notation

$$u''_\ell := u'_{\ell+1} - u'_\ell \quad \text{and} \quad u''''_\ell := u'_{\ell-1} - 2u'_\ell + u'_\ell.$$

**Theorem 6.1.** Let $w, q \in \mathcal{U}$, $u := w + q$, and $F_0 \in \mathbb{R}$. Then, for all $v \in \mathcal{U}$,

$$|\langle \delta E^a(u) - \delta E^{cb}(w) - \delta E^\Gamma(q; F_0), v \rangle| \lesssim \left[ \|w''\|_{\ell^2(\mathbb{Z}_{\geq 0})}^2 + \|w'''\|_{\ell^2(\mathbb{Z}_{>0})}^2 + \|q'' \cdot w''\|_{\ell^2(\mathbb{Z}_{>0})} \right] \|v\|_{\ell^2}.$$

**Proof.** The difference in the first variations is given by

$$\langle \delta E^a(u) - \delta E^{cb}(w) - \delta E^\Gamma(q; F_0), v \rangle = v_0' \left[ \left\{ \partial_F V^{\text{surf}}(u'_0) + \partial_1 V(u'_0, u'_1) \right\} - \left\{ \partial_F W(F_0) \right\} \right.$$

$$- \left\{ \partial_F V^{\text{surf}}(F_0 + q'_0) + \partial_1 V(F_0 + q'_0, F_0 + q'_1) - \partial_F W(F_0) \right\} \right]$$

$$+ \sum_{\ell=1}^{\infty} v'_\ell \left[ \left\{ \partial_2 V(u'_{\ell-1}, u'_\ell) + \partial_1 V(u'_\ell, u'_{\ell+1}) \right\} - \left\{ \partial_F W(w'_\ell) \right\} \right.$$

$$- \left\{ \partial_2 V(F_0 + q'_{\ell-1}, F_0 + q'_\ell) + \partial_1 V(F_0 + q'_\ell, F_0 + q'_{\ell+1}) - \partial_F W(F_0) \right\} \right]$$

$$=: S + B,$$

where $S, B$ denote, respectively, the surface and bulk contributions to the consistency error.
Surface term: Using the Lipschitz continuity of the bulk site energy, we can show that

\[
|S| = \left| v'_0 \left[ \left\{ \partial_F V^\text{surf}(u'_0) + \partial_1 V(u'_0, u'_1) \right\} - \left\{ \partial_F W(F_0) \right\} \right. \right.
\]
\[
- \left. \left\{ \partial_F V^\text{surf}(F_0 + q'_0) + \partial_1 V(F_0 + q'_0, F_0 + q'_1) - \partial_F W(F_0) \right\} \right]\right|
\]
\[
= \left| v'_0 \left| \partial_1 V(F_0 + q'_0, w'_1 + q'_1) - \partial_1 V(F_0 + q'_0, F_0 + q'_1) \right| \right|
\]
\[
\lesssim |v'_0| \cdot |w'_1 - F_0|.
\] (46)

Bulk sum: We write \( B = \sum_{\ell=1}^{\infty} v'_\ell B_\ell \), where

\[
B_\ell = \left\{ \partial_2 V(u'_{\ell-1}, u'_\ell) + \partial_1 V(u'_\ell, u'_{\ell+1}) \right\} - \left\{ \partial_F W(w'_\ell) \right\}
\]
\[
- \left\{ \partial_2 V(F_0 + q'_{\ell-1}, F_0 + q'_\ell) + \partial_1 V(F_0 + q'_\ell, F_0 + q'_{\ell+1}) - \partial_F W(F_0) \right\}.
\]

Using the identity \( \partial_F W(F) = \partial_1 V(F, F) + \partial_2 V(F, F) \) and adding 0, we can split \( B_\ell \) into

\[
B_\ell = \left\{ \partial_2 V(u'_{\ell-1}, u'_\ell) + \partial_1 V(u'_\ell, u'_{\ell+1}) - \partial_2 V(w'_\ell + q'_{\ell-1}, w'_\ell + q'_\ell) - \partial_1 V(w'_\ell + q'_\ell, w'_\ell + q'_{\ell+1}) \right\}
\]
\[
+ \left\{ \partial_2 V(w'_\ell + q'_{\ell-1}, w'_\ell + q'_\ell) + \partial_1 V(w'_\ell + q'_\ell, w'_\ell + q'_{\ell+1}) - \partial_2 V(w'_\ell, w'_\ell) \right\}
\]
\[
- \left\{ \partial_2 V(F_0 + q'_{\ell-1}, F_0 + q'_\ell) + \partial_1 V(F_0 + q'_\ell, F_0 + q'_{\ell+1}) - \partial_2 V(F_0, F_0) - \partial_1 V(F_0, F_0) \right\}
\]
\[
=: B^{(1)}_\ell + B^{(2)}_\ell - B^{(3)}_\ell.
\]

Estimate for \( B^{(1)}_\ell \): Expanding \( \partial V \), we obtain, using \( u = w + q \),

\[
B^{(1)}_\ell = \partial_2 V(w'_\ell + q'_{\ell-1}, w'_\ell + q'_\ell) \cdot \left( \frac{u'_{\ell-1} - w'_\ell - q'_{\ell-1}}{u'_\ell - w'_\ell - q'_\ell} \right)
\]
\[
+ \partial_1 V(w'_\ell + q'_{\ell-1}, w'_\ell + q'_\ell) \cdot \left( \frac{u'_\ell - w'_\ell - q'_\ell}{u'_{\ell+1} - w'_\ell - q'_{\ell+1}} \right) + O(|w''_\ell|^2 + |w''_\ell|^2)
\]
\[
= \partial_1 V(w'_\ell + q'_{\ell-1}, w'_\ell + q'_\ell) \cdot w''_\ell - \partial_2 V(w'_\ell + q'_{\ell-1}, w'_\ell + q'_\ell) \cdot w''_{\ell-1} + O(|w''_\ell|^2 + |w''_\ell|^2).
\]

Expanding the result again yields

\[
B^{(1)}_\ell = \left( \partial_2 V(w'_\ell + q'_{\ell-1}, w'_\ell + q'_\ell) \right) \cdot (w''_\ell - w''_{\ell-1}) + O(|q''_\ell| \cdot |w''_{\ell-1}| + |q''_\ell| \cdot |w''_\ell| + |w''_{\ell-1}|^2 + |w''_\ell|^2).
\]

Thus, we obtain

\[
|B^{(1)}_\ell| \lesssim |w''_\ell| + |w''_{\ell-1}|^2 + |w''_\ell|^2 + |q''_\ell| \cdot |w''_{\ell-1}| + |q''_\ell| \cdot |w''_\ell|.
\] (47)

Estimate for \( B^{(2)}_\ell - B^{(3)}_\ell \): The two terms \( B^{(2)}_\ell \) and \( B^{(3)}_\ell \) are of similar structure and will need
to be treated together. First, we rewrite $B^{(2)}_{\ell}$ and $B^{(3)}_{\ell}$ in the form

$$B^{(2)}_{\ell} = \int_0^1 \partial \partial_2 V(w'_\ell + t_{q_{\ell-1}'}w'_\ell + t_{q_{\ell}}) \cdot \left( \frac{q_{\ell-1}}{q_{\ell}} \right) dt$$

and

$$B^{(3)}_{\ell} = \int_0^1 \partial \partial_1 V(F_0 + t_{q_{\ell-1}}F_0 + t_{q_{\ell}}) \cdot \left( \frac{q_{\ell-1}}{q_{\ell}} \right) dt.$$ 

Subtracting and rearranging terms yields

$$B^{(2)}_{\ell} - B^{(3)}_{\ell} = \int_0^1 \left( \partial \partial_2 V(w'_\ell + t_{q_{\ell-1}'}w'_\ell + t_{q_{\ell}}) - \partial \partial_2 V(F_0 + t_{q_{\ell-1}}F_0 + t_{q_{\ell}}) \right) \cdot \left( \frac{q_{\ell-1}}{q_{\ell}} \right) dt$$

and

$$\int_0^1 \left( \partial \partial_1 V(F_0 + t_{q_{\ell-1}}F_0 + t_{q_{\ell}}) - \partial \partial_1 V(F_0 + t_{q_{\ell-1}}F_0 + t_{q_{\ell}}) \right) \cdot \left( \frac{q_{\ell-1}}{q_{\ell}} \right) dt.$$ 

Making use of the Lipschitz continuity of $\partial^2 V$ once again, we deduce that

$$|B^{(2)}_{\ell} - B^{(3)}_{\ell}| \lesssim \int_0^1 \left( |w'_\ell - F_0| + |w'_\ell - F_0| \right) \cdot \left( \frac{q_{\ell-1}}{q_{\ell}} \right) dt$$

$$\lesssim (|q_{\ell-1}'| + |q_{\ell}'| + |q_{\ell+1}'|)|w'_\ell - F_0|.$$ 

Combining this estimate with (47), summing $\ell$, and applying the Cauchy-Schwarz inequality yields the interior contribution of the stated result.

**Theorem 6.2** (Consistency). Let $\|f\|_{U^{\ast}}$ be sufficiently small and $L$ be sufficiently large so that the conditions of Theorems 2.5 and 2.6 with $F_0 = \nabla u^{cb}(0)$ and of Proposition 2.7 are satisfied. Let $u^{cb}$ and $q_L$ denote the corresponding Cauchy–Born and corrector solutions. Then,

$$\|\delta E^u(\Pi_a u^{cb} + q_L) - f\|_{U^{\ast}} \lesssim \mu^L_q + |\nabla^2 u^{cb}(0)| + \|\nabla^2 u^{cb}\|^2_{L^1} + \|\nabla^3 u^{cb}\|_{L^2} + \|\nabla f\|_{L^2}. \quad (48)$$

**Proof.** As $u^{cb}$ and $q_\infty$ are solutions to their respective problems, $\langle \delta E^{cb}(u^{cb}), v \rangle = \langle \hat{g}, \nabla v \rangle_{\mathbb{R}^2}$ for all $v \in U^{cb}$ with $\hat{g}$ defined as in (38) and $\langle \delta E^\Gamma(q_\infty; F_0), v \rangle = 0$ for all $v \in Q_\infty$. We recall that $U$ can be seen as a subspace of $U^{cb}$ and that $Q_\infty = U$.

Let $\tilde{u} := \Pi_a u^{cb} + q_L$ and $F_0 = \nabla u^{cb}(0)$, then using the fact that $u^{cb}$ solves (17) we can split the consistency error into

$$\langle \delta E^u(\tilde{u}) - f, v \rangle = \langle \delta_{ext} + \delta_{cb} + \delta_{\Gamma} + \delta_{pc}, v \rangle,$$

where

$$\delta_{ext} := \langle f, \cdot \rangle_{\mathbb{R}^2} - \langle f, \cdot \rangle_{Z_\geq 0},$$

$$\delta_{cb} := \delta E^{cb}(\Pi_a u^{cb}) - \delta E^{cb}(u^{cb}),$$

$$\delta_{\Gamma} := \delta E^\Gamma(\Pi_a u^{cb} + q_L) - \delta E^\Gamma(\Pi_a u^{cb}),$$

and

$$\delta_{pc} := \delta E^\Gamma(\Pi_a u^{cb} + q_L) - \delta E^{cb}(\Pi_a u^{cb}) - \delta E^\Gamma(q_\infty; F_0).$$

The term $\delta_{ext}$ represents the error in the action of the external forces. In the atomistic model, the external forces can be written as $\langle f, v \rangle_{Z_\geq 0} = \langle g, v' \rangle_{Z_\geq 0}$, where $g$ is defined as in (38). Using (40), we get that

$$\langle \delta_{ext}, v \rangle = |\langle \hat{g}, \nabla v \rangle_{\mathbb{R}^2} - \langle g, v' \rangle_{Z_\geq 0}| \lesssim \|\nabla f\|_{L^2} \|v'\|_{L^2}$$

for all $v \in U$. \hfill (49)
The term $\delta_{cb}$ represents the error associated with the discretization of the Cauchy–Born problem and was estimated in Theorem 4.2 to be

$$\|\delta_{cb}\|_{U^*} \lesssim \|\nabla^2 u_{cb}\|_{L^4}.$$ 

The term $\delta_{\Gamma}$ represents the error associated with the Galerkin projection of the corrector problem and was estimated in Theorem 2.7:

$$\|\delta_{\Gamma}\|_{U^*} \lesssim \mu_L.$$ 

Finally, $\delta_{pc}$, the error due to the predictor-corrector method is estimated in Theorem 6.1:

$$\|\delta_{pc}\|_{U^*} \lesssim \|\Pi_a u_{cb}\|_{L^4}^2 + \|q'' \cdot (\Pi_a u_{cb})'\|_{L^2} + \mu_{\tilde{q}} L^q.$$ 

where we have written $q \equiv q_{\infty}$ for the sake of simplicity of notation.

To proceed, we need to relate discrete and continuous derivatives. For example,

$$\left|\frac{\partial}{\partial x} \left(\Pi_a u_{cb}\right)_{\ell} \right| = \left|\frac{\partial}{\partial x} \left(\Pi_a u_{cb}\right)_{\ell} - \frac{\partial}{\partial x} \left(\Pi_a u_{cb}\right)_{\ell+1} \right| \approx \int_{\ell}^{\ell+1} \nabla^2 u_{cb}(x+1) - \nabla^2 u_{cb}(x) \, dx \leq \int_{\ell}^{\ell+1} |\nabla^2 u_{cb}(x)| \, dx.$$ 

Analogously, we can prove

$$\left|\frac{\partial^2}{\partial x^2} \left(\Pi_a u_{cb}\right)_{\ell} \right| \approx \int_{\ell}^{\ell+2} |\nabla^3 u_{cb}(x)| \, dx,$$

and

$$\left|\left(\Pi_a u_{cb}\right)_{\ell}' - F_0 \right| \leq \int_{0}^{\ell+1} |\nabla^2 u_{cb}(x)| \, dx.$$ 

(50)

Using these estimates, it is straightforward to establish that

$$P_1 = \|\Pi_a u_{cb}'\|_{L^4}^2 \lesssim \|\nabla^2 u_{cb}\|_{L^4}^2 \quad \text{and} \quad P_2 = \|\Pi_a u_{cb}'\|_{L^2} \lesssim \|\nabla^3 u_{cb}\|_{L^2}.$$ 

The remaining three terms have similar structure. Estimating $|q''| \lesssim \mu_{\tilde{q}} = e^{-\alpha \ell}$ for some $\alpha > 0$, we deduce

$$P_3^2 = \|q'' \cdot (\Pi_a u_{cb})'\|_{L^2}^2 \lesssim \int_{0}^{\infty} e^{-2\alpha x} |\nabla^2 u_{cb}(x)|^2 \, dx.$$ 

Applying (50), and using the fact that $e^{-\alpha x}$ is bounded below on $[0, 1]$, we have

$$P_4^2 = \left|\left(\Pi_a u_{cb}\right)'_0 - F_0\right|^2 \lesssim \int_{0}^{1} e^{-2\alpha x} |\nabla^2 u_{cb}(x)|^2 \, dx.$$ 

(50)
Finally, applying (50) again, together with \( |q'_t| < \mu^t = e^{-\alpha t} \), we can estimate

\[
P_5^2 = \sum_{\ell=1}^{\infty} (|q'_{\ell-1}| + |q'_\ell| + |q'_{\ell+1}|)^2 \cdot (\Pi_a u_{cb})'_\ell - P_0^2 \leq \sum_{\ell=1}^{\infty} \mu^{2t} \left( \int_0^{\ell+1} \| \nabla^2 u_{cb}(x) \| \, dx \right)^2 \leq \int_0^\infty e^{-2\alpha t} \left( \int_0^t \| \nabla^2 u_{cb}(x) \| \, dx \right)^2 \, dt
\]

\[
\lesssim \int_0^\infty e^{-2\alpha t} \int_0^t \| \nabla^2 u_{cb}(x) \|^2 \, dx \, dt = \int_0^\infty \| \nabla^2 u_{cb}(x) \|^2 \, dx \int_0^\infty e^{-2\alpha t} \, dt \, dx
\]

Thus, we can combine

\[
P_3^2 + P_4^2 + P_5^2 \lesssim \int_0^\infty (1 + x)e^{-2\alpha x} \| \nabla^2 u_{cb}(x) \|^2 \, dx.
\]

To finalize, we use the same argument as in the estimate for \( P_5 \) to deduce that

\[
P_3^2 + P_4^2 + P_5^2 \lesssim \| \nabla^2 u_{cb}(0) \|^2 + \int_0^\infty (1 + x)e^{-2\alpha x} \| \nabla^2 u_{cb}(x) - \nabla^2 u_{cb}(0) \|^2 \, dx
\]

\[
\lesssim \| \nabla^2 u_{cb}(0) \|^2 + \int_0^\infty (1 + x)^2e^{-2\alpha x} \| \nabla^3 u_{cb}(x) \|^2 \, dx
\]

\[
\lesssim \| \nabla^2 u_{cb}(0) \|^2 + \| \nabla^3 u_{cb} \|^2_{L^2}.
\]

Combining the estimates for \( \delta_{ext}, \delta_{cb}, \delta_T \) and those for \( P_j, j = 1, \ldots, 5 \), we arrive at the stated result.

\[\square\]

**Theorem 6.3 (Stability).** There exists \( \varepsilon, L_0 > 0 \) such that for all \( f \in U^* \) with \( \| f \|_{U^*} < \varepsilon \) and all \( L \geq L_0 \), we have

\[
\langle \delta^2 \mathcal{E}^a(\Pi_a u_{cb} + q_L)v, v \rangle \geq \frac{c_a}{2} \| v' \|_{L^2}^2
\]

where \( c_a \) denotes the stability constant for \( u_{cb}^* \).

**Proof.** First, let \( f \) be small enough and \( L \) be large enough so that Theorem 2.5, Theorem 2.6 and Proposition 2.7 holds. The second variation of the atomistic energy evaluated at the predictor-corrector solution can be written as

\[
\langle \delta^2 \mathcal{E}^a(\Pi_a u_{cb} + q_L)v, v \rangle = \langle \delta^2 \mathcal{E}^a(u_{cb}^*)v, v \rangle - \langle \delta^2 \mathcal{E}^a(q_L)v, v \rangle - \langle \delta^2 \mathcal{E}^a(\Pi_a u_{cb} + q_L)v, v \rangle
\]

The highlighted difference terms can all be bound using the Lipschitz continuity of the second variation of the atomistic energy:

\[
|\langle \delta^2 \mathcal{E}^a(u_{cb}^*)v, v \rangle - \langle \delta^2 \mathcal{E}^a(q_L)v, v \rangle| \lesssim \| (u_{cb}^*)' - (q_L)' \|_{L^2} \| v' \|_{L^2} (51)
\]

\[
|\langle \delta^2 \mathcal{E}^a(q_L)v, v \rangle - \langle \delta^2 \mathcal{E}^a(\Pi_a u_{cb} + q_L)v, v \rangle| \lesssim \| (q_L)' \|_{L^2} \| v' \|_{L^2} (52)
\]

\[
|\langle \delta^2 \mathcal{E}^a(\Pi_a u_{cb} + q_L)v, v \rangle| \lesssim \| (\Pi_a u_{cb} + q_L)' \|_{L^2} \| v' \|_{L^2} (53)
\]

Each of these bounds goes to zero either for large \( L \) or for small \( \| f \|_{U^*} \). The bound in (51) goes to zero as \( \| f \|_{U^*} \to 0 \) by Theorem 2.6, the bound in (52) goes to zero as \( L \to \infty \) by Proposition 2.7 and the bound in (53) goes to zero as \( f \to 0 \) by Theorem 2.5. Finally, \( \langle \delta^2 \mathcal{E}^a(u_{cb}^*)v, v \rangle \geq c_a \| v' \|_{L^2}^2 \) by definition. Thus, there exists an \( L_0 > 0 \) and an \( \varepsilon > 0 \) such that the theorem statement holds. \[\square\]
7 Appendix

Proposition 7.1 (First Variations.). Let \( u, v \in \mathcal{U} \). Then,

\[
\langle \delta \mathcal{E}^a(u), v \rangle = v_0' \left\{ \partial_1 V_{\text{surf}}(u_0) + \partial_1 V(u_0', u_1') \right\} + \sum_{\ell=1}^{\infty} v_\ell' \left\{ \partial_2 V(u_{\ell-1}, u_\ell') + \partial_1 V(u_\ell', u_{\ell+1}') \right\},
\]

\[
\langle \delta \mathcal{E}^\Gamma(q; u^{cb}), v \rangle = v_0' \left\{ \partial_1 V_{\text{surf}}(F_0 + q_0) + \partial_1 V(F_0 + q_0, F_0 + q_1) - \partial_F W(F_0) \right\},
\]

\[
+ \sum_{\ell=1}^{\infty} v_\ell' \left\{ \partial_2 V(F_0 + q_{\ell-1}, F_0 + q_\ell) + \partial_1 V(F_0 + q_\ell, F_0 + q_{\ell+1}) - \partial_F W(F_0) \right\}.
\]

Let \( u, v \in \mathcal{U}^{cb} \). Then,

\[
\langle \delta \mathcal{E}^{cb}(u), v \rangle = \int_0^{\infty} \partial_F W(\nabla u) \cdot \nabla v dx.
\]

Proposition 7.2 (Second Variations.). Let \( u, v, w \in \mathcal{U} \). Then,

\[
\langle \delta^2 \mathcal{E}^a(u)w, v \rangle = v_0' F_0 \left\{ \partial_2^2 V_{\text{surf}}(u_0') + \partial_2^2 V(u_0', u_1') \right\} + v_0' w_1' \left\{ \partial_2^2 V(u_0', u_1') \right\}
\]

\[
+ \sum_{\ell=1}^{\infty} \left[ w_{\ell-1}' \left\{ \partial_2^{12} V(u_{\ell-1}', u_\ell') \right\} + w_\ell' \left\{ \partial_2^{12} V(u_{\ell-1}', u_\ell') + \partial_2^{11} V(u_\ell', u_{\ell+1}') \right\} \right],
\]

\[
\langle \delta^2 \mathcal{E}^\Gamma(q; u^{cb})w, v \rangle = v_0' F_0 \left\{ \partial_2^2 V_{\text{surf}}(F_0 + q_0) + \partial_2^2 V(F_0 + q_0, F_0 + q_1) \right\}
\]

\[
+ v_0' w_1' \left\{ \partial_2^{12} V(F_0 + q_0, F_0 + q_1) \right\}
\]

\[
+ \sum_{\ell=1}^{\infty} \left[ w_{\ell-1}' \left\{ \partial_2^{12} V(F_0 + q_{\ell-1}, F_0 + q_\ell) \right\} + w_\ell' \left\{ \partial_2^{12} V(F_0 + q_{\ell-1}, F_0 + q_\ell) + \partial_2^{11} V(F_0 + q_\ell, F_0 + q_{\ell+1}) \right\} \right]
\]

\[
+ w_{\ell+1}' \left\{ \partial_2^{12} V(F_0 + q_\ell, F_0 + q_{\ell+1}) \right\},
\]

Let \( u, v, w \in \mathcal{U}^{cb} \). Then,

\[
\langle \delta^2 \mathcal{E}^{cb}(u)w, v \rangle = \int_0^{\infty} \partial_2^2 W(\nabla u) \cdot \nabla w \cdot \nabla v dx.
\]

7.1 Inverse Function Theorem

Theorem 7.3. Let \( \mathcal{H} \) be a Hilbert space equipped with norm \( \| \cdot \|_{\mathcal{H}} \), and let \( \mathcal{G} \in C^1(\mathcal{H}, \mathcal{H}^*) \) with Lipschitz-continuous derivative \( \delta \mathcal{G} : \)

\[
\| \delta \mathcal{G}(u) - \delta \mathcal{G}(v) \|_{\mathcal{L}} \leq M \| u - v \|_{\mathcal{H}} \quad \text{for all } u, v \in \mathcal{H},
\]

where \( \| \cdot \|_{\mathcal{L}} \) denotes the \( \mathcal{L}(\mathcal{H}, \mathcal{H}^*) \)-operator norm.
Let $\bar{u} \in \mathcal{H}$ satisfy

$$\|G(\bar{u})\|_{\mathcal{H}^*} \leq \eta$$

$$\langle \delta G(\bar{u})v, v \rangle \geq \gamma \|v\|_{\mathcal{H}}^2$$

for all $v \in \mathcal{H}$, such that $M, \eta, \gamma$ satisfy the relation

$$\frac{2M\eta}{\gamma^2} < 1.$$ 

Then, there exists a (locally unique) $u \in \mathcal{H}$ such that $G(u) = 0$,

$$\|u - \bar{u}\|_{\mathcal{H}} \leq 2 \frac{\eta}{\gamma},$$

and

$$\langle \delta G(u)v, v \rangle \geq \left(1 - \frac{2M\eta}{\gamma^2}\right) \gamma \|v\|_{\mathcal{H}}^2$$

for all $v \in \mathcal{H}$.

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