COUPLING ATOMISTIC, ELASTICITY AND BOUNDARY ELEMENT MODELS

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Abstract. We formulate a new atomistic/continuum (a/c) coupling scheme that employs the boundary element method (BEM) to obtain an improved far-field boundary condition. We establish sharp error bounds in a 2D model problem for a point defect embedded in a homogeneous crystal.

1. Introduction

Atomistic-to-continuum (a/c) coupling is a class of multi-scale methods that couple atomistic models with continuum elasticity models to reduce computational cost while preserving a significant level of accuracy. In the continuum model coarse finite element methods are often used. We refer to [13] and the references therein for a comprehensive introduction and a framework for error analysis.

The present work explores the feasibility and effectiveness of employing boundary elements in addition to the existing a/c framework to better approximate the far-field energy which is most typically truncated. Specifically we combine a quasi-nonlocal (QNL) type method with a BEM, in a 2D model problem.

The QNL-type coupling, first introduced in [19, 6], is an energy-based a/c method that introduces an interface region between the atomistic and continuum model so that the model is "free of ghost-forces" (a notion of consistency related to the patch test, see §2.2). The first explicit construction of such schemes for two-dimensional domains with corners is developed in [17] for a nearest-neighbour many-body site potential. We call this coupling scheme "G23" for future reference. An error analysis of the G23 coupling equipped with coarse finite elements of order two or higher is described in [5].

The boundary element method is a numerical method for solving linear partial differential equations by discretising the boundary integral formulation. For a general introduction and analysis we refer to [21]. In the present work we first approximate a nonlinear elasticity model by a quadratic energy functional which is then discretised by the BEM.

The idea of employing a BEM-like scheme to model the elastic far-field is not new. For example, in [10, 20] an atomistic Green’s function method is employed to determine a far-field boundary condition which yields a sequential multi-scale scheme, while [22, 11] formulate concurrent multi-scale schemes coupling atomistic mechanics to a Green’s function method. In this setting, a preliminary error analysis can already be found in [8]. By contrast, our new scheme employs a BEM, i.e., a continuum elasticity Green’s function approach to model the elastic far-field. Moreover, our formulation allows a seamless transition between atomistic mechanics,
nonlinear continuum mechanics (FEM) and linearised continuum mechanics (BEM). This flexibility is particularly interesting for an error analysis since we are able to determine quasi-optimal error balancing between the two difference approximations. To conclude the introduction we remark that the BEM far-field boundary condition can of course be employed for other A/C coupling schemes as well as more complex (in terms of geometry and interaction law) atomistic models, but in particular the latter generalisation requires some additional work. With this in mind, the present work may be considered a proof of concept.

1.1. Outline. In the present work we estimate the accuracy of a QNL-type atomistic/continuum coupling method employing a P1 FEM in the continuum region and P0 BEM on the boundary against an exact solution obtain from a fully atomistic model. We review the atomistic model in §2.1, the QNL coupling scheme in §2.2 and §2.3, and the modification to incorporate a BEM for the elastic far-field in §2.4. In §3 we collect notation, assumptions and preliminary results required to state the main results in §4. We then deduce the optimal approximation parameters (atomistic region size, continuum region size, FEM and BEM meshes) in §4.4. We will conclude that omitting the FEM region entirely yields the best possible convergence rate.

2. Method Formulation

2.1. Atomistic model. In order to employ the G23 coupling in [17], we follow the same model construction therein. We consider an infinite 2D triangular lattice as our model geometry,

\[ \Lambda := \mathbb{AZ}^2, \quad \text{with } A = \begin{pmatrix} 1 & \cos(\pi/3) \\ 0 & \sin(\pi/3) \end{pmatrix}. \]

We define the six nearest-neighbour lattice directions by \( a_1 := (1, 0) \), and \( a_j := Q_6^{j-1} a_1, j \in \mathbb{Z} \), where \( Q_6 \) denotes the rotation through the angle \( \pi/3 \). We equip \( \Lambda \) with an atomistic triangulation, as shown in Figure 1 which will be used in both error analysis and numerical simulations. We denote this triangulation by \( \mathcal{T} \) and its elements by \( T \in \mathcal{T} \). In addition, we denote \( \mathbf{a} := (a_j)_{j=1}^6 \), and \( \mathbf{Fa} := (\mathbf{Fa}_j)_{j=1}^6 \), for \( \mathbf{F} \in \mathbb{R}^{m \times 2} \).
We identify a discrete displacement map \( u : \Lambda \rightarrow \mathbb{R} \) with its continuous piecewise affine interpolant, with weak derivative \( \nabla u \), which is also the pointwise derivative on each element \( T \in \mathcal{T} \). For \( m = 1, 2, 3 \), we define the spaces of displacements as
\[
\mathcal{U}_0 := \{ u | \Lambda \rightarrow \mathbb{R}^m : \text{supp}(\nabla u) \text{ is compact} \}, \quad \text{and}
\mathcal{U}^{1,2} := \{ u | \Lambda \rightarrow \mathbb{R}^m : \nabla u \in L^2 \}.
\]
We equip \( \mathcal{U}^{1,2} \) with the \( H^1 \)-semi norm and denote \( \| u \|_{\mathcal{U}^{1,2}} := \| \nabla u \|_{L^2(\mathbb{R}^2)} \). From \cite{[15]} we know that \( \mathcal{U}_0 \) is dense in \( \mathcal{U}^{1,2} \) in the sense that, if \( u \in \mathcal{U}^{1,2} \), then there exist \( u_j \in \mathcal{U}_0 \) such that \( \nabla u_j \rightarrow \nabla u \) strongly in \( L^2 \).

A homogeneous displacement is a map \( u_F : \Lambda \rightarrow \mathbb{R}^m, u_F(x) := Fx \), where \( F \in \mathbb{R}^{m \times 2} \).

For a map \( u : \Lambda \rightarrow \mathbb{R}^m \), we define the finite difference operator
\[
D_j u(x) := u(x + a_j) - u(x), \quad x \in \Lambda, j \in \{1, 2, ..., 6\}, \quad \text{and}
Du(x) := (D_j u(x))_{j=1}^6.
\]
Note that \( Du_F(x) = Fa \).

We assume that the atomistic interaction is represented by a nearest-neighbour many-body site energy potential \( V \in C^r(\mathbb{R}^{m \times 6}), r \geq 5 \), with \( V(0) = 0 \) and \( \nabla^j V \in L^\infty(\mathbb{R}^{m \times 6}) \) for \( j = 2, \ldots, 5 \). In addition, we assume that \( V \) satisfies the point symmetry
\[
V((-g_j+3)_{j=1}^6) = V(g) \quad \forall g \in \mathbb{R}^{m \times 6}.
\]
Because \( V(0) = 0 \), the energy of a displacement \( u \in \mathcal{U}_0 \)
\[
\mathcal{E}^a(u) := \sum_{\ell \in \Lambda} V(Du(\ell)),
\]
is well-defined. We need the following lemma to extend \( \mathcal{E}^a \) to \( \mathcal{U}^{1,2} \) to formulate a variational problem in the energy space \( \mathcal{U}^{1,2} \).

**Lemma 2.1.** \( \mathcal{E}^a : (\mathcal{U}_0, \| \nabla \cdot \|_{L^2}) \rightarrow \mathbb{R} \) is continuous and has a unique continuous extension to \( \mathcal{U}^{1,2} \), which we still denote by \( \mathcal{E}^a \). Moreover, the extended \( \mathcal{E}^a : (\mathcal{U}^{1,2}, \| \nabla \cdot \|_{L^2}) \rightarrow \mathbb{R} \) is \( r \)-times continuously Fréchet differentiable.

**Proof.** See Lemma 2.1 in \cite{[8]}. \( \square \)

We model a point defect by including an external potential \( f \in C^r(\mathcal{U}^{1,2}) \) with \( \partial_{u(\ell)} f(u) = 0 \) for all \( |\ell| \geq R_f \), where \( R_f \) is the defect core radius, and \( f(u + c) = f(u) \) for all constants \( c \). For instance, we can think of \( f \) modelling a substitutional impurity. See also \cite{[12], [14]} for similar approaches.

Then we seek the solution to
\[
u^a \in \arg \min \{ \mathcal{E}^a(u) - f(u) | u \in \mathcal{U}^{1,2} \}.
\]

For \( u, \varphi, \psi \in \mathcal{U}^{1,2} \) we define the first and second variations of \( \mathcal{E}^a \) by
\[
\langle \delta \mathcal{E}^a(u), \varphi \rangle := \lim_{t \to 0} t^{-1} (\mathcal{E}^a(u + t\varphi) - \mathcal{E}^a(u)),
\]
\[
\langle \delta^2 \mathcal{E}^a(u) \varphi, \psi \rangle := \lim_{t \to 0} t^{-1} (\langle \delta \mathcal{E}^a(u + t\varphi), \psi \rangle - \langle \delta \mathcal{E}^a(u), \psi \rangle).
\]
We define analogously all energy functionals introduced in later sections.
2.2. GR-AC coupling. The Cauchy–Born strain energy function \[ W(F) := \frac{1}{\Omega_0} V(Fa), \quad \text{for } F \in \mathbb{R}^{m \times 2}, \]
where \( \Omega_0 := \sqrt{3}/2 \) is the volume of a unit cell of the lattice \( \Lambda \). Hence \( W(F) \) is the energy per volume of the homogeneous lattice \( F\Lambda \). It is shown in [9] that, in a triangular lattice with anti-plane elasticity, \( \nabla^2 W(0) = \mu I_{2 \times 2} \) for some constant \( \mu > 0 \) (the shear modulus), which will be used in the formulation of BEM in later sections.

Let \( A \subset \Lambda \) be the set of all lattices sites for which we require full atomistic accuracy. We define the set of interface lattice sites as \( I := \{ \ell \in \Lambda \setminus A \mid \ell + a_j \in A \text{ for some } j \in \{1, \ldots, 6\} \} \) and we define the remaining lattice sites as \( C := \Lambda \setminus (A \cup I) \). Let \( \Omega_\ell \) be the Voronoi cell associated with site \( \ell \). We define the continuum region \( \Omega^c := \mathbb{R}^2 \setminus \bigcup_{\ell \in A \cup I} \Omega_\ell \); see Figure 2. We also define \( \Omega^a \) and \( \Omega^i \) analogously.

A general form for the GRAC-type a/c coupling energy [6, 17] is
\[
\mathcal{E}^{ac}(u) = \sum_{\ell \in A} V(Du(\ell)) + \sum_{\ell \in I} V\left((\mathcal{R}_\ell D_j u(\ell))_{j=1}^6\right) + \int_{\Omega^c} W(\nabla u(x)) \, dx, \tag{2.3}
\]
where \( \mathcal{R}_\ell D_j u(\ell) := \sum_{i=1}^6 C_{\ell,j,i} D_i u(\ell) \). The parameters \( C_{\ell,j,i} \) are determined such that the coupling scheme satisfies the “patch tests”:

\( \mathcal{E}^{ac} \) is locally energy consistent if, for all \( F \in \mathbb{R}^{m \times 2} \),
\[
V(\mathcal{R}_\ell D_j u(\ell)) = V(Fa) \quad \forall \ell \in I. \tag{2.4}
\]

\( \mathcal{E}^{ac} \) is force consistent if, for all \( F \in \mathbb{R}^{m \times 2} \),
\[
\delta \mathcal{E}^{ac}(u_F) = 0, \quad \text{where } u_F(x) := Fx. \tag{2.5}
\]

\( \mathcal{E}^{ac} \) is patch test consistent if it satisfies both (2.4) and (2.5).

For simplicity we write
\[
V(\mathcal{R}_\ell D_j u(\ell)) := V((\mathcal{R}_\ell D_j u(\ell))_{j=1}^6).
\]

Following [17] we make the following standing assumption (see Figure 3 for examples).
Figure 3. The first two configurations are allowed. The third configuration is not allowed as the interface atom at the corner has no nearest neighbour in the continuum region, and should instead be taken as an atomistic site. This illustration is taken from [5].

Figure 4. The geometry reconstruction coefficients $\lambda_{x,j}$ at the interface sites. This illustration is taken from [5].

(A0) Each vertex $\ell \in \mathcal{I}$ has exactly two neighbours in $\mathcal{I}$, and at least one neighbour in $\mathcal{C}$.

Under this assumption, the geometry reconstruction operator $R_\ell$ is then defined by

$$R_\ell D_j y(\ell) := (1 - \lambda_{t,j})D_{j-1} y(\ell) + \lambda_{t,j} D_j y(\ell) + (1 - \lambda_{t,j})D_{j+1} y(\ell),$$

$$\lambda_{x,j} := \begin{cases} 2/3, & x + a_j \in \mathcal{C} \\ 1, & \text{otherwise} \end{cases};$$

see Figure 4. The resulting a/c coupling method is called G23 and the corresponding energy functional $E_{g23}$. It is proven in [17] that this choice of coefficients (and only this choice) leads to patch test consistency (2.4) and (2.5).

For future reference we decompose the canonical triangulation $\mathcal{T}$ as follows:

$$\mathcal{T}_A := \{ T \in \mathcal{T} \mid T \cap (\mathcal{I} \cup \mathcal{C}) = \emptyset \},$$

$$\mathcal{T}_C := \{ T \in \mathcal{T} \mid T \cap (\mathcal{I} \cup \mathcal{A}) = \emptyset \} \quad \text{and} \quad (2.6)$$

$$\mathcal{T}_I := \mathcal{T} \setminus (\mathcal{T}_C \cup \mathcal{T}_A).$$

2.3. The finite element scheme. In the atomistic region $\Omega^a$ and the interface region $\Omega^i$, the interactions are represented by discrete displacement maps, which are identified with their linear interpolant. In these regions there is no approximation error.

On the other hand, as formulated in (2.3), the interactions are approximated by the Cauchy–Born energy in the continuum region $\Omega^c_h$. 

Let $K > 0$ be the inner radius of the atomistic region,

$$K := \sup \{ r > 0 \mid B_r \cap \Lambda \subset A \},$$

where $B_r$ denotes the ball of radius $r$ centred at 0. We assume throughout that $K \geq R_f$ to ensure that the defect core is contained in the atomistic region.

Let $\Omega_h$ be the entire computational domain and $N > 0$ be the inner radius of $\Omega_h$, i.e.,

$$N := \sup \{ r > 0 \mid B_r \subset \Omega_h \}.$$

Let $T_h$ be a finite element triangulation of $\Omega_h$ which satisfies, for $T \in T_h$,

$$T \cap (A \cup I) \neq \emptyset \Rightarrow T \in T.$$

In other words, $T_h$ and $T$ coincide in the atomistic and interface regions, whereas in the continuum region the mesh size may increase towards the domain boundary.

We observe that the concrete construction of $T_h$ will be based on the choice of the domain parameters $K$ and $N$; hence we will write $T_h(K,N)$ to emphasize this dependence.

To eliminate the possibility of extreme angles on elements, we assume throughout that the family $(T_h(K,N))_{K,N}$ is uniformly shape-regular, i.e., there exists $c > 0$ such that,

$$\text{diam}(T)^2 \leq c|T|, \quad \forall T \in T_h(K,N), \forall K \leq N, \quad (2.7)$$

and that the induced mesh on $\Gamma_h := \partial \Omega_h$ is uniformly quasi-uniform.

Hence in the analysis we can avoid deteriorated constants in finite element interpolation error estimates. In later sections we will again drop the parameters from the notation by writing $T_h \equiv T_h(K,N)$ but implicitly will always keep the dependence.

Similar to (2.6), we denote the atomistic, interface and continuum elements by $T_a$, $T_i$ and $T_c$, respectively. We observe that $T_a = T_A$ and $T_i = T_I$. We also let $N_h$ be the number of degrees of freedom of $T_h$.

We define the finite element space of admissible displacements as

$$U_h := \{ u \in C(\mathbb{R}^2; \mathbb{R}^m) \mid u|_T \in \mathbb{P}^1(T) \text{ for } T \subset T_h \}. \quad (2.8)$$

2.4. GR-AC coupling with BEM. In [5], we employed finite element methods to approximate the solution. We applied P2-FEM with Dirichlet boundary conditions. To improve the far-field description, we now consider applying a boundary element method to approximate the far-field energy.

Recall that the general form (2.3) of the GR-AC type coupling energy is

$$\mathcal{E}^{ac}(u) = \sum_{\ell \in A} V(Du(\ell)) + \sum_{\ell \in I} V^i(Du(\ell)) + \int_{\Omega_c} W(\nabla u(x)) \, dx.$$

In the far-field we can approximate the Cauchy–Born energy by the linearization (recall that $\nabla^2 W(0) = \mu I_{2 \times 2}$)

$$\mathcal{E}_{\text{lin}}^{ac}(u) = \sum_{\ell \in A} V(Du(\ell)) + \sum_{\ell \in I} V^i(Du(\ell)) + \int_{\Omega_h} W(\nabla u(x)) \, dx + \int_{\mathbb{R}^2 \setminus \Omega_h} \frac{\mu}{2} |\nabla u|^2$$

$$=: \mathcal{E}_h^{ac}(u) + \int_{\mathbb{R}^2 \setminus \Omega_h} \frac{\mu}{2} |\nabla u|^2. \quad (2.9)$$

We seek the minimizer of above energy functional

$$u^* := \arg\min \{ \mathcal{E}_{\text{lin}}^{ac}(u) - f(u) : u \in \mathcal{U}^{1,2} \}.$$
For numerical simulations, we exploit the boundary integral to represent the quadratic term \( \int_{\mathbb{R}^2} \Omega_h^\mu \frac{\mu}{2} |\nabla u|^2. \)

In preparation, let \( \Gamma_h := \partial \Omega_h, \quad \gamma_0^\text{int} : C(\Omega_h) \to C(\Gamma_h) \) and \( \gamma_0^\text{ext} : C(\Omega_h^\mathbb{E}) \to C(\Gamma_h) \) be the interior and exterior trace operators respectively, then we define

\[
E^{ac}_*(u) := E^{ac}_h(u) + \inf_{\gamma_0^\text{ext}v = \gamma_0^\text{int}u} \frac{\mu}{2} \int_{\Omega_h^\mathbb{E}} |\nabla v|^2. \tag{2.10}
\]

Let \( \bar{u}_h := \arg\min_{u \in \mathcal{U}_h} \{E^{ac}_*(u) : u \in \mathcal{U}_h\} \)

and

\[
v_h := \arg\min \left\{ \int_{\Omega_h^\mathbb{E}} |\nabla v|^2 : v \in \dot{H}^1(\Omega_h^\mathbb{E}), \gamma_0^\text{ext}v = \gamma_0^\text{int}\bar{u}_h \right\}, \tag{2.11}
\]

\[
u_h^* := \arg\min \left\{ E^{lin}\dot{u}(u) - f(u) : u \in (\mathcal{U}_h + \dot{H}^1(\Omega_h^\mathbb{E})) \cap \dot{H}^1(\mathbb{R}^2) \right\},
\]

then clearly \( u_h^* = \bar{u}_h \) in \( \Omega_h \) while \( u_h^* = v_h \) in \( \Omega_h^\mathbb{E} \). The inf-problem (2.11) can be expressed as an exterior Laplace problem

\[
-\Delta v = 0, \quad \text{in } \Omega_h^\mathbb{E},
\]

\[
v = \gamma_0^\text{int}\bar{u}_h, \quad \text{on } \Gamma_h,
\]

\[
|v(x) - u_0| = O \left( \frac{1}{|x|} \right) \quad \text{as } |x| \to \infty,
\]

where \( u_0 \) is a constant determined by the inner boundary condition \( v = \gamma_0^\text{int}\bar{u}_h \) on \( \Gamma_h \). This exterior Laplace problem can be solved by boundary integrals and be approximated by boundary element methods.

### 2.4.1. Boundary Integrals

In this section, we formally outline how we combine the BEM with a/c coupling. Technical details will be presented in later sections. For a complete introduction to BEM we refer to \[21\].

To define Sobolev spaces of fractional order, we use the Slobodeckij semi-norm.

**Definition 2.1.** Let \( \Gamma \subset \mathbb{R}^d \) be a Lipschitz boundary, then for \( 0 < s < 1 \), we define

\[
|v|_{H^s(\Gamma)} := \left( \int_\Gamma \int_\Gamma \frac{|v(x) - v(y)|^2}{|x - y|^{d+2s}} \mathrm{d}S(x) \mathrm{d}S(y) \right)^{1/2},
\]

\[
\|v\|_{H^s(\Gamma)} := \left( \|v\|_{L^2(\Gamma)}^2 + |v|^2_{H^s(\Gamma)} \right)^{1/2}, \quad \text{and}
\]

\[
H^s(\Gamma) := \{ u \in L^2(\Gamma) \mid |v|_{H^s(\Gamma)} < \infty \}.
\]

For \( 0 < s < 1 \), \( H^{-s}(\Gamma) \) is defined as the dual space of \( H^s(\Gamma) \):

\[
\|v\|_{H^{-s}(\Gamma)} := \sup_{0 \neq w \in H^s(\Gamma)} \frac{\langle v, w \rangle_{\Gamma}}{\|w\|_{H^s(\Gamma)}},
\]

with respect to the duality pairing

\[
\langle v, w \rangle_{\Gamma} := \int_\Gamma v(x) w(x) \mathrm{d}x.
\]
Using the Trace Theorem (see Theorem 3.2), we can conclude that for $u_h \in \mathcal{U}_h \subset H^1(\Omega_h)$,
\[
\gamma_0^{\text{int}} u_h \in H^{1/2}(\Gamma_h) \quad \text{and} \quad \|\gamma_0^{\text{int}} u_h\|_{H^{1/2}(\Gamma_h)} \leq C_{\Omega_h} \|u_h\|_{H^1(\Omega_h)}.
\]

In addition to the trace operators $\gamma_0^{\text{int}}$ and $\gamma_0^{\text{ext}}$, we define the interior and exterior conormal derivative, for $x \in \Gamma_h$, by
\[
\gamma_1^{\text{int}} u(x) := \lim_{\Omega_h \ni y \to x} n(y) \cdot \nabla u(y), \quad \text{and} \quad \gamma_1^{\text{ext}} u(x) := \lim_{\Omega_h^c \ni y \to x} n(y) \cdot \nabla u(y),
\]
where $n$ is the outward unit normal vector to $\Omega_h$, i.e. pointing into $\Omega_h^c$.

Denote the fundamental solution to the Laplace operator in 2D by $G(x, y)$, i.e.
\[
G(x, y) := -\frac{1}{2\pi \log |x - y|}.
\]

For $y_0 \in \Omega_h$ and $R > 2 \text{diam}(\Omega_h)$, let $B_R(y_0)$ be a ball centred at $y_0$ with radius $R$. Then, by Green’s First Identity, we can solve the exterior Laplace problem (2.12) using the following representation formula, for $x \in B_R(y_0) \setminus \Omega_h$,
\[
v(x) = \int_{\Gamma_h} (\gamma_0^{\text{ext}} \bar{u}_h)(y) \gamma_1^{\text{ext}} G(x, y) \, dS(y) - \int_{\Gamma_h} G(x, y) \gamma_1^{\text{ext}} v(y) \, dS(y) + \\
+ \int_{\partial B_R(y_0)} G(x, y) \gamma_1^{\text{int}} v(y) \, dS(y) - \int_{\partial B_R(y_0)} \gamma_1^{\text{ext}} G(x, y) \gamma_0^{\text{int}} v(y) \, dS(y).
\]

Taking limit $R \to \infty$ gives, for $x \in \Omega_h^c$,
\[
v(x) = u_0 + \int_{\Gamma_h} (\gamma_0^{\text{ext}} \bar{u}_h)(y) \gamma_1^{\text{ext}} G(x, y) \, dS(y) - \int_{\Gamma_h} G(x, y) \gamma_1^{\text{ext}} v(y) \, dS(y), \quad (2.13)
\]
where $u_0$ is the far-field constant in (2.12).

Let us define the following boundary integrals, for $x \in \mathbb{R}^2 \setminus \Gamma_h$,
\[
A \psi(x) := \int_{\Gamma_h} G(x, y) \psi(y) \, dS(y) \quad \text{(single layer potential),}
\]
\[
B \psi(x) := \int_{\Gamma_h} \psi(y) \gamma_1^{\text{int}} G(x, y) \, dS(y) \quad \text{(double layer potential)}.
\]

Then for $x \in \Gamma_h$ we define
\[
V u(x) := \gamma_0^{\text{int}} (A u)(x), \quad K u(x) := \gamma_0^{\text{int}} (B u)(x)
\]
\[
K^\prime u(x) := \gamma_1^{\text{int}} (A u)(x), \quad D u(x) := -\gamma_1^{\text{int}} (B u)(x).
\]

Applying the exterior trace operator and the exterior conormal operator to (2.13) gives, for $x \in \Gamma_h$,
\[
\gamma_0^{\text{int}} v(x) = u_0 + \lambda(x) \gamma_0^{\text{int}} \bar{u}_h + (K \gamma_0^{\text{int}} \bar{u}_h)(x) - V(\gamma_1^{\text{ext}} v)(x), \quad (2.14)
\]
\[
\gamma_1^{\text{ext}} v(x) = (1 - \lambda(x)) \gamma_1^{\text{ext}} v(x) - (K^\prime \gamma_1^{\text{ext}} v)(x) - (D \gamma_0^{\text{int}} \bar{u}_h)(x), \quad (2.15)
\]
where by Lemma 6.8 in [21]
\[
\lambda(x) := \lim_{\epsilon \to 0} \frac{1}{2\pi \epsilon} \int_{y \in \Omega_h : |y - x| = \epsilon} \, dS(y) = \frac{1}{2} \text{ a.e.}
\]
Denote another fractional norm on the boundary: for $u \in \mathcal{H}$ its derivation is shown in \[21, \] and in addition, in order to ensure that the regularity constants are independent of the size of the boundary $\Gamma$ we need the following restriction on the boundary spaces.

Let us define subspaces
\[
H_{-1/2}^* (\Gamma_h) := \{ w \in H^{-1/2}(\Gamma_h) : \langle w, 1 \rangle_{\Gamma_h} = 0 \} \quad \text{and} \\
H_{1/2}^* (\Gamma_h) := \{ v \in H^{1/2}(\Gamma_h) : v = V(w) \text{ for some } w \in H_{-1/2}^* \}.
\]

Then Lemma 3.5 shows that $V : H_{-1/2}^* (\Gamma_h) \rightarrow H_{1/2}^* (\Gamma_h)$ is an isomorphism and consequently $u_0 = 0$.

**Remark 2.2.** For any Lipschitz boundary $\Gamma$, there exist an unique $w_\Gamma \in H^{-1/2}(\Gamma) \setminus H_{-1/2}^* (\Gamma)$ such that $\langle w_\Gamma, 1 \rangle_{\Gamma} = 1$ and
\[
u = \langle u, w_\Gamma \rangle_{\Gamma} \in H^{1/2}_{-1} (\Gamma), \quad \text{for any } u \in H^{1/2}(\Gamma).
\]
Its derivation is shown in \[21, \text{§} 6.6.1\].

Therefore \[2.14\] gives
\[-\gamma_1^{\text{ext}} u = V^{-1}(-K + \frac{1}{2} I) \gamma_0^{\text{int}} \bar{u}_h, \quad \text{if } \gamma_0^{\text{int}} \bar{u}_h \in H_{1/2}^* (\Gamma_h).
\]

Denote $g^{-1} := V^{-1}(-K + \frac{1}{2} I)$, which is called Steklov–Poincaré operator. Then the total energy \[2.10\] is equivalent to, for $u \in \mathcal{U}_h \cap H_{1/2}^* (\Gamma_h)$,
\[
\mathcal{E}_h^{ac}(u) \equiv \mathcal{E}_{\text{tot}}(u) := \mathcal{E}_h^{ac}(u) + \frac{\mu}{2} \int_{\Gamma_h} (\gamma_0^{\text{int}} u) g^{-1}(\gamma_0^{\text{int}} u).
\]

Theorem 3.6 establishes that Steklov–Poincaré operator $g^{-1} : H_{1/2}^* (\Gamma_h) \rightarrow H_{-1/2}^* (\Gamma_h)$ is positive definite. Lemma 3.7 shows that $g^{-1}$ is in fact in-variant under rescaling. In addition, in order to ensure that the regularity constants are independent of the size of the boundary $\Gamma_h$, we employ a rescaling argument in Section 3.2 to introduce another fractional norm on the boundary: for $u \in H^{1/2}(\Gamma_h)$
\[
\| u \|^2_{H_2^{1/2}(\Gamma_h)} := \left[ \frac{1}{2} \text{diam}(\Gamma_h) \right]^{-1} \| u \|^2_{L^2(\Gamma_h)} + \| u \|^2_{H_2^{1/2}(\Gamma_h)}.
\]

By Lemma 3.8 we have that for all $u \in H^{1/2}_{-1/2} (\Gamma_h)$
\[
\langle g^{-1} u, u \rangle \geq C_1 \| u \|^2_{H_2^{1/2}(\Gamma_h)} \quad \text{and} \quad \| g^{-1} u \|_{H_2^{1/2}(\Gamma_h)} \leq C_2 \| u \|_{H_2^{1/2}(\Gamma_h)},
\]

where $C_1$ and $C_2$ are independent of the radius of $\Omega_h$.

Now we take in account of the displacement inside $\Omega_h$ to introduce the following norm for the error analysis. For $u \in \mathcal{U}_h \cap H^{1/2}_{-1/2} (\Gamma_h)$, define
\[
\| u \|^2_{2} := \| \nabla u \|^2_{L^2(\Omega_h)} + \| u \|^2_{H^{1/2}_{-1/2}(\Gamma_h)}.
\]
It is clear that this norm is rescale in-variant.
2.4.2. Boundary element method. We introduce a numerical discretization scheme to approximate the boundary integral equations. Let
\[ S_h^0(\Gamma_h) = \text{span}\{ \phi_k^0 \}_{k=1}^M \subset H^{-1/2}_*(\Gamma_h), \]
where \( \phi_k^0 \) are piecewise constant basis functions on the discretized boundary with elements \( \mathcal{T}_h \cap \Gamma_h \). For a Dirichlet data \( u \in H^{1/2}(\Gamma) \), we define \( g_h^{-1}u := \bar{v}_h \in S_h^0(\Gamma_h) \) as the solution to
\[ \langle V\bar{v}_h, \tau_h \rangle = \langle (K + (\lambda - 1)I)u, \tau_h \rangle, \quad \text{for all } \tau_h \in S_h^0(\Gamma_h). \] (2.19)
Then we define
\[ \mathcal{E}_h^{\text{tot}}(u_h) := \mathcal{E}_h^{\text{ac}}(u_h) + \frac{\mu}{2} \int_{\Gamma_h} (\gamma_0^{\text{int}} u_h) g_h^{-1}(\gamma_0^{\text{int}} u_h), \] (2.20)
where \( \gamma_0^{\text{int}} u_h \in S_h^0(\Gamma_h) \). We seek the solution to
\[ u_h := \arg \min \{ \mathcal{E}_h^{\text{tot}}(u) - f(u) : u \in \mathcal{U}_h^o \}, \] (2.21)
where
\[ \mathcal{U}_h^o := \{ u_h \in \mathcal{U}_h \cap S_h^0(\Gamma_h) : u_h|_{\Gamma_h} \in H^{1/2}_*(\Gamma_h) \}. \]
and the error estimate \( \| \nabla u_h - \nabla \bar{v}_h \| \) in a suitable norm.

For the simplicity of analysis, we impose the following assumption on the boundary \( \Gamma_h \) and the atomistic triangulation \( \mathcal{T} \):
\begin{itemize}
  \item \textbf{(A3)} The boundary \( \Gamma_h \) is aligned with the canonical triangulation \( \mathcal{T} \) in the sense that, for all \( T \in \mathcal{T} \),
    \begin{enumerate}
      \item \( T \cap \Gamma_h \neq \emptyset \implies \text{int}(T) \cap \Gamma_h = \emptyset \).
      \item \( \text{Let } \mathcal{V}_{\text{FEM}} \text{ be the set of vertices of } \mathcal{T}_h, \text{ and } \mathcal{V}_{\text{can}} \text{ be the set of vertices of } \mathcal{T}, \text{ then } \mathcal{V}_{\text{FEM}} \cap \Gamma_h \subset \mathcal{V}_{\text{can}}. \)
    \end{enumerate}
\end{itemize}
\textbf{(A3)} is employed in §7.1.1 for the construction of a dual interpolant. We expect that, without it, the main results are still true, but would require some additional technicalities to prove. For the sake of clarity we therefore impose \textbf{(A3)} to emphasize the main concepts of the error analysis.

3. Preliminaries

In order to measure the “smoothness” of displacement maps \( u \in \mathcal{U}^{1,2} \), we review from [12] a smooth interpolant \( \tilde{u} \), namely a \( C^{2,1} \)-conforming multi-quintic interpolant.

\textbf{Lemma 3.1.} \( (a) \) For each \( u : \Lambda \rightarrow \mathbb{R}^m \), there exists a unique \( \tilde{u} \in C^{2,1}(\mathbb{R}^2; \mathbb{R}^m) \) such that, for all \( \ell \in \Lambda \),
\[ \tilde{u}|_{\ell + A(0,1)^2} \text{ is a polynomial of degree } 5, \]
\[ \tilde{u}(\ell) = u(\ell), \]
\[ \partial_{a_i} \tilde{u}(\ell) = \frac{1}{2} (u(\ell + a_i) - u(\ell - a_i)), \]
\[ \partial_{a_i}^2 \tilde{u}(\ell) = u(\ell + a_i) - 2u(\ell) + u(\ell - a_i), \]
where \( i \in \{1,2\} \) and \( \partial_{a_i} \) is the derivative in the direction of \( a_i \).
\( (b) \) Moreover, for \( q \in [1, \infty], 0 \leq j \leq 3, \)
\[ \| \nabla^j \tilde{u} \|_{L^q(\ell + A(1,0)^2)} \lesssim \| D^j u \|_{L^q(\ell + A(-1,0,1,2)^2)} \quad \text{and} \quad |D^j u(\ell)| \lesssim \| \nabla^j \tilde{u} \|_{L^1(\ell + A(-1,1)^2)}, \] (3.1)
where $D$ is the difference operator defined in (2.1). In particular,
\[ \| \nabla \tilde{u} \|_{L^q} \lesssim \| \nabla u \|_{L^q} \lesssim \| \nabla \tilde{u} \|_{L^q}, \]
where $u$ is identified with its piecewise affine interpolant.

Proof. This is the same proof as Lemma 6.1 in [5]. □

3.1. Properties of Steklov–Poincaré operator. As mentioned in Section 2.4, we require some regularity properties of the Steklov–Poincaré operator $g^{-1}$. First of all we have the following trace theorem.

Theorem 3.2 (Trace Theorem). For $\frac{1}{2} \leq s \leq 1$, the interior trace operator
\[ \gamma_0 : H^s(\Omega_h) \to H^{s-1/2}(\Gamma_h) \]
is bounded satisfying
\[ \| \gamma_0 v \|_{H^{s-1/2}(\Gamma_h)} \leq c_T \| v \|_{H^s(\Omega_h)}, \quad \forall v \in H^s(\Omega_h). \]

Proof. This is a standard result, see for example [2]. □

The boundedness and ellipticity of the boundary integrals are proved in [4] for Lipschitz domains.

Theorem 3.3 (Boundedness). The boundary integral operators
\[ V : H^{-1/2+s}(\Gamma_h) \to H^{1/2+s}(\Gamma_h), \]
\[ K : H^{1/2+s}(\Gamma_h) \to H^{1/2+s}(\Gamma_h), \]
\[ K' : H^{1/2+s}(\Gamma_h) \to H^{1/2+s}(\Gamma_h), \]
\[ D : H^{1/2+s}(\Gamma_h) \to H^{-1/2+s}(\Gamma_h) \]
are bounded for all $s \in (-\frac{1}{2}, \frac{1}{2})$.

Proof. See Theorem 1 in [4]. □

Theorem 3.4 (Ellipticity). The operators $V$ and $D$ are strongly elliptic in the sense that, there exists $C^V, C^D > 0$ such that for all $v \in H^{-1/2}(\Gamma_h), u \in H^{1/2}(\Gamma_h)$
\[ \langle V v, v \rangle \geq C^V \| v \|_{H^{-1/2}(\Gamma_h)}, \quad (3.2) \]
\[ \langle D u, u \rangle \geq C^D \| u \|_{H^{1/2}(\Gamma_h)}, \quad (3.3) \]

Proof. This is a special case of Theorem 2 in [4]. In 2D, the far-field constant $u_0$ vanishes only if the Dirichlet data is in the subspace $H^{1/2}(\Gamma_h)$. See Appendix A for a full proof. □

Lemma 3.5. $V : H^{-1/2}(\Gamma_h) \to H^{1/2}(\Gamma_h)$ is an isomorphism.

Proof. This is a consequence of Theorems 3.3 and 3.4 and the Lax-Milgram Theorem. □
Therefore, with the boundedness and ellipticity, we can prove the positive definiteness of the Steklov–Poincaré operator.

**Theorem 3.6.** The Steklov–Poincaré operator $g^{-1} : H^{1/2}_s(\Gamma_h) \rightarrow H^{-1/2}_s(\Gamma_h)$ is well-defined. Furthermore, there exist $C_1^g, C_2^g > 0$ such that for all $u \in H^{1/2}_s(\Gamma_h)$

\[
\langle g^{-1}u, u \rangle \geq C_1^g \|u\|_{H^{1/2}(\Gamma_h)}^2 \quad \text{and} \quad \|g^{-1}u\|_{H^{-1/2}(\Gamma_h)} \leq C_2^g \|u\|_{H^{1/2}(\Gamma_h)}.
\]  

**Proof.** Since $V : H^{-1/2}_s(\Gamma_h) \rightarrow H^{1/2}_s(\Gamma_h)$ is an isomorphism and $K : H^{1/2}(\Gamma_h) \rightarrow H^{1/2}(\Gamma_h)$ is bounded, we have $g^{-1} = V^{-1}(-K + (1 - \lambda)I)$ is well-defined. The upper bound $C_2^g$ follows from the Lax-Milgram Theorem.

For positive-definiteness, we use an analogous argument to that in [21]. We first observe that for any $u \in H^{1/2}_s(\Gamma_h)$, there exists an unique solution $v$ to the Laplace problem

\[
-\Delta v = 0, \quad \text{in } \Omega^c_h
\]

\[
v = u, \quad \text{on } \Gamma_h
\]

\[
|v(x)| = O\left(\frac{1}{|x|}\right) \quad \text{as } |x| \rightarrow \infty
\]

with $g^{-1}u = -\gamma^\text{int} v$. Similar to (2.14) and (2.15), we have the relationships

\[
v(x) = \lambda(x)u + (Ku)(x) - V(\gamma^\text{ext}_1 v)(x) \quad \text{and}
\]

\[
\gamma^\text{ext}_1 v(x) = (1 - \lambda(x))\gamma^\text{ext}_1 u(x) - (K\gamma^\text{ext}_1 v)(x) - Du(x).
\]

Combining these two equations we obtain an alternative representation for $g^{-1}$:

\[
g^{-1}(u) = -\gamma^\text{ext}_1 v = Du + (K' - (1 - \lambda)I)V^{-1}(K - (1 - \lambda)I)(u).
\]

Consequently we have

\[
\langle g^{-1}u, u \rangle = \langle Du, u \rangle + \langle V^{-1}(K - (1 - \lambda)I)u, (K - (1 - \lambda)I)u \rangle \geq \langle Du, u \rangle \geq C^D \|u\|_{H^{1/2}(\Gamma_h)}^2.
\]

\[\square\]

### 3.2. Re-scaling of the boundary integrals.

In the analysis of a/c coupling methods, we are concerned with the convergence rate against the size of the domain. Therefore, we need to explore how boundary integrals scale with the size of the domain.

Suppose that $f_1 : \Gamma_1 := \partial \Omega_1 \rightarrow \mathbb{R}^2$ and $f_1 \in H^{1/2}(\partial \Omega_1)$, where $\Omega_1$ is a Lipschitz domain with radius 1. Let $f_R : \Gamma_R := \partial \Omega_R \rightarrow \mathbb{R}^2$ and $f_R(x) := f_1(x/R)$, where $\Omega_R = R\Omega_1$. Then we have

\[
\|f_R\|_{L^2(\Gamma_R)}^2 = \int_{\Gamma_R} |f_R(x)|^2 \, dx = \int_{\Gamma_R} |f_1(x/R)|^2 \, dx = \int_{\Gamma_1} |f_1(y)|^2 R \, dy = R \|f_1\|_{L^2(\Gamma_1)}^2
\]
Lemma 3.7. Let \( \text{rescaled } H \) while

\[
|f_R|_{H^{1/2}(\Gamma_h)}^2 := \int_{\Gamma_R} \int_{\Gamma_R} \frac{|f_R(x) - f_R(y)|^2}{|x - y|^2} dS(x) dS(y)
\]

\[
= \int_{\Gamma_R} \int_{\Gamma_R} \frac{|f_1(x/R) - f_1(y/R)|^2}{|x - y|^2} dS(x) dS(y)
\]

\[
= \int_{\Gamma_1} \int_{\Gamma_1} \frac{|f_1(x') - f_1(y')|^2}{|Rx' - Ry'|^2} R^2 dS(x') dS(y')
\]

\[
= \int_{\Gamma_1} \int_{\Gamma_1} \frac{|f_1(x') - f_1(y')|^2}{|x' - y'|^2} dS(x') dS(y')
\]

\[
= |f_1|_{H^{1/2}(\Gamma_1)}^2.
\]

Thus we define a re-scaled norm in \( H^{1/2}(\Gamma_h) \),

\[
\|f\|_{H^{1/2}_h}^2 := \left[ \frac{1}{2} \text{diam}(\Gamma_h) \right]^{-1} \|f\|_{L^2(\Gamma_h)}^2 + |f|_{H^{1/2}(\Gamma_h)}^2,
\]

then we have \( \|f_1\|_{H^{1/2}(\Gamma_1)} = \|f_R\|_{H^{1/2}_h} \) with \( R = \frac{1}{2} \text{diam}(\Gamma_h) \). Similarly, we define a rescaled \( H^1 \) norm

\[
\|f\|_{H^1_h}^2 := \left[ \frac{1}{2} \text{diam}(\Gamma_h) \right]^{-1} \|f\|_{L^2(\Gamma_h)}^2 + \left[ \frac{1}{2} \text{diam}(\Gamma_h) \right] \|\nabla f\|_{L^2(\Gamma_h)}^2,
\]

then we have \( \|f_1\|_{H^1(\Gamma_1)} = \|f_R\|_{H^1_h} \) with \( R = \frac{1}{2} \text{diam}(\Gamma_h) \).

**Lemma 3.7.** Let \( V_1, K_1, V_R, K_R \) be the boundary integrals \( V \) and \( K \) on \( \Gamma_1 \) and \( \Gamma_R \) respectively. Denote

\[
g_1^{-1} := V_1^{-1}(-K_1 + (1 - \lambda)I) \quad \text{and} \quad g_R^{-1} := V_R^{-1}(-K_R + (1 - \lambda)I).
\]

Then for \( u_1 \in H^{1/2}_h(\Gamma_1) \) and \( u_R := u_1(x/R) \), we have \( u_R \in H^{1/2}_h(\Gamma_R) \) and

\[
\langle g_1^{-1} u_1, u_1 \rangle_{\Gamma_1} = \langle g_R^{-1} u_R, u_R \rangle_{\Gamma_R}.
\]

**Proof.** See Appendix B. □

Using the re-scaled norm we have the following Lemma.

**Lemma 3.8.** The Steklov–Poincaré operator \( g^{-1} : H^{1/2}_h(\Gamma_h) \rightarrow H^{-1/2}_h(\Gamma_h) \) has the following regularity, for \( u \in H^{1/2}_h(\Gamma_h) \)

\[
\langle g^{-1} u, u \rangle \geq C_1 \|u\|_{H^1_h}^2 \quad \text{and} \quad \|g^{-1} u\|_{H^{-1/2}_h(\Gamma_h)} \leq C_2 \|u\|_{H^1_h}^2,
\]

where \( C_1 \) and \( C_2 \) are independent of the radius of \( \Omega_h \).

**Proof.** The result follows directly from Theorem 3.6 and Lemma 3.7. □
3.3. Boundary element approximation error. We also need the following boundary element approximation error estimate to compare \( g^{-1} \) and \( g_h^{-1} \).

**Theorem 3.9.** If \( u \in H^{1/2}(\Gamma_h) \), then the approximation solution \( g_h^{-1}u \) to (2.19) exists and we have the following stability property

\[
\|g_h^{-1}u\|_{H^{-1/2}(\Gamma_h)} \leq \frac{C_2}{C_1} \|u\|_{H^{1/2}_h},
\]

(3.8)

Furthermore, if \( g^{-1}u \in H^{1}(\Gamma_h) \), then

\[
\|g^{-1}u - g_h^{-1}u\|_{H^{-1/2}(\Gamma_h)} \leq Ch^{3/2}\|g^{-1}u\|_{H^{1}(\Gamma_h)},
\]

(3.9)

where \( h \) is the size of each boundary element and \( C \) is independent of the size of \( \Gamma_h \).

**Proof.** Since \( S_0^1(\Gamma_h) \) is a conforming trial space in \( H^{-1/2}(\Gamma_h) \) and \( g^{-1}u \) is bounded and elliptic according to Lemma 3.8, then by the Lax-Milgram Theorem \( g_h^{-1}u \) exists and we have (3.8). For (3.9), by Cea’s Lemma we have

\[
\|g^{-1}u - g_h^{-1}u\|_{H^{-1/2}(\Gamma_h)} \leq \frac{C_2}{C_1} \inf_{v_h \in H^{-1/2}(\Gamma_h)} \|g^{-1}u - v_h\|_{H^{-1/2}(\Gamma_h)}.
\]

By Theorem 10.4 in [21], we have

\[
\inf_{v_h \in H^{-1/2}(\Gamma_h)} \|g^{-1}u - v_h\|_{H^{-1/2}(\Gamma_h)} \leq ch^{3/2}\|g^{-1}u\|_{H^{1}(\Gamma_h)}.
\]

\[\square\]

4. Main results

4.1. Regularity of \( u^a \). The approximation error estimates in later sections requires the decay of the elastic fields away from the defect core which follows from a natural stability assumption:

(A1) The atomistic solution is strongly stable, that is, there exists \( C_0 > 0 \),

\[
\langle \delta^2 \mathcal{E}^a(u^a) \varphi, \varphi \rangle \geq C_0 \| \nabla \varphi \|^2_{L^2}, \quad \forall \varphi \in \mathcal{U}^{1,2},
\]

(4.1)

where \( u^a \) is a solution to (2.2).

**Corollary 4.1.** Suppose that (A1) is satisfied, then there exists a constant \( C > 0 \) such that, for \( 1 \leq j \leq 3 \),

\[
|D^j u^a(\ell)| \leq C|\ell|^{-1-j} \quad \text{and} \quad |\nabla^j \tilde{u}^a(x)| \leq C|x|^{-1-j}.
\]

**Proof.** See Theorem 2.3 in [8].

\[\square\]

4.2. Stability. In [16] it is proven that there is a “universal” instability in 2D interfaces for QNL-type a/c couplings. It is impossible to show that \( \delta^2 \mathcal{E}^{G23}(u^a) \) is a positive definite operator for general cases, even with the assumption (4.1). In fact, this potential instability is universal to a wide class of generalized geometric reconstruction methods. Nevertheless, it is rarely observed in practice. To circumvent this difficulty, we make the following standing assumption:

(A2) The homogeneous lattice is strongly stable under the G23 approximation, that is, there exists \( C_0^a > 0 \) which is independent of \( K \) such that, for \( K \) sufficiently large,

\[
\langle \delta^2 \mathcal{E}^{a0}_h(0) \varphi_h, \varphi_h \rangle \geq C_0^a \| \nabla \varphi_h \|^2_{L^2}, \quad \forall \varphi_h \in \mathcal{U}_h.
\]

(4.2)
Because\(^{(4.2)}\) does not depend on the solution it can be tested numerically. But a precise understanding under which conditions \((4.2)\) is satisfied is still missing. In\(^{(16)}\) a method of stabilizing 2D QNL-type schemes with flat interfaces is formulated, which could replace this assumption, but we are not yet able to extend this method to interfaces with corners, such as the configurations discussed in this paper. From these two assumptions, we can deduce the following stability result when the BEM formulation is added.

**Lemma 4.2.** For any \(\varphi_h \in \mathcal{U}_h^*\), we have
\[
\langle \delta^2 \mathcal{E}_h^{\text{tot}}(0) \varphi_h, \varphi_h \rangle \geq C_0^{\text{tot}} \| \varphi_h \|_E^2,
\]
where \(\| \cdot \|_E\) is the norm defined in\(^{(2.18)}\) and \(C_0^{\text{tot}}\) is independent of the size of \(\Omega_h\).

**Proof.** This is an immediate consequence of the property \((3.7)\) of \(g^{-1}\):
\[
\langle \delta^2 \mathcal{E}_h^{\text{tot}}(0) \varphi_h, \varphi_h \rangle = \langle \delta^2 \mathcal{E}_h^{\text{ac}}(0) \varphi_h, \varphi_h \rangle + \mu \int_{\Gamma_h} \varphi_h g^{-1} \varphi_h \\
\geq C^{\text{ac}} \| \nabla \varphi_h \|_{L^2(\Omega_h)}^2 + C_1 \| \varphi_h \|_{H^{1/2}}^2 \\
\geq \min\{C^{\text{ac}}, C_1\} \| \varphi_h \|_E^2.
\]

Then we have the following stability estimate.

**Theorem 4.3.** Under assumptions (A1) and (A2) there exists \(\gamma > 0\) such that, when the atomistic region radius \(K\) is sufficiently large,
\[
\langle \delta \mathcal{G}_h(\Pi_h u^a) \varphi_h, \varphi_h \rangle \geq \gamma \| \varphi_h \|_E^2 \quad \text{for all } \varphi_h \in \mathcal{U}_h^*.
\]

**Proof.** After employing Lemma 4.2 this is a straightforward adaptation of the proof of\(^{(12)}\) Lemma 4.9.

\(\Box\)

### 4.3 Main results

Our two main results are a consistency error estimate for the A/C+BEM coupling scheme and the resulting error estimate.

**Theorem 4.4 (Consistency).** If \(u^a\) is a solution to\(^{(2.2)}\), then for all \(v_h \in \mathcal{U}_h^*\)
\[
\langle \delta \mathcal{E}_h^{\text{tot}}(\Pi_h u^a), v_h \rangle \\
\preceq \left( \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega)} + \| \nabla^3 \tilde{u}^a \|_{L^2(\mathbb{R}^2 \setminus \Omega^a)} + \| \nabla^2 \tilde{u}^a \|_{L^2(\mathbb{R}^2 \setminus \Omega^a)}^2 + \| h^{-1/2} \nabla \tilde{u}^a \|_{L^2(\Gamma_h)} + N^{-3} \right) \| v_h \|_E.
\]

**Proof.** See Section 7.6.

\(\Box\)

Combining Theorem 4.4 with the stability result Theorem 4.3 we obtain the following error estimate.

**Theorem 4.5.** If \(u^a\) is a solution to\(^{(2.2)}\) and Assumptions (A1) and (A2) are satisfied then, for \(K\) sufficiently large, there exists a solution \(u_h \in \mathcal{U}_h^*\) to\(^{(2.21)}\) satisfying
\[
\| \tilde{u}^a - u_h \|_E \preceq \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega)} + \| \nabla^3 \tilde{u}^a \|_{L^2(\mathbb{R}^2 \setminus \Omega^a)} + \| \nabla^2 \tilde{u}^a \|_{L^2(\mathbb{R}^2 \setminus \Omega^a)}^2 + \| h^{-1/2} \nabla \tilde{u}^a \|_{L^2(\Gamma_h)} + N^{-3}.
\]

\(\Box\)
Proof. See Section 7.7. □

Remark 4.6. The term $N^{-3}$ is in fact the linearization error. Recall that in (2.9) we approximate the Cauchy–Born strain energy $W(\nabla u)$ by the linearised elasticity strain energy $\frac{1}{2}\mu|\nabla u|^2$. The linearization error in first variation can (formally) be estimated by

$$\int_{\Omega_h} [\partial_k W(\nabla u)\nabla v - \mu \nabla u \cdot \nabla v] \lesssim \int_{\Omega_h} |\nabla u|^2 |\nabla v| \lesssim \|\nabla u\|_{L^2(\Omega_h)}^2 \|\nabla v\|_{L^2(\Omega_h)}.$$

Taking account of the decay of $\tilde{u}^a$ from Corollary 4.1, we have

$$\|\nabla \tilde{u}^a\|_{L^4(\Omega_h)}^2 \lesssim N^{-3}.$$

For technical reasons we cannot directly perform such an estimate, but the $O(N^{-3})$ term arises in an indirect way; cf. §7.5.3 and 7.5.4. □

4.4. Optimal approximation parameters. In [5] we discussed the optimization of mesh parameters for P1-FEM and P2-FEM. We now perform a similar analysis for the setting of the present work, including the BEM approximation of the elastic far-field.

Recall that $K$ is the radius of atomic region $\Omega^a$ and $N$ is the radius of $\Omega_h$. To simplify the discussion we assume that the FE mesh grading is linear, $|h(x)| \approx |x|/K$, which ensures quasi-optimal computational cost, up to logarithmic terms. In this setting it is easy to see that the various error contributions in (4.6) are bounded by

- Modelling error: $\|\nabla^2 \tilde{u}^a\|_{L^2(\Omega^a)} + \|\nabla^3 \tilde{u}^a\|_{L^2(\Omega^a)} + \|\nabla^2 \tilde{u}^a\|_{L^4(\Omega^a)} \lesssim K^{-5/2}$,
- FEM error: $\|h\nabla^2 \tilde{u}^a\|_{L^2(\Omega_h)} \lesssim (K^{-4} - K^{-2}N^{-2})^{1/2}$,
- BEM error: $\|h^{3/2}\nabla^2 \tilde{u}^a\|_{L^2(\Gamma_h)} \lesssim K^{-3/2}N^{-1}$, and
- Linearisation error: $N^{-3}$.

The key observation is that the modelling error, which cannot be reduced by choice of $N$ or $h$ is $O(K^{-5/2})$. By choosing $N \leq K + C$ for some fixed constant, both the FEM and the BEM errors also become $O(K^{-5/2})$, whereas for $N \gg K$, we obtain that the FEM error contribution becomes $O(K^{-2})$ which is strictly larger.

This quasi-optimal balance of approximation parameters means that we ought to remove the nonlinear elasticity region and directly couple the atomistic model to the BEM. The resulting error estimate is

$$\|\tilde{u}^a - u_h\|_E \lesssim K^{-5/2},$$

(4.7)

which is the best possible rate that can be achieved for a sharp-interface coupling method.

We remark, however, that the interface region (and therefore a thin layer of Cauchy–Born elasticity) cannot be removed entirely since the BEM must be coupled to a local elasticity model (FEM) rather than directly to the atomistic model. Coupling directly to the atomistic model would lead to a new consistency error usually dubbed “ghost forces”.
5. Conclusion

In this work we have explored the natural combination of atomistic, finite element and boundary element modelling from the perspective of error analysis. The conclusion is an interesting, albeit not entirely unexpected, one. The rapid decay of elastic fields in the point defect case \(|\nabla^j \tilde{u}(x)| \lesssim |x|^{-1-j}|\) means that the continuum model error \(|\nabla^3 \tilde{u}|\) and and linearisation error \(|\nabla \tilde{u}|^2|\) are balanced. It is therefore reasonable to entirely bypass the nonlinear elasticity model and couple the atomistic region directly to a linearised elasticity model. This observation, as well as additional complexities due to finite element and boundary element discretisation errors are made precise in Theorem 4.5 and in the discussion in § 4.4.

Because the characteristic decay of elastic fields is different for different material defects (or other materials modelling situations) our conclusion cannot immediately applied to other contexts. However in those situations our analysis can still provide guidance on how to generalise our results and optimally balance approximation errors due to continuum approximations, linearisation, finite element and boundary element approximations.

6. Proofs: Reduction to consistency

Assuming the existence of an atomistic solution \(u^a\) to (2.2), we seek to prove the existence of \(\bar{u}^\ast\) satisfying

\[
\langle \delta \mathcal{E}_h^\text{tot}(u^a_h), \varphi_h \rangle = \langle \delta f(u_h), \varphi_h \rangle, \quad \text{for all } \varphi_h \in \mathcal{U}_h^*,
\]

and to estimate the error \(\|u^a - u^a_h\|_E\).

The error analysis consists of a best-approximation analysis (§ 6.1), consistency and stability estimates (§ 6.3). Once these are established we apply a formulation of the inverse function theorem (§ 6.2) to obtain the existence of a solution \(u^a_h\) and the error estimate.

6.1. The best approximation operator. We define a quasi-best approximation map \(\Pi_h : C(\mathbb{R}^2; \mathbb{R}^m) \to \mathcal{U}_h\) to be the nodal interpolation operator, i.e., for \(f \in C(\mathbb{R}^2; \mathbb{R}^m), \Pi_h(f)|_T \in \mathbb{P}^1(T)\) for \(T \subset \mathcal{T}_h\) and

\[
\Pi_h(f)(x) = f(x) - f_0 \quad \text{for all } x \in \mathcal{N}_h,
\]

where \(f_0\) is a constant such that \(f(x) - f_0 \in H^{1/2}_v(\Gamma_h)\) for \(x \in \Gamma_h\). Then it is clear that \(\Pi_h u^a \in \mathcal{U}_h^*\).

6.2. Inverse Function Theorem. The proof of this theorem is standard and can be found in various references, e.g. [18, Lemma 2.2].

**Theorem 6.1 (The inverse function theorem).** Let \(\mathcal{U}_h\) be a subspace of \(\mathcal{U}\), equipped with \(\|\nabla \cdot \|_{L^2}\), and let \(\mathcal{G}_h \in C^1(\mathcal{U}_h, \mathcal{U}_h^*)\) with Lipschitz-continuous derivative \(\delta \mathcal{G}_h\):

\[
\|\delta \mathcal{G}_h(u_h) - \delta \mathcal{G}_h(v_h)\|_{\mathcal{L}} \leq M \|\nabla u_h - \nabla v_h\|_{L^2} \quad \text{for all } u_h, v_h \in \mathcal{U}_h,
\]

where \(\|\cdot\|_{\mathcal{L}}\) denotes the \(\mathcal{L}(\mathcal{U}_h, \mathcal{U}_h^*)\)-operator norm.

Let \(\bar{u}_h \in \mathcal{U}_h\) satisfy

\[
\|\mathcal{G}_h(\bar{u}_h)\|_{\mathcal{U}_h^*} \leq \eta, \quad \langle \delta \mathcal{G}_h(\bar{u}_h)v_h, v_h \rangle \geq \gamma \|\nabla v_h\|_{L^2}^2 \quad \text{for all } v_h \in \mathcal{U}_h,
\]

(6.2) (6.3)
such that $M, \eta, \gamma$ satisfy the relation
\[ \frac{2M\eta}{\gamma^2} < 1. \]

Then there exists a (locally unique) $u_h \in U_h$ such that $G_h(u_h) = 0$,
\[ \| \nabla u_h - \nabla \bar{u}_h \|_{L^2} \leq \frac{\eta}{\gamma}, \quad \text{and} \]
\[ \langle \delta G_h(u_h) v_h, v_h \rangle \geq \left( 1 - \frac{2M\eta}{\gamma^2} \right) \gamma \| \nabla v_h \|_{L^2}^2 \quad \text{for all } v_h \in U_h. \]

To put Theorem 6.1 (Inverse Function Theorem) into our context, let $G_h(v) := \delta \mathcal{E}_h(v) - \delta f(v)$ and $\bar{u}_h := \Pi_h u^a$,
where $u^a$ is a solution to (2.2).

To make (6.2) and (6.3) concrete we will show that there exist $\eta, \gamma > 0$ such that, for all $v_h \in U_h^*$,
\[ \langle \delta \mathcal{E}_h(u^a), \varphi_h \rangle - \langle \delta f(u^a), \varphi_h \rangle \leq \eta \| \varphi_h \|_E, \quad \text{(consistency)} \]
\[ \langle \delta^2 \mathcal{E}_h(u^a), \varphi_h \rangle - \langle \delta^2 f(u^a), \varphi_h \rangle \geq \gamma \| \varphi_h \|_E^2. \quad \text{(stability)} \]

Ignoring some technical requirements, the inverse function theorem implies that, if $\eta/\gamma$ is sufficiently small, then there exists $u_h^{ac} \in U_h^*$ such that
\[ \langle \delta \mathcal{E}_h(u_h^{ac}), \varphi_h \rangle - \langle \delta f(u_h^{ac}), \varphi_h \rangle = 0, \quad \forall \varphi_h \in U_h^*, \quad \text{and} \]
\[ \| u_h^{ac} - \Pi_h u^a \|_E \leq \frac{2\eta}{\gamma}. \]

Finally adding the best approximation error $\| \Pi_h u^a - u^a \|_H$ gives the error estimate
\[ \| u_h^{ac} - u^a \|_E \leq \| \Pi_h u^a - u^a \|_E + \frac{2\eta}{\gamma}. \]

6.3. **Stability and Lipschitz condition.** The Lipschitz and consistency estimates require bounds on the partial derivatives of $V$. For $\mathbf{g} \in \mathbb{R}^{m \times 6}$, define the first and second partial derivatives, for $i, j = 1, \ldots, 6$, by
\[ \partial_j V(\mathbf{g}) := \frac{\partial V(\mathbf{g})}{\partial g_j} \in \mathbb{R}^m, \quad \text{and} \quad \partial_{ij} V(\mathbf{g}) := \frac{\partial^2 V(\mathbf{g})}{\partial g_i \partial g_j} \in \mathbb{R}^{m \times m}, \]
and similarly for the third derivatives $\partial_{ijk} V(\mathbf{g}) \in \mathbb{R}^{m \times m \times m}$. We assumed in §2.1 that second and higher derivatives are bounded, hence we can define the constants
\[ M_2 := \sum_{i,j=1}^{6} \sup_{\substack{\mathbf{g} \in \mathbb{R}^{m \times 6} \\text{\ s.t. } |h_1|=|h_2|=1}} \sup_{h_1, h_2 \in \mathbb{R}^2} \partial_{ij} V(\mathbf{g})[h_1, h_2] < \infty, \quad \text{and} \quad (6.4) \]
\[ M_3 := \sum_{i,j,k=1}^{6} \sup_{\substack{\mathbf{g} \in \mathbb{R}^{m \times 6} \\text{\ s.t. } |h_1|=|h_2|=|h_3|=1}} \sup_{h_1, h_2, h_3 \in \mathbb{R}^2} \partial_{ijk} V(\mathbf{g})[h_1, h_2, h_3] < \infty. \quad (6.5) \]

With the above bounds it is easy to show that
\[
\sum_{i=1}^{6} |\partial_i V(g) - \partial_i V(h)| \leq M_2 \max_{j=1,\ldots,6} |g_j - h_j|, \quad \text{and} \\
\sum_{i,j=1}^{6} |\partial_i \partial_j V(g) - \partial_i \partial_j V(h)| \leq M_3 \max_{k=1,\ldots,6} |g_k - h_k|, \quad \text{for } g, h \in \mathbb{R}^{m \times 6}.
\] (6.6)

We can now obtain the following Lipschitz continuity and stability results.

**Lemma 6.2.** There exists \( M > 0 \) such that
\[
\|\delta \mathcal{G}_h(u_h) - \delta \mathcal{G}_h(v_h)\| \leq M \|u_h - v_h\|_E \quad \text{for all } u_h, v_h \in \mathcal{U}_h^*,
\] (6.7)
where \( \|\cdot\|_E \) denotes the operator norm associated with \( \|\cdot\|_E \).

### 7. Proofs: Consistency

#### 7.1. Interpolants

In this section we introduce two interpolants that are necessary tools for our analysis.

**7.1.1. Test function \(v\).** The consistency error \(\delta \mathcal{E}^\text{tot}_h(\Pi_h u^a)\) will be bounded by estimating
\[
\langle \delta \mathcal{E}^\text{tot}_h(\Pi_h u^a), v_h \rangle - \langle \delta \mathcal{E}^\text{tot}(u^a), v \rangle \leq \eta_h \|v_h\|_E \quad \forall v_h \in \mathcal{U}_h^*,
\]
with \( v \in \hat{\mathcal{U}}^{1,2} \) chosen arbitrarily. The purpose of this section is to construct such \( v = \Pi_h^* v_h \), where \( \Pi_h^*: \mathcal{U}_h^* \to \hat{\mathcal{U}}^{1,2} \).

Given some \( v_h \in \mathcal{U}_h^* \) the first step is to extend \( v_h \) to \( \mathbb{R}^2 \). Let \( v^E_h \) be the solution to the exterior Dirichlet problem
\[
-\Delta v^E_h = 0, \quad \text{in } \Omega^E_h, \\
v^E_h = v_h, \quad \text{on } \partial\Omega_h, \\
v^E_h = v_h, \quad \text{in } \Omega_h,
\] (7.1)
where we note that the last condition can be imposed because \( v_h \in \mathcal{U}_h^* \).

Next, we adapt the quasi-interpolation operator introduced in [3] to “project” \( v^E_h \) to \( \hat{\mathcal{U}}^{1,2} \). Let \( \phi_\ell \) be the piecewise linear hat-functions on the atomistic triangulation \( \mathcal{T} \), i.e., the canonical triangulation associated with \( \Lambda \). Define
\[
\phi_\ell^{\text{PU}} := \frac{\phi_\ell}{\sum_{k \in \mathcal{C}} \phi_k} \quad \forall \ell \in \mathcal{C},
\]
where \( \mathcal{C} \) is the continuum lattice sites as defined in Section 2.2. It is clear that \( \{\phi_\ell^{\text{PU}}\}_{\ell \in \mathcal{C}} \) is a partition of unity of \( \mathbb{R}^2 \setminus \Omega^a \cup \Omega^i \).

In order to estimate the interpolation error and modelling error in (7.10), we need \( v - v^E_h \) to vanish in \( \Omega^a \cup \Omega^i \) and on \( \Gamma_h \). This is made possible due to assumption (A3).

Now we refer to [3] for the construction of a linear interpolant of \( v^E_h \in \mathcal{U}_h^* \). We shall define the interpolant as follows:
\[
\Pi_h^* v_h(x) := v(x) := v_1(x) + v_2(x), \quad \forall x \in \mathbb{R}^2,
\] (7.2)
Lemma 7.1. The Dirichlet problem
\[ -\Delta w = 0, \quad \text{in } B_R^\epsilon, \]
\[ w = u_R^a, \quad \text{on } \partial B_R, \]
\[ |w(x)| = O \left( \frac{1}{|x|} \right) \quad \text{as } |x| \to \infty. \]  

\[ \|\nabla w - \nabla \tilde{u}^a\|_{L^2(B_R^\epsilon)} \lesssim R^{-3}. \]  

7.1.2. Linearized elasticity approximation \( w \). Recall that \( u^a \in \bar{U}^{1,2} \) is the exact atomistic solution and Lemma 3.1 shows that there exists a \( C^{2,1} \)-regular interpolant \( \tilde{u}^a \) of \( u^a \).

In order to make use of existing BEM approximation error estimates (3.9), we need the conormal derivative in \( H^1(\Gamma_h) \) of a solution to Laplace’s equation (\( u^a \) only solves Laplace’s equation approximately). To that end, we introduce an intermediate problem on a domain with smooth boundary inside \( \Omega_h \). Let \( B_R \subset \Omega_h \) be a ball with radius \( R = \frac{2}{3}N \). To ensure the appropriate Dirichlet boundary condition, we use (2.16) to define the following function: let \( u_R^a \) be a constant such that
\[ u_R^a := \tilde{u}^a - u_0^a \quad \text{and } u_R^a|_{\partial B_R} \in H^{1/2}(\partial B_R). \]

Let \( w \) be the solution to the exterior Dirichlet problem
\[ -\Delta w = 0, \quad \text{in } B_R^\epsilon, \]
\[ w = u_R^a, \quad \text{on } \partial B_R, \]
\[ |w(x)| = O \left( \frac{1}{|x|} \right) \quad \text{as } |x| \to \infty. \]  

Lemma 7.1. The Dirichlet problem (7.5) has a unique solution and
\[ \|\nabla w - \nabla \tilde{u}^a\|_{L^2(B_R^\epsilon)} \lesssim R^{-3}. \]  

Note that with the assumption (A3), we have
\[ v(x) - v_h(x) = 0, \quad \forall x \in \Gamma_h. \]

We can use [3, Theorem 3.1] to conclude that
\[ \|\nabla v\|_{L^2(\mathbb{R}^2)} \lesssim \|\nabla v_h^E\|_{L^2(\mathbb{R}^2)}, \quad \forall v_h \in U_h. \]

Furthermore, since \( v_h^E \) is the extension of \( v_h \) via the exterior Laplace problem (7.1), we can link its energy norm to boundary norm of \( v_h \). By the regularity of \( g^{-1} \) in Lemma 3.8 we have
\[ \|\nabla v_h^E\|_{L^2(\Omega_h^\epsilon)} = \langle g^{-1}v_h, v_h \rangle \lesssim \|v_h\|^2_{H^{1/2}_h}. \]  

Therefore we have
\[ \|\nabla v\|_{L^2(\mathbb{R}^2)} \lesssim \|\nabla v_h\|_{L^2(\Omega_h)} + \|\nabla v_h^E\|_{L^2(\Omega_h^\epsilon)} \lesssim \|\nabla v_h\|_{L^2(\Omega_h)} + \|v_h\|_{H^{1/2}_h} \lesssim \|v_h\|_E. \]  

where
\[ v_1(\ell) := \left\{ \begin{array}{ll}
 v_h^E(\ell), & \ell \in A \cup I \cup I^+ \cup (\Gamma_h \cap C), \\
 \frac{f_{2\pi}(\ell)}{f_{2\pi}(\phi_{\ell})}, & \ell \in C \setminus (I^+ \cup \Gamma_h),
\end{array} \right.
\]
\[ v_1(x) := \sum_{\ell \in \Lambda} v_1(\ell) \phi_{\ell}(x), \quad \forall x \in \mathbb{R}^2, \]
\[ v_2(\ell) := \left\{ \begin{array}{ll}
 \frac{f_{2\pi}(\ell^E - v_h^E)\phi_{\ell}}{f_{2\pi}(\phi_{\ell})}, & \ell \in C \setminus (I^+ \cup \Gamma_h), \\
 0, & \ell \in A \cup I \cup I^+ \cup (\Gamma_h \cap C),
\end{array} \right.
\]
\[ v_2(x) := \sum_{\ell \in \Lambda} v_2(\ell) \phi_{\ell}(x), \quad \forall x \in \mathbb{R}^2. \]
Proof. From Section 3.1 we know that this exterior Dirichlet problem has a unique solution. To estimate (7.6), we let
\[ \phi := \tilde{u}^a - w \text{, extended by zero to } B_R \]
then
\[ \| \nabla \phi \|_{L^2(B_R^c)}^2 = \int_{B_R^c} (\nabla \tilde{u}^a - \nabla w) \cdot \nabla \phi = \int_{\mathbb{R}^2} \nabla \tilde{u}^a \cdot \nabla \phi =: B \]

Next, we use the fact that \( B \) is a linearised continuum approximation to the atomistic equilibrium equations. Recalling that \( u^a \) is an atomistic solution, i.e.,
\[ \langle \delta E^a(u^a), \phi \rangle = 0 \quad \forall \phi \in \dot{U}^{1,2} \]
and that \( \partial_F^2 W(0) = \mu I \), we can split \( B \) into
\[ B = \int_{\mathbb{R}^2} \nabla \tilde{u}^a \cdot \nabla \phi - \mu^{-1} \langle \delta E^a(u^a), \phi \rangle \]
\[ = \left( \int_{\mathbb{R}^2} \nabla \tilde{u}^a \cdot \nabla \phi - \mu^{-1} \int_{\mathbb{R}^2} \partial_F W(\nabla \tilde{u}^a) \cdot \nabla \phi \right) + \mu^{-1} \left( \int_{\mathbb{R}^2} \partial_F W(\nabla \tilde{u}^a) \cdot \nabla \phi - \langle \delta E^a(u^a), \phi \rangle \right) \]
\[ =: B_1 + B_2. \]

For \( B_1 \), we apply Taylor’s expansion and use \( \partial_F^2 W(0) = \mu I \) to obtain
\[ |B_1| \leq \left| \int_{\mathbb{R}^2} \nabla \tilde{u}^a - \mu^{-1} \partial_F W(0) - \mu^{-1} \partial_F^2 W(0) \nabla \tilde{u}^a \right| \cdot \nabla \phi + C \int_{\mathbb{R}^2} |D\tilde{u}^a|^2 |\nabla \phi| \]
\[ = C \int_{\mathbb{R}^2} |\nabla \tilde{u}^a|^2 |\nabla \phi| \leq C \| \nabla \tilde{u}^a \|_{L^4(B_R^c)} \| \nabla \phi \|_{L^2} \leq CR^{-3} \| \nabla \phi \|_{L^2}, \]
where the constant \( C \) is independent of \( \tilde{u}^a \) and \( \phi \).

\( B_2 \) is the Cauchy–Born modelling error which is well understood, e.g., in [17] it is proven that
\[ B_2 \leq \int_{\mathbb{R}^2} (C_1 |\nabla^3 \tilde{u}^a| + C_2 |\nabla^2 \tilde{u}^a|^2) |\nabla \phi|, \]
hence we obtain
\[ B_2 \leq \left( \| \nabla^3 \tilde{u}^a \|_{L^2(B_R^c)} + \| \nabla^2 \tilde{u}^a \|_{L^4(B_R^c)} \right) \| \nabla \phi \|_{L^2}
\[ \leq (R^{-3} + R^{-5}) \| \nabla \phi \|_{L^2}. \]
Combining the estimates for \( B_1 \) and \( B_2 \) yields the stated result. \( \square \)

The second estimate we require for \( w \) is for the decay of \( \nabla^2 w \).

**Lemma 7.2.** Let \( w \) be given by (7.5), and \( R \leq \frac{2}{3} N \), where \( N \) is the inner radius of \( \Omega_h \), then
\[ |\nabla^2 w(x)| \lesssim |x|^{-3} \quad \text{for } |x| \geq N \] (7.7)
and in particular,
\[ \| \nabla^2 w \|_{L^2(\Omega_h^c)} \lesssim N^{-5/2} \] (7.8)
Proof. Since the auxiliary problem (7.5) involves a circular boundary $\partial \Omega^c_R$, we can exploit separation of variables and Fourier series to estimate $\nabla^2 w$. We write $\tilde{u}^a$ and $w$ in polar coordinates as

$$\tilde{u}^a(r, \theta) = \sum_{k \in \mathbb{Z}} \hat{a}_k(r)e^{ik\theta},$$

$$w(r, \theta) = \sum_{k \in \mathbb{Z}} \hat{W}_k(r)e^{ik\theta}.$$  \hspace{1cm} (7.9)

The boundary condition $w = \tilde{u}^a$ on $\partial B_R$ becomes

$$w(R, \theta) = \tilde{u}^a(R, \theta), \hspace{0.5cm} i.e., \hspace{0.5cm} \hat{W}_k(R) = \hat{a}_k(R).$$

The Laplace operator in polar coordinates in 2D is given by

$$-\Delta_{x,y} = -r^{-1}\partial_r(r^{-1}\partial_r) - r^{-2}\partial_{\theta}^2.$$ Substituting (7.9) we obtain

$$\sum_{k \in \mathbb{Z}} \partial_r^2 \hat{W}_k + r^{-1}\partial_r \hat{W}_k - k^2 r^{-2} \hat{W}_k = 0.$$ Solving the resulting ODE for each $\hat{W}_k$ and taking into account the decay and boundary condition from (7.5), we deduce that

$$w(r, \theta) = \sum_{k \in \mathbb{Z}} \hat{a}_k(R) \left( \frac{r}{R} \right)^{|k|} e^{ik\theta}.$$ Using the fact that, for $p \in \mathbb{N}$ and $q \geq 1 + \epsilon$,

$$\sum_{k \in \mathbb{Z}} |k|^p q^{-2|k|} \leq C_{p, \epsilon} q^2.$$ We can now estimate

$$|\nabla^2_r w(r, \theta)| = \left| r^{-2} \sum_{k \in \mathbb{Z}} |k|(|k| + 1) \hat{a}_k(R) \left( \frac{r}{R} \right)^{-|k|} e^{ik\theta} \right|$$

$$\leq r^{-2} \left( \sum_{k \in \mathbb{Z}} |\hat{a}_k(R)|^2 \right)^{1/2} \left( \sum_{k \in \mathbb{Z}} |k|^4 \left( \frac{r}{R} \right)^{-2|k|} \right)^{1/2}$$

$$\lesssim r^{-2} (r/R)^2 \left( \frac{1}{R} \int_{\partial B_R} |\tilde{u}^a|^2 \right)^{1/2},$$

where in the last line we also used Plancherel’s Theorem. Using the fact that $|\tilde{u}^a(x)| \lesssim |x|^{-1}$ we finally obtain

$$|\nabla^2_r w(r, \theta)| \lesssim (r/R)^{-3}.$$ Analogous arguments for $\nabla^2_\theta w$ and $\nabla_r \nabla_\theta w$ yield

$$|\nabla^2_\theta w(r, \theta)| \lesssim (r/R)^{-3}.$$ The first result (7.7) follows from the assumption that $R \leq \frac{2}{3} N$. The second result (7.8) is an immediate consequence of (7.7). \hfill \Box
7.2. Consistency decomposition. Given a solution $u^a$ to (2.2) and a discrete test function $v_h$, let $\Pi_h u^a$ be as defined in §6.1 let $v = \Pi_h^c v_h$ be defined by (7.2), and let $w$ be given by (7.5). Moreover, let

$$\tilde{u}_h := \tilde{u}^a - c_h$$

such that $\tilde{u}_h |_{\Gamma_h} \in H^{1/2}(\Gamma_h)$, then we decompose the consistency error into

$$\langle \delta E^{\text{tot}}_h (\Pi_h u^a), v_h \rangle = \langle \delta E^{\text{tot}}_h (\Pi_h u^a), v_h \rangle - \langle \delta E^a(u^a), v \rangle$$

$$= \langle \delta E^{ac}_h (\Pi_h u^a), v_h \rangle + \mu\langle g_h^{-1} \Pi_h u^a, v_h \rangle_{\Gamma_h} - \langle \delta E^a(u^a), v \rangle$$

$$= \langle \delta E^{ac}_h (\Pi_h u), v_h \rangle - \langle \delta E^{ac}(\tilde{u}^a), v \rangle$$

(7.10)

interpolation error

$$+ \langle \delta E^{ac}(\tilde{u}^a) - \delta E^a(\tilde{u}^a), v \rangle - \int_{\Omega_h} (\partial W(\nabla \tilde{u}^a) - \mu \nabla \tilde{u}^a) \cdot \nabla v$$

modelling error

$$+ \mu \langle g_h^{-1} \Pi_h u^a, v_h \rangle_{\Gamma_h} - \mu \int_{\Omega_h^c} \nabla \tilde{u}^a \cdot \nabla v.$$

BEM error

7.3. The interpolation error. The first part of the consistency error, the interpolation error, has already been estimated in [5].

Lemma 7.3. The interpolation error can be estimated by

$$\langle \delta E^{ac}_h (\Pi_h u^a), v_h \rangle - \langle \delta E^{ac}_h (\tilde{u}^a), v \rangle$$

$$\leq c(M_2 \| h \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h \setminus \Omega^i)} + M_2 \| \nabla^3 \tilde{u}^a \|_{L^2(\Omega^i \setminus \Omega^c)} + M_3 \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega^i \setminus \Omega^c)}} \| \nabla v_h \|_{L^2}.$$  

(7.11)

Proof. We split the interpolation error into

$$\langle \delta E^{ac}_h (\Pi_h u^a), v_h \rangle - \langle \delta E^{ac}_h (\tilde{u}^a), v \rangle = \langle \delta E^{ac}_h (\Pi_h u^a) - \delta E^{ac}_h (\tilde{u}^a), v_h \rangle - \langle \delta E^{ac}_h (\tilde{u}^a), v - v_h \rangle.$$  

The first term can be bounded by a standard interpolation error estimate and the uniform boundedness of $\delta^2 E^{ac}_h$,

$$\langle \delta E^{ac}_h (\Pi_h u^a) - \delta E^{ac}_h (\tilde{u}^a), v_h \rangle \leq \langle \delta^2 E^{ac}_h (\theta)(\nabla \Pi_h u^a - \nabla \tilde{u}^a), v_h \rangle$$

$$\leq cM_2 \| h \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^c)} \| \nabla v_h \|_{L^2(\Omega_h^c)}.$$

The bound for the second term follows from the exactly same argument as in the proof of [3, Theorem 3.2]. Since the interpolant $v$ defined in (7.2) has property

$$v(x) - v_h(x) = 0, \quad \forall x \in \Gamma_h \cup \Omega^c \cup \Omega^i$$

we can integrate by part in $\Omega_h^c$ without obtaining boundary contributions. Let $Q := -\text{div} [\partial_k W(\nabla \tilde{u}^a)]$, then

$$\langle \delta E^{ac}_h (\tilde{u}^a), v - v_h \rangle = \int_{\Omega_h^c} Q \cdot (v_h - v) \, dx = \int_{\Omega_h^c} Q \cdot ((v_h - v_1) - v_2) \, dx.$$  

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Since $v_2$ is a piecewise-linear quasi-interpolant of $v_h - v_1$ as defined in [3], a direct consequence of Theorem 3.1 in [3] is that there exists $C > 0$ such that,

$$\langle \delta E_h^{ac}(\Pi_h u^a) - \delta E_h^{ac}(\tilde{u}^a), v_h \rangle \leq C \| \nabla (v_h - v_1) \|_{L^2(\Omega_h^c)} \left( \sum_{\ell \in C \cap \Omega_h^c} d_{\ell}^2 \int_{w_{\ell}} \phi_{\ell}^{PU} |Q - \langle Q \rangle_{\ell}|^2 \, dx \right)^{1/2},$$

where $w_{\ell} := \text{supp}(\phi_{\ell})$, $\langle Q \rangle_{\ell} := 1/|w_{\ell}| \int_{w_{\ell}} Q(x) \, dx$ and $d_{\ell} := \text{diam}(w_{\ell}) = 1$. With the sharp Poincaré constant derived in [1], we obtain

$$\int_{w_{\ell}} \phi_{\ell}^{PU} |Q - \langle Q \rangle_{\ell}|^2 \, dx \leq \int_{w_{\ell}} |Q - \langle Q \rangle_{\ell}|^2 \, dx \leq \frac{1}{4} d_{\ell}^2 \| \nabla Q \|_{L^2(w_{\ell})}^2.$$ 

On the other hand, $v_1$ is a standard quasi-interpolant of $v_h$ in $\bigcup \mathcal{T}_h^{c}$, which implies that there exists $C' > 0$ such that

$$\| \nabla (v_h - v_1) \|_{L^2(\Omega_h^c)} \leq C' \| \nabla v_h \|_{L^2(\Omega_h^c)}.$$ 

Due to the fact that $d_{\ell} = 1$ and that each point in $\mathbb{R}^2 \setminus \Omega^a$ is covered by at most three $w_{\ell}$, we have

$$\langle \delta E_h^{ac}(\Pi_h u^a) - \delta E_h^{ac}(\tilde{u}^a), v_h \rangle \leq C \max_{\ell} d_{\ell}^2 \| \nabla Q \|_{L^2(\Omega_h^c)} \| \nabla v_h \|_{L^2(\Omega_h^c)}$$

$$\leq C \left( M_2 \| \nabla^3 \tilde{u}^a \|_{L^2(\Omega_h^c)} + M_3 \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^c)} \right) \| \nabla v_h \|_{L^2(\Omega_h^c)},$$

where we used the following estimate, for some $c > 0$,

$$\| \nabla Q \|_{L^2(\Omega_h^c)} = \| \nabla \text{div} [\partial_\ell W(\nabla \tilde{u}^a)] \|_{L^2(\Omega_h^c)}$$

$$= \| \nabla \left( \partial_\ell^2 W(\nabla \tilde{u}^a) \nabla^2 \tilde{u}^a \right) \|_{L^2(\Omega_h^c)}$$

$$= \| \partial_\ell^2 W(\nabla \tilde{u}^a) \nabla^3 \tilde{u}^a + \partial_\ell^2 W(\nabla \tilde{u}^a) (\nabla^2 \tilde{u}^a)^2 \|_{L^2(\Omega_h^c)}$$

$$\leq c \left( M_2 \| \nabla^3 \tilde{u}^a \|_{L^2(\Omega_h^c)} + M_3 \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^c)} \right),$$

employing the global bounds (6.4) and (6.5). \hfill \Box

### 7.4. The modelling error

In this section we rely on the following theorem from [17] of the pure modelling error estimate of G23 coupling method.

**Theorem 7.4 (G23 modeling error).** For any $v \in \mathcal{U}_{1,2}$ we have the G23 consistency error

$$\langle \delta \mathcal{E}^{ac}(u^a), v \rangle - \langle \delta \mathcal{E}^a(u^a), v \rangle \leq c \left( M_2 \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega)} + M_3 \| \nabla^3 \tilde{u}^a \|_{L^2(\Omega^c)} \right) \| \nabla v \|_{L^2(\mathbb{R}^2)}$$ \hspace{1cm} (7.12)

Furthermore, the second term of the modelling error can be estimated as follows.

**Lemma 7.5.** For any $v \in \mathcal{U}_{1,2}$ we have

$$\int_{\Omega_h^c} (\partial W(\nabla \tilde{u}) - \mu \nabla \tilde{u}) \cdot \nabla v \lesssim \| \nabla \tilde{u}^a \|_{L^2(\Omega_h^c)}^2 \| \nabla v \|_{L^2(\Omega_h^c)}.$$
Proof. This is a direct result from applying Taylor expansion,
\[
\int_{\Omega_h^2} (\partial W(\nabla \tilde{u}) - \mu \nabla \tilde{u}) \cdot \nabla v = \int_{\Omega_h^2} \left[ \partial W(0) + \partial^2 W(0) \nabla \tilde{u}^a + \frac{1}{2} \partial^3 W(0)(\nabla \tilde{u}^a)^2 \right] \nabla v \\
- \int_{\Omega_h^2} \mu \nabla \tilde{u}^a \nabla v \\
\leq \frac{M_3}{2} \int_{\Omega_h^2} (\nabla \tilde{u}^a)^2 \nabla v \\
\lesssim \|\nabla \tilde{u}^a\|^2_{L^2(\Omega_h^2)} \|\nabla v\|_{L^2(\Omega_h^2)},
\]
where we use the fact that \(\partial W(0) = 0\) and that \(\partial^2 W(0) = \mu I\). \(\square\)

Therefore the modelling error can be estimated by
\[
\langle \delta \mathcal{E}^{ac}(\tilde{u}^a) - \delta \mathcal{E}^a(\tilde{u}^a), v \rangle - \int_{\Omega_h^2} (\partial W(\nabla \tilde{u}^a) - \mu \nabla \tilde{u}^a) \cdot \nabla v \\
\lesssim \left( \|\nabla^2 \tilde{u}^a\|_{L^2(\Omega)} + \|\nabla^3 \tilde{u}^a\|_{L^2(\Omega)} + \|\nabla^2 \tilde{u}^a\|_{L^2(\Omega)} \right) \|\nabla v\|_{L^2(\Omega)} \\
\lesssim \left( \|\nabla^2 \tilde{u}^a\|_{L^2(\Omega)} + \|\nabla^3 \tilde{u}^a\|_{L^2(\Omega)} + \|\nabla^2 \tilde{u}^a\|_{L^2(\Omega)} \right) \|v_h\|_E,
\]
where we used the face that \(\|\nabla v\|_{L^2(\Omega)} \lesssim \|v_h\|_E\) from (7.4).

7.5. The BEM error. To complete the analysis of our numerical scheme it remains to estimate the BEM error contribution to the consistency error (7.10). Recall that we need to estimate
\[
\langle g_h^{-1} \Pi_h u^a, v_h \rangle - \int_{\Omega_h^2} \nabla \tilde{u}^a \cdot \nabla v,
\]
where \(v\) is the interpolant defined in Section 7.1.1. Recall that \(v_h^E\) solves the exterior Laplace problem (7.1). Then we have
\[
\int_{\Omega_h^2} \nabla \tilde{u}^a \cdot \nabla v_h^E = \langle g^{-1} \tilde{u}_h^a, v_h \rangle v_h.
\]
Then the BEM error can be decomposed into
\[
\langle g_h^{-1} \Pi_h u^a, v_h \rangle - \int_{\Omega_h^2} \nabla \tilde{u}^a \cdot \nabla v = \langle g_h^{-1} \Pi_h u^a, v_h \rangle - \langle g^{-1} \tilde{u}_h^a, v_h \rangle + \int_{\Omega_h^2} \nabla \tilde{u}^a \cdot (\nabla v_h^E - \nabla v) \\
= \langle g_h^{-1} (\Pi_h u^a - \tilde{u}_h^a), v_h \rangle + \langle (g_h^{-1} - g^{-1})w, v_h \rangle \\
+ \langle g^{-1} (w - \tilde{u}_h^a), v_h \rangle + \langle g_h^{-1} (\tilde{u}_h^a - w), v_h \rangle \\
+ \int_{\Omega_h^2} \nabla \tilde{u}^a \cdot (\nabla v_h^E - \nabla v) \\
=: A_1 + A_2 + A_3 + A_4 + A_5,
\]
where we use the fact that \(v_h = v_h^E\) on \(\Gamma_h\).

We will employ stability of \(g_h^{-1}\) and \(g^{-1}\), as stated in Theorems 3.3 and 3.4. In addition, the estimate of \(A_1\) relies on best approximation error bounds; \(A_2\) is the standard BEM approximation error; \(A_3\) and \(A_4\) require the results on the auxiliary function \(w\) that we established in § 7.1.2 while estimating \(A_5\) is analogous of the proof of Lemma 7.3.
7.5.1. Estimate of $A_1$. In this section we first discuss the best approximation error $\| \nabla \Pi_h u^a - \nabla \tilde{u}^a \|_{L^2(\Gamma_h)}$. We will exploit the theorems below, which are well established in the literature.

**Theorem 7.6 (Interpolation).** Recall that the rescaled norms $H_{\Gamma_h}^{1/2}$ and $H_{\Gamma_h}^1$ are defined in (3.5) and (3.6), respectively. Let $u \in H_{\Gamma_h}^1$ then we have

$$\| u \|_{H_{\Gamma_h}^{1/2}} \leq \| u \|_{H_{\Gamma_h}^1}^{1/2} \| u \|_{H_{\Gamma_h}^{1/2}}^{1/2}.$$  

*Proof.* Let $u_1(x) := u(Rx)$ and $\Gamma_1$ be the image of mapping $\Gamma_h \ni x \mapsto \frac{x}{R}$. Then, by definitions (3.5) and (3.6), we have

$$\| u \|_{H_{\Gamma_h}^{1/2}} = \| u_1 \|_{H_{\Gamma_1}^{1/2}},$$

$$\| u \|_{H_{\Gamma_h}^1} = \| u_1 \|_{H_{\Gamma_1}},$$

and

$$\| u \|_{H_{\Gamma_h}^{1/2}} = \| u_1 \|_{H_{\Gamma_1}}.$$  

The standard interpolation theorem (see, for example, Theorem 2.18 in [21]) states that

$$\| u_1 \|_{H_{\Gamma_1}^{1/2}} \leq \| u_1 \|_{H_{\Gamma_1}}^{1/2} \| u_1 \|_{H_{\Gamma_1}}^{1/2}.$$  

Hence the result follows. □

**Theorem 7.7.** Recall that $\Pi_h$ was defined in Section 6.1 as the piecewise linear nodal interpolation operator, then we have, for $v \in H^2(\Gamma_h)$,

$$\| v - \Pi_h v \|_{L^2(\Gamma_h)} \leq c \| h^2 \nabla^2 v \|_{L^2(\Gamma_h)},$$

and

$$\| v - \Pi_h v \|_{H^1(\Gamma_h)} \leq c \| h \nabla v \|_{L^2(\Gamma_h)}.$$  

*Proof.* This is a direct result of Bramble-Hilbert Lemma. It is worth noting that in fact we only need the tangential part of $\nabla^2 v$ for this estimate. □

Thus, using also $\left[ \frac{1}{2} \text{diam}(\Gamma_h) \right] \approx N$, we can conclude that

$$\| \Pi_h u^a - \tilde{u}_h^a \|_{H_{\Gamma_h}^{1/2}} \leq \| \Pi_h u^a - \tilde{u}_h^a \|_{H_{\Gamma_h}^{1/2}}^{1/2} \| \Pi_h u^a - \tilde{u}_h^a \|_{H_{\Gamma_h}^{1/2}}^{1/2}$$

$$\lesssim \left( N \| h \nabla^2 \tilde{u}_h^a \|_{L^2(\Gamma_h)}^2 + N^{-1} \| h^2 \nabla^2 \tilde{u}_h^a \|_{L^2(\Gamma_h)}^2 \right)^{1/4}$$

$$\approx \left( N^{-1} \| h^2 \nabla^2 \tilde{u}_h^a \|_{L^2(\Gamma_h)}^2 \right)^{1/4}$$  

$$\lesssim \| h \nabla^2 \tilde{u}_h^a \|_{L^2(\Gamma_h)} \| h \nabla^2 \tilde{u}_h^a \|_{L^2(\Gamma_h)}$$

where, in the last line, we used the fact that $N^{-2}h \lesssim 1$ and that $h$ is quasi-uniform on $\Gamma_h$.

By the stability estimate (3.8), we have

$$\| g_h^{-1}(\Pi_h u - \tilde{u}_h^a) \|_{H^{-1/2}(\Gamma_h)} \leq c \| \Pi_h u - \tilde{u}_h^a \|_{H_{\Gamma_h}^{1/2}}.$$  

Therefore we can estimate $A_1$ as follows

$$A_1 \leq C \| \Pi_h u^a - \tilde{u}_h^a \|_{H_{\Gamma_h}^{1/2}} \| v_h \|_{H_{\Gamma_h}^{1/2}} \lesssim \| h^{3/2} \nabla \tilde{u}_h^a \|_{L^2(\Gamma_h)} \| v_h \|_{H_{\Gamma_h}^{1/2}}.$$  

(7.15)
7.5.2. Estimate of $A_2$. Since $w$ is the solution to the Laplace equation (7.5) with smooth boundary $\partial B_R$, its conormal derivative $g^{-1}w$ on $\Gamma_h$ is in $H^1(\Gamma_h)$. Hence we can apply Theorem 3.9 and then Lemma 3.8 to estimate
\[
A_2 \leq \|(g_h^{-1} - g^{-1})w\|_{H^{-1/2}(\Gamma_h)} \|v_h\|_{H^{1/2}_{r_h}}
\]
\[
\leq c h^{3/2} \|\nabla (g^{-1}w)\|_{L^2(\Gamma_h)} \|v_h\|_{H^{1/2}_{r_h}}
\]
\[
\lesssim h^{3/2} \|\nabla^2 w\|_{L^2(\Gamma_h)} \|v_h\|_{H^{1/2}_{r_h}}
\]
\[
\lesssim h^{3/2} N^{-5/2} \|v_h\|_{H^{1/2}_{r_h}},
\] (7.16)
where the last line results from (7.7) and the Trace Theorem.

7.5.3. Estimates of $A_3$ and $A_4$. By the stability of $g^{-1}$, we have
\[
A_3 \leq C_2 \|\hat{u}_h^a - w\|_{H^{1/2}_{r_h}} \|v_h\|_{H^{1/2}_{r_h}}.
\]
Since $g^{-1}$ is positive-definite and bounded by Lemma 3.8, we can link $\|\cdot\|_{H^{1/2}_{r_h}}$ to $\|\nabla \cdot\|_{L^2(\Omega_h^c)}$ through exterior Laplace problems.

Recall that $\hat{u}_h^a := \hat{u}_h^a - c_h \in H^{1/2}_{r_h}(\Gamma_h)$. Then by Theorem 3.6 the following exterior Laplace problem has a unique solution
\[
-\Delta y = 0, \quad \text{in } \Omega_h^c,
\]
\[
y = \hat{u}_h^a, \quad \text{on } \Gamma_h,
\]
\[
|y(x)| = O \left(\frac{1}{|x|}\right) \quad \text{as } |x| \to \infty.
\] (7.17)
Then arguing exactly as in the proof of Lemma 7.1, we have
\[
\|\nabla y - \nabla \hat{u}_h^a\|_{L^2(\Omega_h^c)} \lesssim N^{-3}.
\]
In addition, by the positive-definiteness of $g^{-1}$ in Lemma 3.8 we have
\[
C_1 \|\hat{u}_h^a - w\|_{H^{1/2}_{r_h}}^2 \leq \langle g^{-1}(\hat{u}_h^a - w), (\hat{u}_h^a - w) \rangle = \int_{\Omega_h^c} |\nabla y - \nabla w|^2.
\]
Therefore we have
\[
A_3 \lesssim \|\hat{u}_h^a - w\|_{H^{1/2}_{r_h}} \|v_h\|_{H^{1/2}_{r_h}}
\]
\[
\lesssim \left(\|\nabla y - \nabla \hat{u}_h^a\|_{L^2(\Omega_h^c)} + \|\nabla w - \nabla \hat{u}_h^a\|_{L^2(\Omega_h^c)}\right) \|v_h\|_{H^{1/2}_{r_h}}
\]
\[
\lesssim (N^{-3} + R^{-3}) \|v_h\|_{H^{1/2}_{r_h}}
\]
\[
\lesssim N^{-3} \|v_h\|_{H^{1/2}_{r_h}}.
\] (7.18)

For $A_4$, using the stability of $g_h^{-1}$ in (3.8) and the same argument as for $A_4$, we have
\[
A_4 \lesssim N^{-3} \|v_h\|_{H^{1/2}_{r_h}}.
\] (7.19)
7.5.4. Estimate of $A_5$. Now we consider

$$A_5 = \int_{\Omega_h^E} \nabla \tilde{u}^a \cdot (\nabla v^E_h - \nabla v).$$

Recall that $v$ is the quasi-interpolant of $v^E_h$ defined in (7.21). Under the assumption (A3) we know that

$$v^E_h(x) - v(x) = 0 \quad \forall x \in \Gamma_h.$$ 

So we can use analogous argument to the proof of Lemma 7.3 to get

$$A_5 \lesssim \| \nabla \text{div}(\nabla \tilde{u}^a) \|_{L^2(\Omega_h^E)} \| \nabla v^E_h \|_{L^2(\Omega_h^E)}$$

By (7.3) we have

$$\| \nabla v^E_h \|_{L^2(\Omega_h^E)} \lesssim \| v_h \|_{H^{1/2}_h}.$$ 

Therefore we have

$$A_5 \lesssim \| \nabla \tilde{u}^a \|_{L^2(\Omega_h^E)} \| v_h \|_{H^{1/2}_h} \lesssim N^{-3} \| v_h \|_{H^{1/2}_h}. \quad (7.20)$$

Summarising all five components of the BEM error estimates (7.15), (7.16), (7.18), (7.19) and (7.20) we obtain

$$\text{BEM error} \lesssim \left( N^{-3} + \| h^{3/2} \nabla^2 \tilde{u}^a \|_{L^2(\Gamma_h)} \right) \| v_h \|_{H^{1/2}_h}. \quad (7.21)$$

7.6. Proof of Theorem 4.4. Finally, recalling the decomposition in (7.10), we add the estimates for all three components (7.11), (7.13) and (7.21) together to get the following estimate. We have, for any $v_h \in U_h^*$

$$\langle \delta E_{h,\text{tot}}^\text{int}(\Pi_h u^a), v_h \rangle$$

$$\lesssim \left( \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega)} + \| \nabla \tilde{u}^a \|_{L^2(\Omega_h^E)} + \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^E)} \right) \| v_h \|_E$$

$$+ \| h^{3/2} \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^E)} \| v_h \|_{H^{1/2}_h}$$

$$+ \| h^{3/2} \nabla^2 \tilde{u}^a \|_{L^2(\Gamma_h)} \| v_h \|_{H^{1/2}_h}.$$ 

Therefore the result follows.

7.7. Proof of Theorem 4.5. We shall use the Inverse Function Theorem 6.1. To put into the context of Theorem 6.1 let

$$\mathcal{G}_h(v) := \delta E_{h,\text{tot}}^\text{int}(v) - \delta f(v) \quad \text{and} \quad \bar{u}_h := \Pi_h u^a.$$ 

Then Theorem 4.4 gives property (6.2) and Theorem 4.3 gives property (6.3). Then we can conclude that, for $K, N$ sufficiently large, there exists $u_h \in U_h^*$ such that

$$\mathcal{G}_h(u_h) = 0, \quad \text{and}$$

$$\| u_h - \Pi_h u^a \|_E \lesssim \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega)} + \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^E)} + \| \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^E)}$$

$$+ \| h^{3/2} \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^E)} + \| h^{3/2} \nabla^2 \tilde{u}^a \|_{L^2(\Gamma_h)} + N^{-3}.$$ 

Finally we add the best approximation error

$$\| \Pi_h u^a - u_h \|_{E}^2 = \| \nabla \Pi_h u^a - \nabla u_h \|_{L^2(\Omega_h)}^2 + \| \Pi_h u^a - u_h \|_{H^{1/2}_h}^2$$

$$\lesssim \| h^{3/2} \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h^E)}^2 + \| h^{3/2} \nabla^2 \tilde{u}^a \|_{L^2(\Gamma_h)}^2,$$
where the last term comes from (7.14). Thus the result follows.

**Appendix A. Proof of Theorem 3.4**

The proof follows exactly as Theorem 2 in [4] but with details specific for 2D, showing how the subspace $H^{-1/2}_s(\Gamma_h)$ ensures that the far-field value $u_0 = 0$.

To construct the proofs for Theorem 3.4 we need several intermediate results from literature.

**Lemma A.1.** Suppose $v \in H^{-1/2}(\Gamma_h)$, $y_0 \in \Omega_h$ and $u(x) = (Av)(x)$ for $x \in \mathbb{R}^2 \setminus \Gamma_h$, then we have

$$|u(x)| \leq c_1 \frac{1}{|x - y_0|} \quad \text{and} \quad |
abla u(x)| \leq c_2 \frac{1}{|x - y_0|^2/2}, \quad \text{for } |x - y_0| > \max\{1, 2\text{diam}(\Omega_h)\}.$$

**Proof.** See Lemma 6.21 in [21].

**Lemma A.2.** For $w \in H^{-1/2}(\Gamma_h)$ and $u = Av$, we have the following jump relation:

$$\gamma^\text{int}_1 u - \gamma^\text{ext}_1 u = w. \quad (A.1)$$

**Proof.** See Lemma 4 in [4].

**Lemma A.3.** The interior and exterior conormal derivatives $\gamma^\text{int}_1 : H^1(\Omega_h) \rightarrow H^{-1/2}(\Gamma_h)$ and $\gamma^\text{ext}_1 : H^1(\Omega_h^\text{c}) \rightarrow H^{-1/2}(\Gamma_h)$ are continuous in the sense that

$$\|\gamma^\text{int}_1 u\|_{H^{-1/2}(\Gamma_h)} \leq c^\text{int}\|\nabla u\|_{L^2(\Omega_h)} \quad (A.2)$$

$$\|\gamma^\text{ext}_1 u\|_{H^{-1/2}(\Gamma_h)} \leq c^\text{ext}\|\nabla u\|_{L^2(\Omega_h^\text{c})}. \quad (A.3)$$

**Proof.** See Lemma 3.2 in [4].

**Proof of Theorem 3.4.** It is clear that if $v \in H^{1/2}_s(\Gamma)$, $u = Av(x)$ is a solution to the interior Dirichlet boundary value problem

$$-\Delta u = 0, \quad \text{in } \Omega_h,$$

$$u = \gamma^\text{int}_0(Av)(x) = (Vv)(x), \quad \text{on } \Gamma_h.$$  

By choosing $w \in H^1(\Omega_h)$ we integrate by part to get

$$a_{\Omega_h}(u, w) := \int_{\Omega_h} \nabla u(x) \nabla w(x) \, dx = \langle \gamma^\text{int}_1 u, \gamma^\text{int}_0 w \rangle_{\Gamma_h}. \quad (A.4)$$

On the other hand, for $y_0 \in \Omega_h$ and $R > 2\text{diam}(\Omega_h)$, let $B_R(y_0)$ be a ball centred at $y_0$ with radius $R$. Then $u = Av(x)$ is also the unique solution to the exterior Dirichlet boundary value problem

$$-\Delta u = 0, \quad \text{in } B_R(y_0) \setminus \widehat{\Omega}_h,$$

$$u = \gamma^\text{ext}_0(Av)(x) = (Vv)(x), \quad \text{on } \Gamma_h,$$

$$u = (Av)(x), \quad \text{on } \partial B_R(y_0).$$
We also integrate by part and get
\[ a_{B_R(y_0)}(u, w) := \int_{B_R(y_0)} \nabla u(x) \nabla w(x) \, dx = -\langle \gamma^\text{ext}_1 u, \gamma^\text{ext}_0 w \rangle_{\Gamma_h} + \langle \gamma^\text{int}_1 u, \gamma^\text{int}_0 w \rangle_{\partial B_R(y_0)}. \]

Since \( u = Av(x) \) with \( v \in H^{1/2}_s(\Gamma) \), by Lemma A.1 we have
\[
|\langle \gamma^\text{int}_1 u, \gamma^\text{int}_0 u \rangle_{\partial B_R(y_0)}| \leq C \int_{|x-y_0|=R} \frac{1}{|x-y_0|^3} \, dS(x) \leq CR^{-2} \to 0, \text{ as } R \to \infty.
\]

Thus we have
\[ a_{\Omega h}(u, w) = -\langle \gamma^\text{ext}_1 u, \gamma^\text{ext}_0 w \rangle_{\Gamma_h}. \quad (A.5) \]

Consequently we have by Lemma A.2
\[ a_{\Omega}(u, u) + a_{\Omega h}(u, u) = \langle \gamma^\text{int}_1 u - \gamma^\text{ext}_1 u, \gamma^\text{int}_0 u \rangle_{\Gamma_h} = \langle v, \gamma^\text{int}_0 u \rangle_{\Gamma_h} = \langle Vv, v \rangle_{\Gamma_h}. \quad (A.6) \]

Applying (A.2) and (A.3) gives the ellipticity of \( V \). Analogous argument follows for the ellipticity of \( D \).

\[ \square \]

**Appendix B. Proof of Lemma 3.8**

*Proof.* First we show that \( u_R \in H^{1/2}_s(\Gamma_R) \). Since \( u_1 \in H^{1/2}_s(\Gamma_1) \), there exists \( \phi_1 \in H^{1/2}_s(\Gamma_1) \) such that \( V_1 \phi_1 = u_1 \). Let \( \phi_R(x) := \frac{1}{R} \phi_1(x/R) \), then it is clear that \( \phi_R \in H^{-1/2}_s(\Gamma_R) \). Then we can write
\[
\begin{align*}
u_R(x) = u_1(x/R) &= -\frac{1}{2\pi} \int_{\Gamma_1} \log \left| \frac{x}{R} - y \right| \phi_1(y) \, dS(y) \\
&= -\frac{1}{2\pi} \int_{\Gamma_R} \log \left| \frac{x}{R} - y \right| \phi_1 \left( \frac{y}{R} \right) \frac{1}{R} \, dS(y) \\
&= -\frac{1}{2\pi} \int_{\Gamma_R} \log \left| \frac{x}{R} - y \right| \phi_R(y) \, dS(y) \\
&= -\frac{1}{2\pi} \int_{\Gamma_R} (\log |x-y| - \log R) \phi_R(y) \, dS(y) \\
&= -\frac{1}{2\pi} \int_{\Gamma_R} \log |x-y| \phi_R(y) \, dS(y) = V_R \phi_R \in H^{1/2}_s(\Gamma_R),
\end{align*}
\]

where we used the fact that \( \langle \phi_R, 1 \rangle_{\Gamma_R} = 0 \). By a similar argument of change of variables, we have
\[
[(-K_1 + (1-\lambda)I)u_1 = [-K_R + (1-\lambda)I]u_R.
\]

Now we shall prove that \( V^{-1} \) is also scale in-variant. Let \( \tilde{u}_1 \) be the solution to the homogeneous Laplace equation
\[
-\Delta \tilde{u}_1 = 0, \quad \text{in } \mathbb{R}^2 \setminus \Gamma_1, \\
\tilde{u}_1 = u_1, \quad \text{on } \Gamma_1,
\]

\[
|\tilde{u}_1(x)| = O\left( \frac{1}{|x|} \right) \quad \text{as } |x| \to \infty.
\]
Then $\bar{u}_R := \bar{u}_1(x/R)$ also solves
\[-\Delta \bar{u}_R = 0, \quad \text{in } \mathbb{R}^2 \setminus \Gamma_R,
\]
\[\bar{u}_R = u_R, \quad \text{on } \Gamma_R,
\]
\[|\bar{u}_R(x)| = \mathcal{O}\left(\frac{1}{|x|}\right), \quad \text{as } |x| \to \infty.
\]
For $i = 1, R$, define $v_i$ and $\bar{v}_i$ in the same way as $u_i$ and $\bar{u}_i$. Then we can apply (A.4), (A.5) and the jump relation in Lemma A.2 to get
\[
\int_{\Omega_i} \nabla \bar{u}_i \nabla \bar{v}_i + \int_{\mathbb{R}^2 \setminus \Omega_i} \nabla \bar{u}_i \nabla \bar{v}_i =: a_{\Omega_i}(\bar{u}_i, \bar{v}_i) + a_{\mathbb{R}^2 \setminus \Omega_i}(\bar{u}_i, \bar{v}_i)
\]
\[= \langle \gamma^\text{int}_1 \bar{u}_i - \gamma^\text{ext}_1 \bar{u}_i, \gamma^\text{int}_0 \bar{v}_i \rangle_{\Gamma_i}
\]
\[= \langle \phi_i, v_i \rangle_{\Gamma_i}
\]
\[= \langle V_i^{-1} u_i, v_i \rangle_{\Gamma_i}, \quad \text{for } i = 1, R,
\]
where $\phi_i = V_i^{-1} u_i$. Clearly
\[a_{\Omega_i}(\bar{u}_1, \bar{v}_1) + a_{\mathbb{R}^2 \setminus \Omega_i}(\bar{u}_1, \bar{v}_1) = a_{\Omega_R}(\bar{u}_R, \bar{v}_R) + a_{\mathbb{R}^2 \setminus \Omega_R}(\bar{u}_R, \bar{v}_R).
\]
Thus $\langle V_i^{-1} u_i, v_i \rangle_{\Gamma_i} = \langle V_R^{-1} u_R, v_R \rangle_{\Gamma_R}$ and hence the result follows. \qed

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