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ON THE DERIVATION OF GUARANTEED AND p -ROBUST A POSTERIORI ERROR ESTIMATES FOR THE HELMHOLTZ EQUATION*

T. CHAUMONT-FRELET^{1,2}, A. ERN^{3,4}, AND M. VOHRALÍK^{4,3}

ABSTRACT. We propose a novel *a posteriori* error estimator for conforming finite element discretizations of two- and three-dimensional Helmholtz problems. The estimator is based on an equilibrated flux that is computed through the solve of patchwise mixed finite element problems. We show that the estimator is reliable up to a prefactor that tends to one with mesh refinement or with polynomial degree increase. We also derive a fully computable upper bound on this prefactor for several common settings of domains and boundary conditions, leading to a guaranteed estimate in all wavenumber regimes without any assumption on the mesh size or the polynomial degree. We finally demonstrate that the estimator is locally efficient as soon as the mesh exhibits sufficiently many degrees of freedom per wavelength. In such a regime, the estimator is also robust with respect to the polynomial degree. We present numerical experiments that illustrate our analysis and indicate that our theoretical results are sharp.

KEY WORDS. A posteriori error estimates; Finite element methods; Helmholtz problems; High order methods.

1. INTRODUCTION

In this work, we are concerned with the following Helmholtz equation: find $u : \Omega \rightarrow \mathbb{C}$ such that

$$(1.1) \quad \begin{cases} -k^2 u - \Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \nabla u \cdot \mathbf{n} - iku = g & \text{on } \Gamma_A. \end{cases}$$

Here $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3 , is a Lipschitz domain with polygonal or polyhedral boundary $\partial\Omega$ that is partitioned into two disjoint relatively open sets Γ_D and Γ_A , \mathbf{n} denotes the unit vector normal to $\partial\Omega$ pointing outward Ω , $f : \Omega \rightarrow \mathbb{C}$ and $g : \Gamma_A \rightarrow \mathbb{C}$ are prescribed data, and $k \in \mathbb{R}_+^*$ is the wavenumber.

Problem (1.1) can accurately model the propagation of time-harmonic acoustic or polarized electromagnetic waves. It is also insightful for more elaborate wave propagation

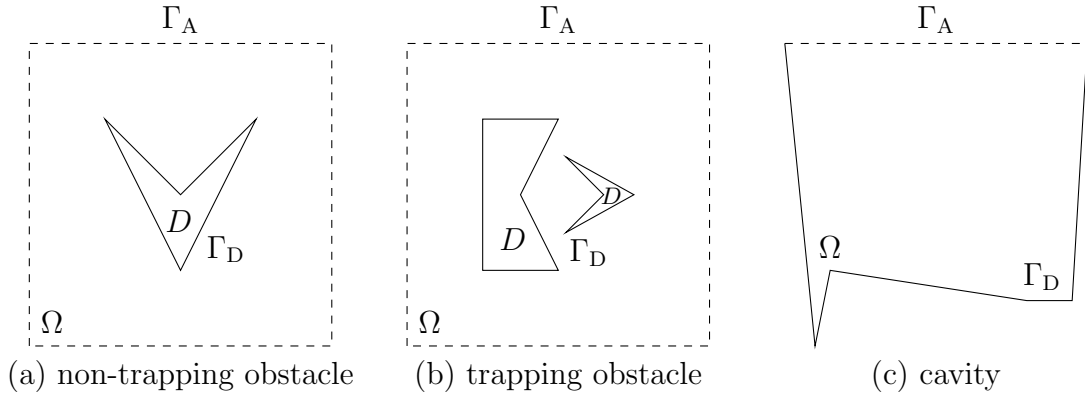
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FIGURE 1. Examples of domains Ω and boundaries Γ_D and Γ_A

models employed, for instance, in elasticity and electromagnetics, with industrial applications in acoustics, radar, and medical or subsurface imaging, see, e.g. [16, 19, 23, 40, 53] and the references therein.

The above setting can represent the *scattering problem* by a sound-soft obstacle D , see Figure 1, (a) and (b). Then $\Gamma_D = \partial D$ represents the boundary of the obstacle, $\Gamma_A = \partial\Omega_0$ where Ω_0 is some “computational box” that includes and surrounds D , and $\Omega = \Omega_0 \setminus D$. An important scenario is the case of a *non-trapping obstacle* D in which both D and Ω_0 are star-shaped with respect to a common center, see Figure 1, (a). In *cavity* problems, see Figure 1, (c), Γ_D represents the basis of a cavity and Γ_A is typically planar. The obstacle-free case with $\Gamma_D = \emptyset$ represents the propagation of a wave in *free space*. Finally, the so-called *interior problem* where $\Gamma_A = \emptyset$ is well-posed provided that k^2 is not an eigenvalue of the Laplace operator in Ω .

Numerical discretizations, often based on the finite element method, are nowadays vastly used to find approximate solutions to (1.1). Here, a finite-dimensional space V_h is constructed which typically consists of piecewise polynomials of degree $p \geq 1$ defined over a computational mesh \mathcal{T}_h of Ω with a maximal cell size h . In this case, $(\frac{kh}{2\pi p})^{-1}$ is a measure of the number of degrees of freedom per wavelength. Another important quantity, following [28, 43], is the best approximation constant¹

$$(1.2) \quad \sigma_{\text{ba}} := k \sup_{\phi \in L^2(\Omega) \setminus \{0\}} \inf_{v_h \in V_h} \frac{|u_\phi^* - v_h|_{1,\Omega}}{\|\phi\|_{0,\Omega}},$$

where $\overline{u_\phi^*}$ is the (adjoint) solution to (1.1) with data $f = \overline{\phi}$ and $g = 0$; here $\bar{\cdot}$ denotes the complex conjugate. The real number σ_{ba} describes the ability of the discrete space V_h to approximate (adjoint) solutions to (1.1). For the case of scattering by a smooth

¹Our definition is slightly different from [43] as we include the factor k in σ_{ba} . This way, the quantity σ_{ba} is adimensional, and invariant under rescaling.

non-trapping obstacle, we have in particular

$$(1.3) \quad \sigma_{\text{ba}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}})C(\kappa) \left(\frac{kh}{p} + kh_{\Omega} \left(\frac{kh}{p} \right)^p \right),$$

where the constants $C(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}})$ and $C(\kappa)$, respectively, only depend on the shape of the computational domain Ω (but not on its diameter h_{Ω}) and on the mesh shape-regularity parameter κ , see [43, Proposition 5.3]. We speak of *unresolved regime* when $\frac{kh}{2\pi p} > 1$, and of *resolved regime* when $\frac{kh}{2\pi p} \leq 1$. We also speak of *asymptotic regime* when $\sigma_{\text{ba}} \leq 1$ and *preasymptotic regime* otherwise. We point out that the condition $\sigma_{\text{ba}} \leq 1$ typically translates into stronger requirements on h and p than the resolved regime.

The sesquilinear form $b(\cdot, \cdot)$ associated with the boundary value problem (1.1) is typically not coercive, as it contains a negative $L^2(\Omega)$ contribution, and thus does not lead to an energy norm. The finite element solution (when it exists), is almost meaningless in the unresolved regime, where even the best approximation of the solution u of (1.1) in the discrete space V_h is inaccurate. In the resolved regime, this best approximation already starts to accurately represent u , but the finite element solution $u_h \in V_h$ is not necessarily quasi-optimal and is typically still inaccurate. This phenomena is known in the literature as the ‘‘pollution effect’’. It is only in the asymptotic regime that the quasi-optimality of the finite element solution is ensured, cf. [43] and the references therein. The typical dependence (1.3) encourages the use of finite elements with high polynomial degree p to solve problems with high wavenumber k , and this is a usual practice, cf. [2, 6, 14, 20, 43, 53] and the references therein.

The design of suitable *a posteriori* estimators is of paramount importance both for control of the error between u and u_h and for the efficiency of algorithms adaptively refining h and/or p [24, 55]. Pioneering works on a posteriori error estimation for the Helmholtz equation are reported in [4, 5]. The authors focus on first-order discretizations ($p = 1$) of one-dimensional problems and prove that in the asymptotic regime, the residual [55] and the Zienkiewicz–Zhu [56] estimators are reliable (yielding an error upper bound) and efficient (yielding an error lower bound). Numerous refinements of these results, including goal-oriented estimation and *hp* adaptivity, can be found in [22, 35, 45, 48, 51, 52], see also the references therein.

More recently, *residual estimators* for high-order finite element as well as discontinuous Galerkin discretizations of two- and three-dimensional problems have been studied in [28, 49], where an upper bound is obtained even in the pre-asymptotic regime, taking the form (when the data f and g are piecewise polynomial)

$$(1.4a) \quad (k^2 \|u - u_h\|_{0,\Omega}^2 + |u - u_h|_{1,\Omega}^2)^{\frac{1}{2}} \leq C_{\text{up}} \eta, \quad C_{\text{up}} = C(\kappa) + \theta_0(\sigma_{\text{ba}}),$$

where η is the a posteriori error estimator which is fully computable from u_h and the data. The constant $C(\kappa)$ is not computable, but only depends on the shape-regularity κ of the mesh \mathcal{T}_h , and $\lim_{t \rightarrow 0} \theta_0(t) = 0$. One sees that in the asymptotic regime where $\sigma_{\text{ba}} \leq 1$, the prefactor C_{up} in (1.4a) simplifies into an (unknown) constant that only depends on the mesh regularity. Moreover, the authors in [28, 49] prove that as long as there are

sufficiently many degrees of freedom per wavelength (the resolved regime where $\frac{kh}{2\pi p} \leq 1$),

$$(1.4b) \quad \eta_K \leq C_{\text{low},\omega_K} (k^2 \|u - u_h\|_{0,\omega_K}^2 + |u - u_h|_{1,\omega_K}^2)^{\frac{1}{2}}, \quad C_{\text{low},\omega_K} = C(\kappa_{\mathcal{T}_K}, p) \left(1 + \frac{kh_{\omega_K}}{p}\right),$$

where the factor $(1 + \frac{kh_{\omega_K}}{p})$ naturally appears for $\Gamma_A = \emptyset$, $\eta = (\sum_{K \in \mathcal{T}_h} \eta_K^2)^{\frac{1}{2}}$, \mathcal{T}_K is the patch of elements around the mesh element K with shape-regularity $\kappa_{\mathcal{T}_K}$ and the corresponding subdomain ω_K , and the constant $C(\kappa_{\mathcal{T}_K}, p)$ deteriorates as the polynomial degree p increases.

Another approach to a posteriori error estimation is based on a construction of an *equilibrated flux*, cf. [25, 37, 46]. In this case, an unknown-constant-free upper bound is obtained for elliptic problems. Moreover, it has been recently shown [7, 29, 30] that such a strategy provides a p -robust estimator which means that the lower bound does not depend on the polynomial degree p . The recent work [20] proposes to use this type of estimators for discontinuous Galerkin discretizations of the Helmholtz problem. The authors consider a simpler configuration of (1.1) with $\Gamma_D = \emptyset$ and $d = 2$ and evaluate the error in the $H^1(\Omega)$ -seminorm $|u - u_h|_{1,\Omega}$ only. While the proposed estimator is p -robust, both reliability and efficiency only hold up to the uncomputable scaled error terms $k\|u - u_h\|_{0,\Omega}$ and $k^{\frac{1}{2}}\|u - u_h\|_{0,\Gamma_A}$. These terms asymptotically vanish, but their actual size is unknown.

In the present work, we follow some of the main arguments developed in [28] but we employ equilibrated flux estimators instead of residual estimators. We establish our results in the *energy norm*

$$(1.5) \quad \| \|u - u_h\|_{1,k,\Omega}^2 := k^2 \|u - u_h\|_{0,\Omega}^2 + k \|u - u_h\|_{0,\Gamma_A}^2 + |u - u_h|_{1,\Omega}^2,$$

and prove the global upper bound

$$(1.6a) \quad \| \|u - u_h\|_{1,k,\Omega} \| \leq C_{\text{up}} \eta, \quad C_{\text{up}} = \sqrt{2} + \theta_1(\sigma_{\text{ba}}),$$

where η is a fully computable equilibrated flux estimator and $\theta_1(t) := \sqrt{2t + 2t^2}$. The factor $\sqrt{2}$ can be further decreased to the optimal value of 1 modulo additional technical developments that we detail in Theorem 2.3 below. Thus, asymptotically, (1.6a) is *unknown-constant-free*, in improvement of (1.4a), and additionally the entire energy norm (including the scaled $L^2(\Omega)$ and $L^2(\Gamma_A)$ terms) is controlled in contrast to [20]. Though the asymptotic nature of the approximability factor σ_{ba} is known, cf. (1.3), σ_{ba} cannot be computed or estimated from (1.3), so that the bound (1.6a) is not guaranteed in general. We succeed in removing this remaining deficiency and find a fully computable upper bound on σ_{ba} in several configurations of interest, see Theorem 2.6 below. Remarkably, the bound (1.6a) then becomes *guaranteed*, and this in *any regime* (unresolved, resolved, asymptotic).

The second main property of our estimators is the local efficiency

$$(1.6b) \quad \eta_K \leq C_{\text{low},\omega_K} \| \|u - u_h\|_{1,k,\omega_K} \|, \quad C_{\text{low},\omega_K} = C(\kappa_{\mathcal{T}_K}) \left(1 + \left(\frac{kh_{\omega_K}}{p}\right)^{\frac{1}{2}} + \frac{kh_{\omega_K}}{p}\right),$$

for every mesh element K , where the term $(\frac{kh_{\omega_K}}{p})^{\frac{1}{2}}$ appears for $\Gamma_A \neq \emptyset$. Importantly, in contrast to (1.4b), the constant $C(\kappa_{\mathcal{T}_K})$ in (1.6b) is independent of the polynomial degree p (only depends on the local shape-regularity parameter $\kappa_{\mathcal{T}_K}$), and, in contrast to [20], the scaled $L^2(\Omega)$ and $L^2(\Gamma_A)$ terms are not omitted. Hence, in the resolved regime $\frac{kh}{2\pi p} \leq 1$, the present estimators are *p-robust*.

Our manuscript is organized as follows. In Section 2, we precise the functional and discrete settings and state our main results. We perform a general analysis of the relationships between the energy error (1.5) and dual norms of the residual in Section 3, and we employ these results in the context of flux equilibration in Section 4. In Section 5, we prove our fully computable upper bounds on the factor σ_{ba} . We present numerical experiments that illustrate our findings in Section 6 and draw our conclusions in Section 7. Finally, in Appendix A, we establish an intermediate result related to boundary and volume data.

2. SETTING AND MAIN RESULTS

This section details the setting and presents our main results.

2.1. Variational formulation. We recast problem (1.1) into a weak form that consists in finding $u \in H_{\Gamma_D}^1(\Omega)$ such that

$$(2.1) \quad b(u, v) = (f, v) + (g, v)_{\Gamma_A} \quad \forall v \in H_{\Gamma_D}^1(\Omega)$$

where

$$(2.2) \quad b(u, v) := -k^2(u, v) - ik(u, v)_{\Gamma_A} + (\nabla u, \nabla v)$$

and

$$H_{\Gamma_D}^1(\Omega) := \{v \in H^1(\Omega) \mid v = 0 \text{ on } \Gamma_D\}.$$

Above and hereafter, for $m \in \mathbb{N}$ and an open set \mathcal{O} , $H^m(\mathcal{O})$ denotes the Sobolev space of order m . We also employ the notations $\|\cdot\|_{m, \mathcal{O}}$ and $|\cdot|_{m, \mathcal{O}}$ for the norm and semi-norm on $H^m(\mathcal{O})$. Also, $(\cdot, \cdot)_{\mathcal{O}}$ denotes the $L^2(\mathcal{O})$ inner-product, and we drop the subscript when $\mathcal{O} = \Omega$. We refer to [1, 18, 31] for the definition and essential properties of the Sobolev spaces. In the following, we assume that (2.1) is uniquely solvable for all $f \in L^2(\Omega)$ and $g \in L^2(\Gamma_A)$ and we equip $H_{\Gamma_D}^1(\Omega)$ with the *energy norm*

$$(2.3) \quad \|v\|_{1, k, \Omega}^2 := k^2 \|v\|_{0, \Omega}^2 + k \|v\|_{0, \Gamma_A}^2 + |v|_{1, \Omega}^2 \quad \forall v \in H_{\Gamma_D}^1(\Omega).$$

Remark that this choice leads to the sharp continuity estimate

$$(2.4) \quad |b(\phi, v)| \leq \| \phi \|_{1, k, \Omega} \| v \|_{1, k, \Omega} \quad \forall \phi, v \in H^1(\Omega),$$

which is of particular interest in the context of goal-oriented error estimation [22, 45, 48].

2.2. Discrete solution. Consider a mesh \mathcal{T}_h of Ω that consists of triangular or tetrahedral elements K such that $\cup_{K \in \mathcal{T}_h} \overline{K} = \overline{\Omega}$ and such that for two distinct elements $K_{\pm} \in \mathcal{T}_h$, the intersection $\overline{K_+} \cap \overline{K_-}$ is either empty, a single vertex, a full edge, or a full face of K_+ and K_- . We further require \mathcal{T}_h to be compatible with the partition $\overline{\Gamma_D} \cup \overline{\Gamma_A}$ of $\partial\Omega$, i.e., that each boundary mesh face $\overline{F} \subset \partial\Omega$ is either included in $\overline{\Gamma_D}$ or in $\overline{\Gamma_A}$. We also define, for every $K \in \mathcal{T}_h$,

$$h_K := \sup_{\mathbf{x}, \mathbf{y} \in K} |\mathbf{x} - \mathbf{y}|, \quad \rho_K := \sup \{r > 0 \mid \exists \mathbf{x} \in K; B(\mathbf{x}, r) \subset K\}.$$

We assume that the mesh is shape-regular in the sense that every $K \in \mathcal{T}_h$ satisfies

$$\kappa_K := \frac{\rho_K}{h_K} \geq \kappa > 0$$

for a fixed constant κ . These hypotheses are standard [18] and not restrictive in particular in the sense that they do not preclude strong grading of the mesh. We will also sometimes use the notation $h := \max_{K \in \mathcal{T}_h} h_K$. If $\mathcal{T} \subset \mathcal{T}_h$ is a subset of cells K , we write $\kappa_{\mathcal{T}} := \min_{K \in \mathcal{T}} \kappa_K$.

For an integer $p \geq 1$, consider the space $\mathcal{P}_p(K)$ of polynomials on K of degree at most p , the broken space

$$\mathcal{P}_p(\mathcal{T}_h) := \{v \in L^2(\Omega) \mid v|_K \in \mathcal{P}_p(K); \forall K \in \mathcal{T}_h\},$$

and define the approximation space

$$(2.5) \quad V_h := \mathcal{P}_p(\mathcal{T}_h) \cap H_{\Gamma_D}^1(\Omega).$$

The discrete version of (2.1) seeks for $u_h \in V_h$ such that

$$(2.6) \quad b(u_h, v_h) = (f, v_h) + (g, v_h)_{\Gamma_A} \quad \forall v_h \in V_h.$$

The present analysis applies for any $u_h \in V_h$ satisfying (2.6).

2.3. Approximation properties of adjoint solutions. The approximation properties of the space V_h from (2.5) play a central role in the forthcoming analysis. Specifically, following [28, 43], we consider the real number σ_{ba} defined in (1.2), i.e.

$$(2.7) \quad \sigma_{\text{ba}} := k \sup_{\phi \in L^2(\Omega) \setminus \{0\}} \inf_{v_h \in V_h} \frac{|u_{\phi}^* - v_h|_{1,\Omega}}{\|\phi\|_{0,\Omega}},$$

where u_{ϕ}^* denotes the unique (adjoint) solution in $H_{\Gamma_D}^1(\Omega)$ such that

$$(2.8) \quad b(w, u_{\phi}^*) = (w, \phi) \quad \forall w \in H_{\Gamma_D}^1(\Omega).$$

The real number σ_{ba} is independent of the data f and g but implicitly depends on Ω , Γ_D , k , and V_h . It describes the ability of the discrete space V_h to approximate the (adjoint) solution to (2.8). Indeed, we have

$$(2.9) \quad k \inf_{v_h \in V_h} |u_{\phi}^* - v_h|_{1,\Omega} \leq \sigma_{\text{ba}} \|\phi\|_{0,\Omega} \quad \forall \phi \in L^2(\Omega).$$

The dependence of σ_{ba} on Ω , Γ_D , k , and V_h (or less precisely but more concretely on the discretization parameters h and p) is not known in general. For the case of scattering by

a smooth non-trapping obstacle [43], see also [13, 14], the upper bound (1.3) is available. More generally, as long as the domain Ω features an elliptic regularity shift for the Laplace operator, one can state that

$$\sigma_{\text{ba}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}}, k, \kappa) \left(\frac{kh}{p} \right)^\varepsilon$$

for some $\varepsilon = \varepsilon(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}}) > 0$, so that $\sigma_{\text{ba}} \rightarrow 0$ as $\frac{kh}{p} \rightarrow 0$. Here and above, $\widehat{\Omega} := (1/h_\Omega)\Omega$ and $\widehat{\Gamma}_{\text{D}} := (1/h_\Omega)\Gamma_{\text{D}}$ denote scaled versions of Ω and Γ_{D} which are independent of the size of the computational domain Ω . We provide a computable upper bound on σ_{ba} in some settings of interest in Theorem 2.6 below.

In addition to (2.7), we also introduce

$$(2.10) \quad \tilde{\sigma}_{\text{ba}} := k^{\frac{1}{2}} \sup_{\psi \in L^2(\Gamma_{\text{A}}) \setminus \{0\}} \inf_{v_h \in V_h} \frac{|\tilde{u}_\psi^* - v_h|_{1,\Omega}}{\|\psi\|_{0,\Gamma_{\text{A}}}},$$

where \tilde{u}_ψ^* is the (adjoint) solution in $H_{\Gamma_{\text{D}}}^1(\Omega)$ such that

$$(2.11) \quad b(w, \tilde{u}_\psi^*) = (w, \psi)_{\Gamma_{\text{A}}} \quad \forall w \in H_{\Gamma_{\text{D}}}^1(\Omega).$$

The quantity $\tilde{\sigma}_{\text{ba}}$ is similar to σ_{ba} since it measures the best-approximation error for the solution of (2.11) which features a boundary right-hand side instead of a volume right-hand side as in (2.8). As in the case of volume data, if the domain Ω features an elliptic regularity shift, we have

$$\tilde{\sigma}_{\text{ba}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}}, k, \kappa) \left(\frac{kh}{p} \right)^{\tilde{\varepsilon}},$$

where $\tilde{\varepsilon} = \tilde{\varepsilon}(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}}) > 0$. In addition, under some reasonable assumption that is satisfied in all the configurations depicted in Figure 1, we prove in Appendix A the estimate

$$(2.12) \quad \tilde{\sigma}_{\text{ba}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}}) C_{\text{qi}}(\kappa) \left(\left(\frac{kh}{p} \right)^{\frac{1}{2}} + \frac{kh}{p} \right) + \left(C(\widehat{\Omega}, \widehat{\Gamma}_{\text{D}}) \frac{1}{kh_\Omega} \left(1 + \frac{1}{kh_\Omega} \right) + 2 \right) \sigma_{\text{ba}},$$

where $C_{\text{qi}}(\kappa)$ is a quasi-interpolation constant that only depends on the shape-regularity parameter [34, 42]. In particular, in the high-wavenumber regime when $kh_\Omega \rightarrow \infty$, we have

$$\tilde{\sigma}_{\text{ba}} \leq 2\sigma_{\text{ba}} + \mathcal{O} \left(\left(\frac{kh}{p} \right)^{\frac{1}{2}} \right).$$

2.4. Equilibrated flux reconstruction. For each vertex \mathbf{a} in the set of vertices \mathcal{V}_h of the mesh \mathcal{T}_h , set

$$(2.13a) \quad d_{\mathbf{a}} := \psi_{\mathbf{a}} \pi_h^p(f) + \psi_{\mathbf{a}} k^2 u_h - \nabla \psi_{\mathbf{a}} \cdot \nabla u_h,$$

and

$$(2.13b) \quad b_{\mathbf{a}} := \begin{cases} -\psi_{\mathbf{a}} \tilde{\pi}_h^p(g) - \psi_{\mathbf{a}} i k u_h & \text{on } \partial\omega_{\mathbf{a}} \cap \Gamma_{\text{A}}, \\ 0 & \text{on } \partial\omega_{\mathbf{a}} \setminus \Gamma_{\text{A}}. \end{cases}$$

Here u_h is the finite element approximation from (2.6) and $\psi_{\mathbf{a}}$ is the ‘‘hat function’’ associated with the vertex \mathbf{a} : the unique function in $\mathcal{P}_1(\mathcal{T}_h) \cap H^1(\Omega)$ such that $\psi_{\mathbf{a}}(\mathbf{a}) = 1$ and $\psi_{\mathbf{a}}(\mathbf{a}') = 0$ for all $\mathbf{a}' \in \mathcal{V}_h \setminus \{\mathbf{a}\}$. Moreover, the elementwise/facewise L^2 projectors π_h^q and $\tilde{\pi}_h^q$ are respectively defined for any integer $q \geq 0$, any $v \in L^2(\Omega)$, and any $w \in L^2(\Gamma_A)$ by

$$(2.14a) \quad \pi_h^q(v)|_K \in \mathcal{P}_q(K), \quad (\pi_h^q(v)|_K, \phi)_K = (v|_K, \phi)_K \quad \forall \phi \in \mathcal{P}_q(K), \forall K \in \mathcal{T}_h,$$

$$(2.14b) \quad \tilde{\pi}_h^q(w)|_F \in \mathcal{P}_q(F), \quad (\tilde{\pi}_h^q(w)|_F, \phi)_F = (w|_F, \phi)_F \quad \forall \phi \in \mathcal{P}_q(F), \forall F \in \mathcal{F}_h, F \subset \overline{\Gamma_A},$$

where \mathcal{F}_h is the set of mesh faces.

For an integer $q \geq 0$, let $\mathcal{P}_q(K)$ be the set of vector-valued functions that have all components in $\mathcal{P}_q(K)$. We introduce the space $\mathbf{RT}_q(K) := \mathbf{x}\mathcal{P}_q(K) + \mathcal{P}_q(K)$ from [44, 47] and define

$$\begin{aligned} \mathcal{P}_q(\mathcal{T}) &:= \{v \in L^2(\omega) \mid v|_K \in \mathcal{P}_q(K); \forall K \in \mathcal{T}\}, \\ \mathbf{RT}_q(\mathcal{T}) &:= \{\mathbf{v} \in \mathbf{L}^2(\omega) \mid \mathbf{v}|_K \in \mathbf{RT}_q(K); \forall K \in \mathcal{T}\} \end{aligned}$$

for any subset of mesh elements $\mathcal{T} \subset \mathcal{T}_h$ with the corresponding open subdomain ω . In particular, for each vertex $\mathbf{a} \in \mathcal{V}_h$, we denote by $\mathcal{T}_{\mathbf{a}}$ the patch of all elements $K \in \mathcal{T}_h$ having \mathbf{a} as a vertex and by $\omega_{\mathbf{a}}$ the corresponding open subdomain.

Following [7, 25, 29], we consider the following inexpensive and fully parallel post-processing procedure:

Definition 2.1 (Equilibrated flux reconstruction). *For every vertex $\mathbf{a} \in \mathcal{V}_h$, let*

$$(2.15) \quad \boldsymbol{\sigma}_h^{\mathbf{a}} := \underset{\substack{\boldsymbol{\tau}_h^{\mathbf{a}} \in \mathbf{RT}_{p+1}(\mathcal{T}_{\mathbf{a}}) \cap \mathbf{H}(\text{div}, \omega_{\mathbf{a}}) \\ \nabla \cdot \boldsymbol{\tau}_h^{\mathbf{a}} = d_{\mathbf{a}} \text{ in } \omega_{\mathbf{a}} \\ \boldsymbol{\tau}_h^{\mathbf{a}} \cdot \mathbf{n} = b_{\mathbf{a}} \text{ on } \Gamma_{\mathbf{a}}}}{\text{argmin}} \|\boldsymbol{\tau}_h^{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h\|_{0, \omega_{\mathbf{a}}},$$

where $\Gamma_{\mathbf{a}} := \partial\omega_{\mathbf{a}} \setminus \Gamma_D$ if $\mathbf{a} \in \overline{\Gamma_D}$ and $\partial\omega_{\mathbf{a}}$ otherwise. The equilibrated flux reconstruction is computed by summing up the patchwise contributions (after zero extension) as

$$(2.16) \quad \boldsymbol{\sigma}_h := \sum_{\mathbf{a} \in \mathcal{V}_h} \boldsymbol{\sigma}_h^{\mathbf{a}} \in \mathbf{RT}_{p+1}(\mathcal{T}_h) \cap \mathbf{H}(\text{div}, \Omega).$$

Since $d_{\mathbf{a}} \in \mathcal{P}_{p+1}(\mathcal{T}_{\mathbf{a}})$ and $b_{\mathbf{a}} \in \mathcal{P}_{p+1}(F)$ for each face $F \subset \partial\omega_{\mathbf{a}}$, we see that the minimization set in (2.15) is non-empty when

$$(2.17) \quad (d_{\mathbf{a}}, 1)_{\omega_{\mathbf{a}}} = (b_{\mathbf{a}}, 1)_{\partial\omega_{\mathbf{a}}} \quad \forall \mathbf{a} \notin \overline{\Gamma_D}.$$

Since $\psi_{\mathbf{a}} \in V_h$ when $\mathbf{a} \notin \overline{\Gamma_D}$, we have from (2.6) in combination with (2.14)

$$(\psi_{\mathbf{a}} \pi_h^p(f), 1)_{\omega_{\mathbf{a}}} = (f, \psi_{\mathbf{a}}) = b(u_h, \psi_{\mathbf{a}}) - (g, \psi_{\mathbf{a}})_{\Gamma_A} = b(u_h, \psi_{\mathbf{a}}) - (\psi_{\mathbf{a}} \tilde{\pi}_h^p(g), 1)_{\Gamma_A}.$$

As a result, the compatibility condition (2.17) follows from the definition (2.2) of $b(\cdot, \cdot)$ and

$$\begin{aligned} (\psi_{\mathbf{a}} \pi_h^p(f), 1)_{\omega_{\mathbf{a}}} &= -k^2(u_h, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} - ik(u_h, \psi_{\mathbf{a}})_{\partial\omega_{\mathbf{a}} \cap \Gamma_A} + (\nabla u_h, \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} - (\psi_{\mathbf{a}} \tilde{\pi}_h^p(g), 1)_{\Gamma_A} \\ &= (\nabla \psi_{\mathbf{a}} \cdot \nabla u_h - k^2 \psi_{\mathbf{a}} u_h, 1)_{\omega_{\mathbf{a}}} + (b_{\mathbf{a}}, 1)_{\partial\omega_{\mathbf{a}}}. \end{aligned}$$

Then the uniqueness of the minimizer in (2.15) follows from standard convexity arguments.

Remark 2.2 (Equilibrated flux). *In practice, the local fluxes $\boldsymbol{\sigma}_h^{\mathbf{a}}$ are obtained by invoking the Euler–Lagrange conditions of the constrained minimization problem (2.15). This leads to the problem of finding the unique pair $(\boldsymbol{\sigma}_h^{\mathbf{a}}, r_h^{\mathbf{a}}) \in \mathbf{RT}_{p+1}(\mathcal{T}_{\mathbf{a}}) \cap \mathbf{H}(\operatorname{div}, \omega_{\mathbf{a}}) \times \mathcal{P}_{p+1}^0(\mathcal{T}_{\mathbf{a}})$ such that $\boldsymbol{\sigma}_h^{\mathbf{a}} \cdot \mathbf{n} = b_{\mathbf{a}}$ on $\Gamma_{\mathbf{a}}$ and*

$$\begin{cases} (\boldsymbol{\sigma}_h^{\mathbf{a}}, \mathbf{v}_h)_{\omega_{\mathbf{a}}} - (r_h^{\mathbf{a}}, \nabla \cdot \mathbf{v}_h)_{\omega_{\mathbf{a}}} = -(\psi_{\mathbf{a}} \nabla u_h, \mathbf{v}_h)_{\omega_{\mathbf{a}}} & \forall \mathbf{v}_h \in \mathbf{RT}_{p+1}(\mathcal{T}_{\mathbf{a}}) \cap \mathbf{H}_{\Gamma_{\mathbf{a}}}(\operatorname{div}, \omega_{\mathbf{a}}), \\ (\nabla \cdot \boldsymbol{\sigma}_h^{\mathbf{a}}, v_h)_{\omega_{\mathbf{a}}} = (d_{\mathbf{a}}, v_h)_{\omega_{\mathbf{a}}} & \forall v_h \in \mathcal{P}_{p+1}^0(\mathcal{T}_{\mathbf{a}}), \end{cases}$$

where $\mathbf{H}_{\Gamma_{\mathbf{a}}}(\operatorname{div}, \omega_{\mathbf{a}})$ imposes zero normal flux through $\Gamma_{\mathbf{a}}$ and where $\mathcal{P}_{p+1}^0(\mathcal{T}_{\mathbf{a}})$ is composed of the functions $v_h \in \mathcal{P}_{p+1}(\mathcal{T}_{\mathbf{a}})$ such that $(v_h, 1)_{\omega_{\mathbf{a}}} = 0$ if $\mathbf{a} \notin \overline{\Gamma_{\mathbf{D}}}$ whereas $\mathcal{P}_{p+1}^0(\mathcal{T}_{\mathbf{a}}) := \mathcal{P}_{p+1}(\mathcal{T}_{\mathbf{a}})$ otherwise.

2.5. Data oscillation. For each element $K \in \mathcal{T}_h$, we define

$$(2.18) \quad \operatorname{osc}_K(f, g) := \frac{h_K}{\pi} \|f - \pi_h^p(f)\|_{0,K} + C_{\operatorname{tr},K} \left(\frac{h_K}{\pi} \right)^{\frac{1}{2}} \|g - \tilde{\pi}_h^p(g)\|_{0,\partial K \cap \Gamma_{\mathbf{A}}}$$

with

$$C_{\operatorname{tr},K}^2 := N_{K,\Gamma_{\mathbf{A}}} \frac{3}{4\pi} \left(1 + \frac{1}{\pi} \right) \left(\frac{h_K}{\rho_K} \right)^d,$$

where $N_{K,\Gamma_{\mathbf{A}}}$ is the number of faces of K that belong to $\Gamma_{\mathbf{A}}$, and the remaining part of $C_{\operatorname{tr},K}$ comes from the standard trace inequality for one face of K , cf. [17, Section 4.2]. Owing to this definition of $\operatorname{osc}_K(f, g)$ and to the Poincaré inequality (recall that K is convex)

$$\|v\|_{0,K} \leq \frac{h_K}{\pi} |v|_{1,K}$$

as well as to the trace inequality

$$\|v\|_{0,\partial K \cap \Gamma_{\mathbf{A}}} \leq C_{\operatorname{tr},K} \left(\frac{h_K}{\pi} \right)^{\frac{1}{2}} |v|_{1,K},$$

we have

$$(2.19) \quad \|f - \pi_h^p(f)\|_{0,K} \|v\|_{0,K} + \|g - \tilde{\pi}_h^p(g)\|_{0,\partial K \cap \Gamma_{\mathbf{A}}} \|v\|_{0,\partial K \cap \Gamma_{\mathbf{A}}} \leq \operatorname{osc}_K(f, g) |v|_{1,K},$$

for any function $v \in H^1(K)$ with zero mean value on K . If $\mathcal{T} = \{K\}$ is a collection of several elements K , we set

$$\operatorname{osc}_{\mathcal{T}}(f, g) := \left(\sum_{K \in \mathcal{T}} \operatorname{osc}_K(f, g)^2 \right)^{\frac{1}{2}},$$

and we omit the subscript when $\mathcal{T} = \mathcal{T}_h$.

2.6. Main results. Let u be the weak solution to (2.1) and let u_h be any conforming finite element approximation solving (2.6). Let the equilibrated flux reconstruction σ_h be prescribed by definition 2.1 and define the local and global error estimators as

$$(2.20) \quad \eta_K := \|\sigma_h + \nabla u_h\|_{0,K}, \quad \eta := \left(\sum_{K \in \mathcal{T}_h} \eta_K^2 \right)^{\frac{1}{2}}.$$

Recall finally the approximability factors σ_{ba} and $\tilde{\sigma}_{\text{ba}}$ defined respectively by (2.7) and (2.10). Our main result on the error upper bound is the following.

Theorem 2.3 (Upper bounds). *The following global upper bound holds true:*

$$(2.21) \quad \| \|u - u_h\| \|_{1,k,\Omega} \leq C_{\text{up}} (\eta + \text{osc}(f, g)),$$

where

$$C_{\text{up}} := \min(\sqrt{2} + \tilde{\theta}_1(\sigma_{\text{ba}}), 1 + \tilde{\theta}_2(\sigma_{\text{ba}}, \tilde{\sigma}_{\text{ba}})),$$

and

$$(2.22) \quad \begin{aligned} 0 \leq \tilde{\theta}_1(t) &:= \sqrt{\left(\frac{1}{2} + \sqrt{\frac{1}{4} + t^2} \right)^2 + \left(\frac{1}{2} + \sqrt{\frac{1}{4} + t^2} \right)^2 + t^2} - \sqrt{2} \\ &\leq \theta_1(t) := \sqrt{2t + 2t^2}, \end{aligned}$$

together with

$$(2.23) \quad \begin{aligned} 0 \leq \tilde{\theta}_2(t, \tilde{t}) &:= \sqrt{\left(\frac{1}{2} + \sqrt{\frac{1}{4} + t^2} \right)^2 + t^2 + \tilde{t}^2} - 1 \\ &\leq \theta_2(t, \tilde{t}) := \sqrt{t + 2t^2 + \tilde{t}^2}. \end{aligned}$$

Note that the bounds $0 \leq \tilde{\theta}_1(t) \leq \theta_1(t)$ and $0 \leq \tilde{\theta}_2(t, \tilde{t}) \leq \theta_2(t, \tilde{t})$ in (2.22) and (2.23), respectively, are straightforward, so that the only estimate to prove is (2.21). This result is established in Propositions 3.4, 3.6, and 4.1.

Remark 2.4 (Upper bounds in the asymptotic regime). *As we show in Appendix A, for most configurations of interest, the upper bound (2.21) together with (2.12) and (2.23) shows that asymptotically, when $\frac{kh}{p} \rightarrow 0$ and $\sigma_{\text{ba}} \rightarrow 0$, we have $C_{\text{up}} \rightarrow 1$.*

Our main result on the error lower bound is as follows.

Theorem 2.5 (Lower bounds). *The following local lower bounds also hold true:*

$$(2.24) \quad \eta_K \leq C_{\text{low},\omega_K} \| \|u - u_h\| \|_{1,k,\omega_K} + C(\kappa_{\mathcal{T}_K}) \text{osc}_{\mathcal{T}_K}(f, g) \quad \forall K \in \mathcal{T}_h$$

with

$$C_{\text{low},\omega_K} := C(\kappa_{\mathcal{T}_K}) \left(1 + \left(\frac{kh_{\omega_K}}{p} \right)^{\frac{1}{2}} + \frac{kh_{\omega_K}}{p} \right),$$

where $C(\kappa_{\mathcal{T}_K})$ only depends on the shape-regularity parameter $\kappa_{\mathcal{T}_K}$ of the mesh in the patch \mathcal{T}_K of elements sharing a vertex with K and h_{ω_K} is the diameter of the corresponding subdomain ω_K .

In addition, the following global lower bound holds true:

$$(2.25) \quad \eta \leq C_{\text{low}} \| \|u - u_h\| \|_{1,k,\Omega} + C(\kappa) \text{osc}(f, g),$$

where

$$C_{\text{low}} := C(\kappa) \left(1 + \left(\frac{kh}{p} \right)^{\frac{1}{2}} + \frac{kh}{p} \right),$$

and $C(\kappa)$ only depends on the shape regularity-parameter κ of the mesh.

The local lower bound (2.24) is established in Proposition 4.5. Though (2.25) is easily obtained from (2.24) by summation over the mesh cells, we provide an estimate with a sharper constant in Proposition 4.6.

Crucially, for several configurations of interest, the upper bound of Theorem 2.3 can be turned into a *guaranteed estimate* in *any regime* starting from the unresolved one (on any mesh \mathcal{T}_h and for any polynomial degree p) through the two following computable upper bounds on the approximability factor σ_{ba} .

Theorem 2.6 (Computable bounds on σ_{ba}).

Case 1a) (Scattering by a non-trapping obstacle). Assume that $\Omega = \Omega_0 \setminus \overline{D}$, $\Gamma_A = \partial\Omega_0$, and $\Gamma_D = \partial D$, where $\Omega_0, D \subset \mathbb{R}^d$ are two open, bounded, connected sets such that \overline{D} is a proper subset of Ω_0 and assume that the subset

$$(2.26) \quad \mathcal{O}_{\Gamma_D, \Gamma_A} := \{ \mathbf{x}_0 \in \mathbb{R}^d \mid (\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n} \leq 0 \ \forall \mathbf{x} \in \Gamma_D, (\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n} > 0 \ \forall \mathbf{x} \in \Gamma_A \}$$

is nonempty (recall that \mathbf{n} points outward Ω). Let

$$(2.27) \quad C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) := \inf_{\mathbf{x}_0 \in \mathcal{O}_{\Gamma_D, \Gamma_A}} C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0),$$

with

$$C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0) := \frac{1}{h_\Omega} \left\{ \sup_{\mathbf{x} \in \widehat{\Omega}} |\mathbf{x} - \mathbf{x}_0| + \sup_{\mathbf{x} \in \widehat{\Gamma}_D} \left(2(\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n} + \frac{|(\mathbf{x} - \mathbf{x}_0) \times \mathbf{n}|^2}{(\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n}} \right) \right\}.$$

Then, we have

$$(2.28) \quad \sigma_{\text{ba}} \leq \left(\left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) kh_\Omega \right) + \left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) kh_\Omega \right)^2 \right)^{\frac{1}{2}}.$$

Case 1b) (Wave propagation in free space). Assume that Ω is convex and $\Gamma_D = \emptyset$, so that $\mathcal{O}_{\Gamma_D, \Gamma_A} = \Omega$. Let $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D)$ be defined as above. Then, we have

$$(2.29) \quad \sigma_{\text{ba}} \leq C_i(\kappa) \left(d + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) kh_\Omega \right) \frac{kh}{p^\beta},$$

where $C_i(\kappa)$ is any approximation constant satisfying

$$(2.30) \quad \inf_{v_h \in \mathcal{V}_h} |v - v_h|_{1,\Omega} \leq C_i(\kappa) \frac{h}{p^\beta} |v|_{2,\Omega} \quad \forall v \in H_{\Gamma_D}^1(\Omega) \cap H^2(\Omega),$$

and such that it only depends on the mesh regularity κ ; typically $\beta = 0$ or $\beta = 1$ in (2.29) and (2.30).

Case 2a) (Interior problem). Assume that $\Gamma_A = \emptyset$. Then

$$(2.31) \quad \sigma_{\text{ba}} \leq k \max_{j \in \mathbb{N}} \sqrt{\frac{\lambda_j}{|\lambda_j - k^2|}},$$

where λ_j is the j -th eigenvalue of the Laplace operator in Ω with Dirichlet boundary conditions.

Case 2b) (Convex interior problem). Assume that $\Gamma_A = \emptyset$ and that Ω is convex. Then

$$(2.32) \quad \sigma_{\text{ba}} \leq C_i(\kappa) \left(1 + \frac{k^2}{\min_{j \in \mathbb{N}} |\lambda_j - k^2|} \right) \frac{h}{p^\beta},$$

where $C_i(\kappa)$ is any approximation constant satisfying (2.30).

The proof of Theorem 2.6 is carried out in Section 5. The estimates (2.31) and (2.32) follow from standard properties of spectral decomposition and we only sketch the proof at the beginning of Section 5. The more involved upper bounds (2.28) and (2.29) are respectively established in Sections 5.2 and 5.3.

Finally, the constant $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D)$ can be easily bounded when Γ_A has a simple geometry (which is usually the case in scattering applications).

Remark 2.7 (Constant $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D)$). In the Case 1a) (resp. 1b) above, if Ω_0 (resp. Ω) is a circle or a ball centered at \mathbf{x}_0 , then $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) \leq \frac{3}{2}$. If Ω_0 (resp. Ω) is a square centered at \mathbf{x}_0 , then $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) \leq \frac{3+\sqrt{2}}{2\sqrt{2}}$. Finally, if Ω_0 (resp. Ω) is a cube centered at \mathbf{x}_0 , then $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) \leq \frac{3+\sqrt{3}}{2\sqrt{3}}$.

Similarly, several expressions for the constant $C_i(\kappa)$ can be found in the literature [3, 10, 36, 39], leading to (2.30) with $\beta = 0$.

Remark 2.8 (Constant $C_i(\kappa)$). A more precise definition than (2.30) is

$$C_i(\kappa) := \frac{p^\beta}{h} \sup_{v \in H_{\Gamma_D}^1(\Omega) \cap H^2(\Omega) \setminus \{0\}} \inf_{v_h \in V_h} \frac{|v - v_h|_{1,\Omega}}{|v|_{2,\Omega}}.$$

The value of $C_i(\kappa)$ can then be estimated by considering any interpolation operator. For any $v \in H_{\Gamma_D}^1(\Omega) \cap H^2(\Omega)$, we can define its \mathcal{P}_1 nodal interpolant $\mathcal{I}_h(v) \in V_h$ by

$$(\mathcal{I}_h(v))(\mathbf{a}) = v(\mathbf{a}) \quad \forall \mathbf{a} \in \mathcal{V}_h.$$

Then we have (with $\beta = 0$)

$$C_i(\kappa) \leq \sup_{v \in H_{\Gamma_D}^1(\Omega) \cap H^2(\Omega) \setminus \{0\}} \frac{|v - \mathcal{I}_h(v)|_{1,\Omega}}{h|v|_{2,\Omega}},$$

where $C_i(\kappa)$ only depends on κ . In particular, following Theorem 1.1 of [3], we have $C_i(\kappa) = 3/\kappa$ if $d = 2$ and $C_i(\kappa) = 8/\kappa$ if $d = 3$. Furthermore, sharper estimates are available for the specific case of triangles when $d = 2$, and we refer the reader to [10, 36, 39].

In particular, for a mesh formed by isosceles right-angled triangles, we will employ the estimate $C_i(\kappa) \leq 0.493/\sqrt{2}$ from [39].

Remark 2.9 (Eigenvalues). *Apart from very simple domain geometries, analytic expressions of the eigenvalues λ_j appearing in (2.31) and (2.32) are not available. However, guaranteed a posteriori error estimators can be employed to reliably estimate their value, and thus σ_{ba} , see [8, 9, 38] and the references therein. We also refer the reader to [11], where related arguments are employed in the context of least-squares discretizations.*

Remark 2.10 (Data oscillation). *Actually, a slightly sharper upper bound than (2.21), with data oscillation integrated to the local error estimators, follows from (4.1) below. Also, upon modifying the treatment of the data f and g as in [27, 29], one could replace in $\text{osc}_K(f, g)$ in (2.18) the projections π_h^p and $\tilde{\pi}_h^p$ by π_h^{p+1} and $\tilde{\pi}_h^{p+1}$ and gain an additional order for data oscillation in the upper bound (2.21). This is, however, not possible in the lower bounds (2.24) and (2.25). We do not present these extensions here for the clarity of exposition.*

3. RELATION BETWEEN THE ERROR AND THE DUAL NORM OF THE RESIDUAL

The aim of this section is to obtain lower and upper bounds on the error between u and u_h by dual residual norms. We define the *residual* $\mathcal{R}(u_h) \in (H_{\Gamma_D}^1(\Omega))'$ stemming from the weak formulation (2.1) by

$$(3.1) \quad \langle \mathcal{R}(u_h), v \rangle := b(u - u_h, v) = (f, v) + (g, v)_{\Gamma_A} - b(u_h, v) \quad \forall v \in H_{\Gamma_D}^1(\Omega).$$

We further introduce the residual norm

$$(3.2) \quad \|\mathcal{R}(u_h)\|_{-1, \Omega} := \sup_{v \in H_{\Gamma_D}^1(\Omega) \setminus \{0\}} \frac{|\langle \mathcal{R}(u_h), v \rangle|}{|v|_{1, \Omega}}.$$

Note that in virtue of (2.6), we have

$$(3.3) \quad \langle \mathcal{R}(u_h), v_h \rangle = 0 \quad \forall v_h \in V_h.$$

3.1. Global upper bounds. We start by an upper bound on the $L^2(\Omega)$ -norm using the approximation factor σ_{ba} defined in (2.7). The proof follows the lines of Lemma 4.7 of [28] and employs the usual Aubin–Nitsche duality argument.

Lemma 3.1 ($L^2(\Omega)$ -norm upper bound by the dual norm of the residual). *We have*

$$(3.4) \quad k\|u - u_h\|_{0, \Omega} \leq \sigma_{\text{ba}}\|\mathcal{R}(u_h)\|_{-1, \Omega}.$$

Proof. We introduce ξ as the unique element of $H_{\Gamma_D}^1(\Omega)$ such that $b(w, \xi) = (w, u - u_h)$ for all $w \in H_{\Gamma_D}^1(\Omega)$. Selecting the test function $w = u - u_h$ and using (3.1) and (3.3), we see that

$$k\|u - u_h\|_{0, \Omega}^2 = k\langle \mathcal{R}(u_h), \xi \rangle = k\langle \mathcal{R}(u_h), \xi - \xi_h \rangle \leq k\|\mathcal{R}(u_h)\|_{-1, \Omega}|\xi - \xi_h|_{1, \Omega}$$

for all $\xi_h \in V_h$. Hence, using (2.7) and its consequence (2.9) and recalling the definition of ξ , we have

$$k\|u - u_h\|_{0,\Omega}^2 \leq \|\mathcal{R}(u_h)\|_{-1,\Omega} \left(k \inf_{\xi_h \in V_h} |\xi - \xi_h|_{1,\Omega} \right) \leq \sigma_{\text{ba}} \|\mathcal{R}(u_h)\|_{-1,\Omega} \|u - u_h\|_{0,\Omega},$$

and (3.4) follows. \square

We now record a useful quadratic inequality.

Lemma 3.2 (Quadratic inequality). *Assume that $x \geq 0$ satisfies*

$$ax^2 \leq c + bx,$$

for some constants $a, b, c > 0$. Then we have

$$ax \leq \frac{b}{2} + \sqrt{\frac{b^2}{4} + ac}.$$

With the help of Lemmas 3.1 and 3.2, we obtain an upper bound on the $H^1(\Omega)$ semi-norm.

Lemma 3.3 ($H^1(\Omega)$ semi-norm upper bound by the dual norm of the residual). *We have*

$$(3.5) \quad |u - u_h|_{1,\Omega} \leq \left(\frac{1}{2} + \sqrt{\frac{1}{4} + (\sigma_{\text{ba}})^2} \right) \|\mathcal{R}(u_h)\|_{-1,\Omega}.$$

Proof. Using the definition (2.2) of b , (3.1), and Lemma 3.1, we have

$$\begin{aligned} |u - u_h|_{1,\Omega}^2 &= \text{Re } b(u - u_h, u - u_h) + k^2 \|u - u_h\|_{0,\Omega}^2 \\ &\leq \|\mathcal{R}(u_h)\|_{-1,\Omega} |u - u_h|_{1,\Omega} + (\sigma_{\text{ba}})^2 \|\mathcal{R}(u_h)\|_{-1,\Omega}^2, \end{aligned}$$

and (3.5) is a direct consequence of Lemma 3.2 with $a = 1$, $b = \|\mathcal{R}(u_h)\|_{-1,\Omega}$, and $c = (\sigma_{\text{ba}})^2 \|\mathcal{R}(u_h)\|_{-1,\Omega}^2$. \square

We are now ready to establish global upper bounds in the energy norm. Our first estimate is explicit in terms of σ_{ba} .

Proposition 3.4 (First upper bound by the dual norm of the residual). *We have*

$$\| \|u - u_h\| \|_{1,k,\Omega} \leq (\sqrt{2} + \tilde{\theta}_1(\sigma_{\text{ba}})) \|\mathcal{R}(u_h)\|_{-1,\Omega},$$

with $\tilde{\theta}_1$ defined in (2.22).

Proof. Employing the definitions (2.2) and (3.1), we have

$$k\|u - u_h\|_{0,\Gamma_A}^2 = -\text{Im } b(u - u_h, u - u_h) \leq \|\mathcal{R}(u_h)\|_{-1,\Omega} |u - u_h|_{1,\Omega},$$

and using Lemma 3.3, it follows that

$$k\|u - u_h\|_{0,\Gamma_A}^2 \leq \left(\frac{1}{2} + \sqrt{\frac{1}{4} + (\sigma_{\text{ba}})^2} \right) \|\mathcal{R}(u_h)\|_{-1,\Omega}^2.$$

Hence, from (2.3) and (3.4)–(3.5), we infer that

$$\|u - u_h\|_{1,k,\Omega}^2 \leq \left((\sigma_{\text{ba}})^2 + \left(\frac{1}{2} + \sqrt{\frac{1}{4} + (\sigma_{\text{ba}})^2} \right) + \left(\frac{1}{2} + \sqrt{\frac{1}{4} + (\sigma_{\text{ba}})^2} \right)^2 \right) \|\mathcal{R}(u_h)\|_{-1,\Omega}^2,$$

and the claim follows from the definition of $\tilde{\theta}_1$. \square

Proposition 3.4 is not completely satisfactory, since the asymptotic value for vanishing σ_{ba} of the prefactor is $\sqrt{2}$. We now provide a sharper analysis that shows that the asymptotic constant can be brought to the optimal value of 1. Recall the definition (2.10) of $\tilde{\sigma}_{\text{ba}}$.

Lemma 3.5 ($L^2(\Gamma_A)$ -norm upper bound by the dual norm of the residual). *We have*

$$(3.6) \quad k^{\frac{1}{2}} \|u - u_h\|_{0,\Gamma_A} \leq \tilde{\sigma}_{\text{ba}} \|\mathcal{R}(u_h)\|_{-1,\Omega}.$$

Proof. We use again a duality argument. We define χ as the unique element of $H_{\Gamma_D}^1(\Omega)$ such that $b(w, \chi) = (w, u - u_h)_{\Gamma_A}$ for all $w \in H_{\Gamma_D}^1(\Omega)$. Selecting the test function $w = u - u_h$, employing the definition of the residual (3.1), and taking advantage of Galerkin's orthogonality (3.3), we have

$$k \|u - u_h\|_{0,\Gamma_A}^2 = kb(u - u_h, \chi) = k \langle \mathcal{R}(u_h), \chi - \chi_h \rangle \leq k \|\mathcal{R}(u_h)\|_{-1,\Omega} |\chi - \chi_h|_{1,\Omega}$$

for all $\chi_h \in V_h$. Then, recalling the above definition of χ and the definition (2.10) of $\tilde{\sigma}_{\text{ba}}$, we obtain (3.6) by taking the infimum over all $\chi_h \in V_h$. \square

Our second estimate is explicit in terms of the two constants σ_{ba} and $\tilde{\sigma}_{\text{ba}}$:

Proposition 3.6 (Second upper bound by the dual norm of the residual). *We have*

$$\|u - u_h\|_{1,k,\Omega} \leq (1 + \tilde{\theta}_2(\sigma_{\text{ba}}, \tilde{\sigma}_{\text{ba}})) \|\mathcal{R}(u_h)\|_{-1,\Omega},$$

where $\tilde{\theta}_2$ is defined in (2.23).

Proof. The proof combines (3.4), (3.5), and (3.6). \square

3.2. Local lower bounds. Define the local Sobolev space $H_{\star}^1(\omega_{\mathbf{a}})$ as

$$H_{\star}^1(\omega_{\mathbf{a}}) := \begin{cases} \{v \in H^1(\omega_{\mathbf{a}}) \mid \int_{\omega_{\mathbf{a}}} v = 0\} & \text{when } \mathbf{a} \notin \overline{\Gamma_D}, \\ \{v \in H^1(\omega_{\mathbf{a}}) \mid v = 0 \text{ on the part of } \Gamma_D \text{ where } \psi_{\mathbf{a}} \neq 0\} & \text{when } \mathbf{a} \in \overline{\Gamma_D}. \end{cases}$$

We will now employ a localized dual norm of the residual from (3.1) that is defined for each $\mathbf{a} \in \mathcal{V}_h$ by

$$(3.7) \quad \|\mathcal{R}(u_h)\|_{-1,\mathbf{a}} := \sup_{v \in H_{\star}^1(\omega_{\mathbf{a}}) \setminus \{0\}} \frac{|\langle \mathcal{R}(u_h), \psi_{\mathbf{a}} v \rangle|}{|v|_{1,\omega_{\mathbf{a}}}},$$

recalling that $\psi_{\mathbf{a}}$ is the hat function associated with the vertex $\mathbf{a} \in \mathcal{V}_h$.

We record that there exists a (Poincaré or Poincaré–Friedrichs) constant $C_{\text{PF},\mathbf{a}}$ that depends only on the local shape-regularity parameter $\kappa_{\mathcal{T}_{\mathbf{a}}} := \min_{K \in \mathcal{T}_{\mathbf{a}}} \kappa_K$ such that

$$(3.8) \quad \|v\|_{0,\omega_{\mathbf{a}}} \leq C_{\text{PF},\mathbf{a}} h_{\mathbf{a}} |v|_{1,\omega_{\mathbf{a}}} \quad \forall v \in H_{\star}^1(\omega_{\mathbf{a}}),$$

where $h_{\mathbf{a}} := \sup_{\mathbf{x}, \mathbf{y} \in \omega_{\mathbf{a}}} |\mathbf{x} - \mathbf{y}|$ is the diameter of the patch subdomain $\omega_{\mathbf{a}}$. When $\omega_{\mathbf{a}}$ is convex and $\mathbf{a} \notin \overline{\Gamma_D}$, we have $C_{\text{PF}, \mathbf{a}} = 1/\pi$, and we refer the reader to [54] and the references therein for a discussion on the value of the constant $C_{\text{PF}, \mathbf{a}}$ in the case of non-convex patches or patches around a Dirichlet boundary vertex. As observed in [7, 29], Leibniz's rule in conjunction with (3.8) shows that

$$(3.9) \quad |\psi_{\mathbf{a}} v|_{1, \omega_{\mathbf{a}}} \leq C_{\text{cont}, \text{PF}, \mathbf{a}} |v|_{1, \omega_{\mathbf{a}}} \quad \forall v \in H_{\star}^1(\omega_{\mathbf{a}}),$$

where the constant $C_{\text{cont}, \text{PF}, \mathbf{a}} := 1 + C_{\text{PF}, \mathbf{a}} |\psi_{\mathbf{a}}|_{1, \infty, \omega_{\mathbf{a}}} h_{\mathbf{a}}$ only depends on $\kappa_{\mathcal{T}_{\mathbf{a}}}$. We will also employ the trace inequality

$$(3.10) \quad \|v\|_{0, \partial \omega_{\mathbf{a}} \cap \Gamma_A} \leq C_{\text{tr}, \mathbf{a}} h_{\mathbf{a}}^{\frac{1}{2}} |v|_{1, \omega_{\mathbf{a}}} \quad \forall v \in H_{\star}^1(\omega_{\mathbf{a}}),$$

where the constant $C_{\text{tr}, \mathbf{a}}$ again only depends on $\kappa_{\mathcal{T}_{\mathbf{a}}}$. Finally, we introduce for each vertex $\mathbf{a} \in \mathcal{V}_h$ the local norm

$$\|v\|_{1, k, \omega_{\mathbf{a}}}^2 := k^2 \|v\|_{0, \omega_{\mathbf{a}}}^2 + k \|v\|_{0, \partial \omega_{\mathbf{a}} \cap \Gamma_A}^2 + |v|_{1, \omega_{\mathbf{a}}}^2 \quad \forall v \in H^1(\omega_{\mathbf{a}}).$$

For all vertices $\mathbf{a} \in \mathcal{V}_h$, if $v \in H_{\Gamma_D}^1(\Omega)$ with $\text{supp } v \subset \omega_{\mathbf{a}}$, there exists a discrete function $Q_{hp}^{\mathbf{a}}(v) \in V_h$ with $\text{supp}(Q_{hp}^{\mathbf{a}}(v)) \subset \omega_{\mathbf{a}}$ such that

$$(3.11) \quad \|v - Q_{hp}^{\mathbf{a}}(v)\|_{1, k, \omega_{\mathbf{a}}} \leq C_{\text{qi}, \mathbf{a}} \left(1 + \frac{kh_{\mathbf{a}}}{p} + \left(\frac{kh_{\mathbf{a}}}{p} \right)^2 \right)^{\frac{1}{2}} |v|_{1, \omega_{\mathbf{a}}},$$

where the constant $C_{\text{qi}, \mathbf{a}}$ only depends on $\kappa_{\mathcal{T}_{\mathbf{a}}}$. We can use a quasi-interpolation operator $Q_{hp}^{\mathbf{a}}$ to achieve (3.11). The construction of such an operator is presented in Theorem 3.3 of [42] in two space dimensions. For three space dimensions, the corresponding operator is constructed in [34].

Lemma 3.7 (Local lower bounds of the error by the dual norm of the residual). *For all vertices $\mathbf{a} \in \mathcal{V}_h$, we have*

$$\|\mathcal{R}(u_h)\|_{-1, \mathbf{a}} \leq C_{\text{lb}, \mathbf{a}} \|u - u_h\|_{1, k, \omega_{\mathbf{a}}},$$

where $C_{\text{lb}, \mathbf{a}} := \min(C_{\text{lb}, \text{hat}, \mathbf{a}}, C_{\text{lb}, \text{qi}, \mathbf{a}})$ and

$$C_{\text{lb}, \text{hat}, \mathbf{a}} := C_{\text{cont}, \text{PF}, \mathbf{a}} \left(1 + \frac{C_{\text{tr}, \mathbf{a}}^2}{C_{\text{cont}, \text{PF}, \mathbf{a}}^2} kh_{\mathbf{a}} + \frac{C_{\text{PF}, \mathbf{a}}^2}{C_{\text{cont}, \text{PF}, \mathbf{a}}^2} (kh_{\mathbf{a}})^2 \right)^{\frac{1}{2}},$$

$$C_{\text{lb}, \text{qi}, \mathbf{a}} := C_{\text{cont}, \text{PF}, \mathbf{a}} C_{\text{qi}, \mathbf{a}} \left(1 + \frac{kh_{\mathbf{a}}}{p} + \left(\frac{kh_{\mathbf{a}}}{p} \right)^2 \right)^{\frac{1}{2}}.$$

Proof. Let $v \in H_{\star}^1(\omega_{\mathbf{a}})$. From (2.4) and (3.1), we observe that

$$(3.12) \quad |\langle \mathcal{R}(u_h), \psi_{\mathbf{a}} v \rangle| = |b(u - u_h, \psi_{\mathbf{a}} v)| \leq \|u - u_h\|_{1, k, \omega_{\mathbf{a}}} \|\psi_{\mathbf{a}} v\|_{1, k, \omega_{\mathbf{a}}}.$$

Then, using (3.8), (3.9), and (3.10), we have

$$\begin{aligned}
\|\psi_{\mathbf{a}}v\|_{1,k,\omega_{\mathbf{a}}}^2 &= k^2\|\psi_{\mathbf{a}}v\|_{0,\omega_{\mathbf{a}}}^2 + k\|\psi_{\mathbf{a}}v\|_{0,\partial\omega_{\mathbf{a}}\cap\Gamma_{\Lambda}}^2 + |\psi_{\mathbf{a}}v|_{1,\omega_{\mathbf{a}}}^2 \\
&\leq k^2\|v\|_{0,\omega_{\mathbf{a}}}^2 + k\|v\|_{0,\partial\omega_{\mathbf{a}}\cap\Gamma_{\Lambda}}^2 + |\psi_{\mathbf{a}}v|_{1,\omega_{\mathbf{a}}}^2 \\
&\leq (C_{\text{PF},\mathbf{a}}^2 k^2 h_{\mathbf{a}}^2 + C_{\text{tr},\mathbf{a}}^2 k h_{\mathbf{a}} + C_{\text{cont,PF},\mathbf{a}}^2) |v|_{1,\omega_{\mathbf{a}}}^2 \\
&= C_{\text{lb,hats},\mathbf{a}}^2 |v|_{1,\omega_{\mathbf{a}}}^2.
\end{aligned}$$

On the other hand, since $Q_{hp}^{\mathbf{a}}(\psi_{\mathbf{a}}v) \in V_h$ with $\text{supp}(Q_{hp}^{\mathbf{a}}(\psi_{\mathbf{a}}v)) \subset \omega_{\mathbf{a}}$, using Galerkin's orthogonality (3.3) in (3.12) and (3.11) with (3.9), we have

$$\begin{aligned}
|\langle \mathcal{R}(u_h), \psi_{\mathbf{a}}v \rangle| &\leq \|u - u_h\|_{1,k,\omega_{\mathbf{a}}} \|\psi_{\mathbf{a}}v - Q_{hp}^{\mathbf{a}}(\psi_{\mathbf{a}}v)\|_{1,k,\omega_{\mathbf{a}}} \\
&\leq C_{\text{qi},\mathbf{a}} \left(1 + \frac{kh_{\mathbf{a}}}{p} + \left(\frac{kh_{\mathbf{a}}}{p} \right)^2 \right)^{\frac{1}{2}} \|u - u_h\|_{1,k,\omega_{\mathbf{a}}} |\psi_{\mathbf{a}}v|_{1,\omega_{\mathbf{a}}} \\
&\leq C_{\text{cont,PF},\mathbf{a}} C_{\text{qi},\mathbf{a}} \left(1 + \frac{kh_{\mathbf{a}}}{p} + \left(\frac{kh_{\mathbf{a}}}{p} \right)^2 \right)^{\frac{1}{2}} \|u - u_h\|_{1,k,\omega_{\mathbf{a}}} |v|_{1,\omega_{\mathbf{a}}} \\
&= C_{\text{lb,qi},\mathbf{a}} \|u - u_h\|_{1,k,\omega_{\mathbf{a}}} |v|_{1,\omega_{\mathbf{a}}}.
\end{aligned}$$

The expected result follows by combining the two bounds together with the definition (3.7) of the localized dual norm. \square

4. BOUNDS ON THE DUAL NORM OF THE RESIDUAL BY EQUILIBRATED FLUXES

In the previous section, we derived upper and lower bounds for the finite element error based on dual norms of the residual. These dual norms are not directly computable, as they are defined using a supremum over infinite-dimensional spaces. In this section, we use the technique of equilibrated flux construction to achieve guaranteed computable upper and lower bounds of these dual norms.

4.1. Global upper bound. Recall the definitions (2.18) of the data oscillation, (2.20) of the error estimator η , (3.1) and (3.2) of the residual and its dual norm, and finally Definition 2.1 of the equilibrated flux σ_h .

Proposition 4.1 (Upper bound on the dual norm of the residual). *The following holds true:*

$$(4.1) \quad \|\mathcal{R}(u_h)\|_{-1,\Omega} \leq \left(\sum_{K \in \mathcal{T}_h} (\eta_K + \text{osc}_K(f, g))^2 \right)^{\frac{1}{2}}.$$

Proof. We first observe that since the hat functions form a partition of unity, we have

$$\sum_{\mathbf{a} \in \mathcal{V}_h} \psi_{\mathbf{a}}(\mathbf{x}) = 1 \quad \forall \mathbf{x} \in \bar{\Omega}.$$

The summation over all vertices $\mathbf{a} \in \mathcal{V}_h$ in (2.16) together with the divergence and normal trace constrains in (2.15) lead to

$$\nabla \cdot \boldsymbol{\sigma}_h = \pi_h^p(f) + k^2 u_h \text{ in } \Omega, \quad \boldsymbol{\sigma}_h \cdot \mathbf{n} = -(\tilde{\pi}_h^p(g) + iku_h) \text{ on } \Gamma_A.$$

Then, if $v \in H_{\Gamma_D}^1(\Omega)$, we have

$$\begin{aligned} b(u_h, v) &= -k^2(u_h, v) - ik(u_h, v)_{\Gamma_A} + (\nabla u_h, \nabla v) \\ &= (\pi_h^p(f), v) + (\tilde{\pi}_h^p(g), v)_{\Gamma_A} - (\pi_h^p(f) + k^2 u_h, v) - (\tilde{\pi}_h^p(g) + iku_h, v)_{\Gamma_A} + (\nabla u_h, \nabla v) \\ &= (\pi_h^p(f), v) + (\tilde{\pi}_h^p(g), v)_{\Gamma_A} - (\nabla \cdot \boldsymbol{\sigma}_h, v) + (\boldsymbol{\sigma}_h \cdot \mathbf{n}, v)_{\Gamma_A} + (\nabla u_h, \nabla v) \\ &= (\pi_h^p(f), v) + (\tilde{\pi}_h^p(g), v)_{\Gamma_A} + (\boldsymbol{\sigma}_h + \nabla u_h, \nabla v). \end{aligned}$$

It follows that

$$\begin{aligned} \langle \mathcal{R}(u_h), v \rangle &= (f - \pi_h^p(f), v) + (g - \tilde{\pi}_h^p(g), v)_{\Gamma_A} + (\pi_h^p(f), v) + (\tilde{\pi}_h^p(g), v)_{\Gamma_A} - b(u_h, v) \\ &= (f - \pi_h^p(f), v) + (g - \tilde{\pi}_h^p(g), v)_{\Gamma_A} - (\boldsymbol{\sigma}_h + \nabla u_h, \nabla v). \end{aligned}$$

Since the restriction of $\pi_h^p v$ to each mesh face $F \subset \Gamma_A$ of the mesh belongs to $\mathcal{P}_p(F)$, and $v - \pi_h^p v$ has zero mean-value on each mesh cell K , we have

$$\begin{aligned} & |(f - \pi_h^p(f), v)_K + (g - \tilde{\pi}_h^p(g), v)_{\partial K \cap \partial \Gamma_A}| \\ &= |(f - \pi_h^p(f), v - \pi_h^p v)_K + (g - \tilde{\pi}_h^p(g), v - \pi_h^p v)_{\partial K \cap \partial \Gamma_A}| \\ &\leq \|f - \pi_h^p(f)\|_{0,K} \|v - \pi_h^p v\|_{0,K} + \|g - \tilde{\pi}_h^p(g)\|_{0,\partial K \cap \partial \Gamma_A} \|v - \pi_h^p v\|_{0,\partial K \cap \partial \Gamma_A} \\ &\leq \text{osc}_K(f, g) |v|_{1,K}, \end{aligned}$$

where we used (2.19). The Cauchy–Schwarz inequality now implies (4.1). \square

At this point, the upper bound (2.21) of Theorem 2.3 follows from Propositions 3.4, 3.6, and 4.1 by setting $C_{\text{up}} = \min\left(\sqrt{2} + \tilde{\theta}_1(\sigma_{\text{ba}}), 1 + \tilde{\theta}_2(\sigma_{\text{ba}}, \tilde{\sigma}_{\text{ba}})\right)$ and bounding (4.1) further by the triangle inequality.

4.2. Local lower bound. We first introduce a residual with projected source terms

$$(4.2) \quad \langle \mathcal{R}_h(u_h), v \rangle := (\pi_h^p(f), v) + (\tilde{\pi}_h^p(g), v)_{\Gamma_A} - b(u_h, v) \quad \forall v \in H_{\Gamma_D}^1(\Omega),$$

where the original right-hand sides f and g have been respectively replaced by their elementwise and facewise L^2 projections. We employ the same notation for the dual norms of $\mathcal{R}_h(u_h)$ as for those of $\mathcal{R}(u_h)$.

Lemma 4.2 (Data oscillations). *We have*

$$\|\mathcal{R}_h(u_h)\|_{-1,\mathbf{a}} \leq \|\mathcal{R}(u_h)\|_{-1,\mathbf{a}} + C(\kappa_{\mathcal{T}_{\mathbf{a}}}) \text{osc}_{\mathcal{T}_{\mathbf{a}}}(f, g) \quad \forall \mathbf{a} \in \mathcal{V}_h,$$

where the constant $C(\kappa_{\mathcal{T}_{\mathbf{a}}})$ only depends on the shape-regularity parameter of the elements in the patch $\mathcal{T}_{\mathbf{a}}$.

Proof. Fix a vertex $\mathbf{a} \in \mathcal{V}_h$. For all $v \in H_*^1(\omega_{\mathbf{a}})$, we have

$$\langle \mathcal{R}_h(u_h), \psi_{\mathbf{a}} v \rangle = \langle \mathcal{R}(u_h), \psi_{\mathbf{a}} v \rangle - (f - \pi_h^p(f), \psi_{\mathbf{a}} v) - (g - \tilde{\pi}_h^p(g), \psi_{\mathbf{a}} v)_{\Gamma_{\mathbf{A}}}.$$

Consequently, we infer that

$$\begin{aligned} & |\langle \mathcal{R}_h(u_h), \psi_{\mathbf{a}} v \rangle| \\ & \leq |\langle \mathcal{R}(u_h), \psi_{\mathbf{a}} v \rangle| + \|f - \pi_h^p(f)\|_{0, \omega_{\mathbf{a}}} \|\psi_{\mathbf{a}} v\|_{0, \omega_{\mathbf{a}}} + \|g - \tilde{\pi}_h^p(g)\|_{0, \partial \omega_{\mathbf{a}} \cap \Gamma_{\mathbf{A}}} \|\psi_{\mathbf{a}} v\|_{0, \partial \omega_{\mathbf{a}} \cap \Gamma_{\mathbf{A}}} \\ & \leq |\langle \mathcal{R}(u_h), \psi_{\mathbf{a}} v \rangle| + \|f - \pi_h^p(f)\|_{0, \omega_{\mathbf{a}}} \|v\|_{0, \omega_{\mathbf{a}}} + \|g - \tilde{\pi}_h^p(g)\|_{0, \partial \omega_{\mathbf{a}} \cap \Gamma_{\mathbf{A}}} \|v\|_{0, \partial \omega_{\mathbf{a}} \cap \Gamma_{\mathbf{A}}}, \end{aligned}$$

and we conclude using a similar estimate as in (2.19) patchwise. \square

In the next lemma, we observe following [7, Theorem 7], [29, Remark 3.15], or [30, Corollary 3.6] that the dual norms of the residual can be characterized using ‘‘continuous versions’’ of the minimization problems defining the equilibrated fluxes $\boldsymbol{\sigma}_h^{\mathbf{a}}$. Recall that $\Gamma_{\mathbf{a}} = \partial \omega_{\mathbf{a}} \setminus \Gamma_{\mathbf{D}}$ if $\mathbf{a} \in \overline{\Gamma_{\mathbf{D}}}$ and $\Gamma_{\mathbf{a}} = \partial \omega_{\mathbf{a}}$ otherwise.

Lemma 4.3 (Dual characterization). *We have*

$$(4.3) \quad \|\mathcal{R}_h(u_h)\|_{-1, \mathbf{a}} = \min_{\substack{\boldsymbol{\tau}^{\mathbf{a}} \in \mathbf{H}(\text{div}, \omega_{\mathbf{a}}) \\ \nabla \cdot \boldsymbol{\tau}^{\mathbf{a}} = d_{\mathbf{a}} \text{ in } \omega_{\mathbf{a}} \\ \boldsymbol{\tau}^{\mathbf{a}} \cdot \mathbf{n} = b_{\mathbf{a}} \text{ on } \Gamma_{\mathbf{a}}}} \|\boldsymbol{\tau}^{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h\|_{0, \omega_{\mathbf{a}}},$$

where $b_{\mathbf{a}}$ and $d_{\mathbf{a}}$ are defined in (2.13).

Proof. We introduce $r_{\mathbf{a}}$ as the unique element of $H_*^1(\omega_{\mathbf{a}})$ such that

$$(\nabla r_{\mathbf{a}}, \nabla v)_{\omega_{\mathbf{a}}} = \langle \mathcal{R}_h(u_h), \psi_{\mathbf{a}} v \rangle \quad \forall v \in H_*^1(\omega_{\mathbf{a}}).$$

Let $v \in H_*^1(\omega_{\mathbf{a}})$. The definitions (2.13) and (4.2) together with the identity $\nabla(\psi_{\mathbf{a}} v) = \psi_{\mathbf{a}} \nabla v + v \nabla \psi_{\mathbf{a}}$ show that

$$\langle \mathcal{R}_h(u_h), \psi_{\mathbf{a}} v \rangle = (d_{\mathbf{a}}, v)_{\omega_{\mathbf{a}}} - (b_{\mathbf{a}}, v)_{\partial \omega_{\mathbf{a}} \cap \Gamma_{\mathbf{A}}} - (\psi_{\mathbf{a}} \nabla u_h, \nabla v)_{\omega_{\mathbf{a}}},$$

and therefore

$$(\nabla r_{\mathbf{a}}, \nabla v)_{\omega_{\mathbf{a}}} = (d_{\mathbf{a}}, v)_{\omega_{\mathbf{a}}} - (b_{\mathbf{a}}, v)_{\partial \omega_{\mathbf{a}} \cap \Gamma_{\mathbf{A}}} - (\psi_{\mathbf{a}} \nabla u_h, \nabla v)_{\omega_{\mathbf{a}}} \quad \forall v \in H_*^1(\omega_{\mathbf{a}}).$$

Thus, $\boldsymbol{\sigma}^{\mathbf{a}} := -(\nabla r_{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h) \in \mathbf{H}(\text{div}, \omega_{\mathbf{a}})$ satisfies $\nabla \cdot \boldsymbol{\sigma}^{\mathbf{a}} = d_{\mathbf{a}}$ and $\boldsymbol{\sigma}^{\mathbf{a}} \cdot \mathbf{n} = b_{\mathbf{a}}$ on $\Gamma_{\mathbf{a}}$ as well as

$$\begin{cases} (\boldsymbol{\sigma}^{\mathbf{a}}, \mathbf{v})_{\omega_{\mathbf{a}}} - (r_{\mathbf{a}}, \nabla \cdot \mathbf{v})_{\omega_{\mathbf{a}}} = -(\psi_{\mathbf{a}} \nabla u_h, \mathbf{v})_{\omega_{\mathbf{a}}} & \forall \mathbf{v} \in \mathbf{H}_{\Gamma_{\mathbf{A}}}(\text{div}, \omega_{\mathbf{a}}), \\ (\nabla \cdot \boldsymbol{\sigma}^{\mathbf{a}}, v)_{\omega_{\mathbf{a}}} = (d_{\mathbf{a}}, v)_{\omega_{\mathbf{a}}} & \forall v \in H_*^1(\omega_{\mathbf{a}}), \end{cases}$$

so that $\boldsymbol{\sigma}^{\mathbf{a}}$ is the unique minimizer in the right-hand side of (4.3). Then, the conclusion follows since we have $\|\mathcal{R}_h(u_h)\|_{-1, \mathbf{a}} = |r_{\mathbf{a}}|_{1, \omega_{\mathbf{a}}} = \|\boldsymbol{\sigma}^{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h\|_{0, \omega_{\mathbf{a}}}$. \square

The following key estimate directly follows from [7, Theorem 7] in two space dimensions and [30, Corollaries 3.3 and 3.8] in three space dimensions.

Lemma 4.4 (Stability of discrete minimization). *For every vertex $\mathbf{a} \in \mathcal{V}_h$, we have*

$$\|\boldsymbol{\sigma}_h^{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h\|_{0, \omega_{\mathbf{a}}} \leq C_{\text{st}, \mathbf{a}} \min_{\substack{\boldsymbol{\tau}^{\mathbf{a}} \in \mathbf{H}(\text{div}, \omega_{\mathbf{a}}) \\ \nabla \cdot \boldsymbol{\tau}^{\mathbf{a}} = d_{\mathbf{a}} \text{ in } \omega_{\mathbf{a}} \\ \boldsymbol{\tau}^{\mathbf{a}} \cdot \mathbf{n} = b_{\mathbf{a}} \text{ on } \Gamma_{\mathbf{a}}}} \|\boldsymbol{\tau}^{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h\|_{0, \omega_{\mathbf{a}}},$$

where $C_{\text{st},\mathbf{a}}$ only depends on $\kappa_{\mathcal{T}_\mathbf{a}}$.

The following proposition gathers intermediate results established throughout Sections 3 and 4 and proves the local lower bound (2.24) of Theorem 2.5. Denote here by \mathcal{V}_K the set of vertices of the mesh cell $K \in \mathcal{T}_h$.

Proposition 4.5 (Local lower bound). *We have*

$$\eta_K \leq C_{\text{low},\omega_K} \| \|u - u_h\| \|_{1,k,\omega_K} + C(\kappa_{\mathcal{T}_K}) \text{osc}_{\mathcal{T}_K}(f, g) \quad \forall K \in \mathcal{T}_h,$$

where

$$C_{\text{low},\omega_K} := (d+1) \max_{\mathbf{a} \in \mathcal{V}_K} C_{\text{st},\mathbf{a}} C_{\text{lb},\mathbf{a}}.$$

Proof. Combining Lemmas 3.7, 4.2, 4.3, and 4.4, we infer that

$$(4.4) \quad \| \boldsymbol{\sigma}_h^\mathbf{a} + \psi_\mathbf{a} \nabla u_h \|_{0,\omega_\mathbf{a}} \leq C_{\text{st},\mathbf{a}} C_{\text{lb},\mathbf{a}} \| \|u - u_h\| \|_{1,k,\omega_\mathbf{a}} + C_{\text{st},\mathbf{a}} C(\kappa_{\mathcal{T}_\mathbf{a}}) \text{osc}_{\mathcal{T}_\mathbf{a}}(f, g).$$

Since

$$\eta_K \leq \sum_{\mathbf{a} \in \mathcal{V}_K} \| \boldsymbol{\sigma}_h^\mathbf{a} + \psi_\mathbf{a} \nabla u_h \|_{0,\omega_\mathbf{a}}$$

and as each $K \in \mathcal{T}_h$ has $(d+1)$ vertices and the neighboring elements have a similar diameter, the assertion follows. \square

Finally, the following estimate is obtained by summation of the local lower bounds (4.4) established in the proof of Proposition 4.5 and proves the global lower bound (2.25) of Theorem 2.5:

Proposition 4.6 (Global lower bound). *We have*

$$\eta \leq C_{\text{low}} \| \|u - u_h\| \|_{1,k,\Omega} + C(\kappa) \text{osc}(f, g),$$

where

$$C_{\text{low}} := (d+1) \max_{\mathbf{a} \in \mathcal{V}_h} C_{\text{st},\mathbf{a}} C_{\text{lb},\mathbf{a}}.$$

Remark 4.7 (Computable lower bound). *Lemma 3.7 shows that $C_{\text{lb},\mathbf{a}} \leq C_{\text{lb},\text{hat},\mathbf{a}}$, where $C_{\text{lb},\text{hat},\mathbf{a}}$ is a fully computable constant. Since we can compute an upper bound for $C_{\text{st},\mathbf{a}}$, see [29, Lemma 3.23], we are able to provide a fully computable lower bound for the error.*

5. PRE-ASYMPTOTIC ERROR ESTIMATES

In this section, we establish the results stated in Theorem 2.6. We will only detail the proof for Case 1a) and 1b), as the other cases (related to the interior problem) easily follow from standard properties of spectral decomposition and the regularity shift

$$|\phi|_{2,\Omega} \leq \| \Delta \phi \|_{0,\Omega},$$

for all $\phi \in H_0^1(\Omega)$ with $\Delta \phi \in L^2(\Omega)$, which is valid when Ω a convex polytope, see [32] for instance. The aim of this section is thus to prove the bounds (2.28) and (2.29) of Theorem 2.6.

5.1. **A stability estimate in $L^2(\Omega)$.** Under the assumptions of Case 1a) or 1b), the cornerstone of the analysis is a stability estimate that we establish hereafter. Similar upper bounds are available in [33, 41] for the setting considered here, and we refer the reader to [12, 13, 50] for more complex geometries. However, these estimates are not as sharp as possible and/or the constant $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0)$ is not computable, since they have been derived having a priori error estimation (or simply, stability analysis) in mind. We provide here sharper, fully-computable estimates.

Lemma 5.1 ($L^2(\Omega)$ stability estimate). *Let $\Omega = \Omega_0 \setminus \overline{D}$, $\Gamma_A = \partial\Omega_0$, and $\Gamma_D = \partial D$, where $\Omega_0, D \subset \mathbb{R}^d$ are two open, bounded, and connected sets such that \overline{D} is a proper subset of Ω_0 . Assume that the subset $\mathcal{O}_{\Gamma_D, \Gamma_A}$ defined in (2.26) is nonempty. For all $\phi \in L^2(\Omega)$, let the (adjoint) solution $u_\phi^* \in H_{\Gamma_D}^1(\Omega)$ solve (2.8), i.e., $b(w, u_\phi^*) = (w, \phi)$ for all $w \in H_{\Gamma_D}^1(\Omega)$. Then, we have*

$$(5.1) \quad k^2 \|u_\phi^*\|_{0, \Omega} \leq \left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) kh_\Omega \right) \|\phi\|_{0, \Omega},$$

with $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D)$ is defined in (2.27).

Proof. Let $\mathbf{x}_0 \in \mathcal{O}_{\Gamma_D, \Gamma_A}$, i.e., we have

$$(\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n} \leq 0 \quad \forall \mathbf{x} \in \Gamma_D \quad (\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n} > 0 \quad \forall \mathbf{x} \in \Gamma_A.$$

Let us set $\mathbf{y}(\mathbf{x}) := \mathbf{x} - \mathbf{x}_0$, $\mathbf{y}_\tau := \mathbf{y} - (\mathbf{y} \cdot \mathbf{n})\mathbf{n}$, $\nabla_\tau u_\phi^* := \nabla u_\phi^* - (\nabla u_\phi^* \cdot \mathbf{n})\mathbf{n}$. In strong form, the (adjoint) solution u_ϕ^* is such that

$$\begin{cases} -k^2 u_\phi^* - \Delta u_\phi^* &= \phi & \text{in } \Omega, \\ u_\phi^* &= 0 & \text{on } \Gamma_D, \\ \nabla u_\phi^* \cdot \mathbf{n} + ik u_\phi^* &= 0 & \text{on } \Gamma_A. \end{cases}$$

The key idea of the proof is to multiply the first equation by the test function $\overline{w} := \mathbf{y} \cdot \nabla \overline{u_\phi^*}$ and employ integration by parts techniques. Let us point out that since Ω is a polytopal domain and Γ_D and Γ_A are well separated, we have $u_\phi^* \in H^{\frac{3}{2}+\varepsilon}(\Omega)$ for some $\varepsilon > 0$, and therefore u_ϕ^* and w are sufficiently smooth to allow the operations performed hereafter (see in particular Section 3.3 of [33]).

First, applying Green's formula, we have

$$2 \operatorname{Re} \left\{ -k^2 \int_\Omega u_\phi^* (\mathbf{y} \cdot \nabla \overline{u_\phi^*}) \right\} = -k^2 \int_\Omega \mathbf{y} \cdot \nabla |u_\phi^*|^2 = dk^2 \|u_\phi^*\|_{0, \Omega}^2 - k^2 \int_{\partial\Omega} |u_\phi^*|^2 \mathbf{y} \cdot \mathbf{n},$$

where we used the fact that $\nabla \cdot \mathbf{y} = d$. Recalling Rellich's identity

$$2 \operatorname{Re} \left\{ \int_\Omega \nabla (\mathbf{y} \cdot \nabla \overline{u_\phi^*}) \cdot \nabla u_\phi^* \right\} = -(d-2) \|u_\phi^*\|_{1, \Omega}^2 + \int_{\partial\Omega} |\nabla u_\phi^*|^2 \mathbf{y} \cdot \mathbf{n},$$

which can be obtained by integration by parts (see [33, proof of Proposition 3.3] for instance), we have

$$\begin{aligned} & 2 \operatorname{Re} \left\{ - \int_{\Omega} \Delta u_{\phi}^* \mathbf{y} \cdot \nabla \overline{u_{\phi}^*} \right\} \\ &= 2 \operatorname{Re} \int_{\Omega} \nabla u_{\phi}^* \cdot \nabla (\mathbf{y} \cdot \nabla \overline{u_{\phi}^*}) - 2 \operatorname{Re} \int_{\Omega} (\nabla u_{\phi}^* \cdot \mathbf{n}) \mathbf{y} \cdot \nabla \overline{u_{\phi}^*} \\ &= -(d-2) |u_{\phi}^*|_{1,\Omega}^2 + \int_{\partial\Omega} |\nabla u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} - 2 \operatorname{Re} \int_{\partial\Omega} (\nabla u_{\phi}^* \cdot \mathbf{n}) \mathbf{y} \cdot \nabla \overline{u_{\phi}^*}. \end{aligned}$$

It follows that

$$\begin{aligned} 2 \operatorname{Re} \int_{\Omega} \phi \mathbf{y} \cdot \nabla \overline{u_{\phi}^*} &= 2 \operatorname{Re} \int_{\Omega} (-k^2 u_{\phi}^* - \Delta u_{\phi}^*) \mathbf{y} \cdot \nabla \overline{u_{\phi}^*} \\ &= dk^2 \|u_{\phi}^*\|_{0,\Omega}^2 - (d-2) |u_{\phi}^*|_{1,\Omega}^2 \\ &\quad - k^2 \int_{\partial\Omega} |u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} + \int_{\partial\Omega} |\nabla u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} - 2 \operatorname{Re} \int_{\partial\Omega} (\nabla u_{\phi}^* \cdot \mathbf{n}) \mathbf{y} \cdot \nabla \overline{u_{\phi}^*}. \end{aligned}$$

We now simplify the boundary term as

$$\begin{aligned} \mathcal{B} &:= \int_{\partial\Omega} |\nabla u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} - 2 \operatorname{Re} \int_{\partial\Omega} (\nabla u_{\phi}^* \cdot \mathbf{n}) \mathbf{y} \cdot \nabla \overline{u_{\phi}^*} \\ &= \int_{\partial\Omega} |\nabla_{\tau} u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} - \int_{\partial\Omega} |\nabla u_{\phi}^* \cdot \mathbf{n}|^2 \mathbf{y} \cdot \mathbf{n} - 2 \operatorname{Re} \int_{\partial\Omega} (\nabla u_{\phi}^* \cdot \mathbf{n}) \mathbf{y}_{\tau} \cdot \nabla_{\tau} \overline{u_{\phi}^*} \\ &= \int_{\Gamma_A} |\nabla_{\tau} u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} - \int_{\Gamma_D} |\nabla u_{\phi}^* \cdot \mathbf{n}|^2 \mathbf{y} \cdot \mathbf{n} - \int_{\Gamma_A} |iku_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} + 2 \operatorname{Re} \left\{ \int_{\Gamma_A} iku_{\phi}^* \mathbf{y}_{\tau} \cdot \nabla_{\tau} \overline{u_{\phi}^*} \right\} \\ &\geq \int_{\Gamma_A} |\nabla_{\tau} u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} - k^2 \int_{\Gamma_A} |u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} + 2 \operatorname{Re} \left\{ \int_{\Gamma_A} iku_{\phi}^* \mathbf{y}_{\tau} \cdot \nabla_{\tau} \overline{u_{\phi}^*} \right\}, \end{aligned}$$

where we used the facts that $\nabla_{\tau} u_{\phi}^* = \mathbf{0}$ on Γ_D , $\nabla u_{\phi}^* \cdot \mathbf{n} = -iku_{\phi}^*$ on Γ_A , and $\mathbf{y} \cdot \mathbf{n} \leq 0$ on Γ_D . We now have

$$\begin{aligned} 2 \operatorname{Re} \int_{\Omega} \phi \mathbf{y} \cdot \nabla \overline{u_{\phi}^*} &\geq dk^2 \|u_{\phi}^*\|_{0,\Omega}^2 + \int_{\Gamma_A} |\nabla_{\tau} u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} - (d-2) |u_{\phi}^*|_{1,\Omega}^2 \\ &\quad - 2k^2 \int_{\Gamma_A} |u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} + 2 \operatorname{Re} \int_{\Gamma_A} iku_{\phi}^* \mathbf{y}_{\tau} \cdot \nabla_{\tau} \overline{u_{\phi}^*}, \end{aligned}$$

that we can rewrite as

$$\begin{aligned} & dk^2 \|u_{\phi}^*\|_{0,\Omega}^2 + \int_{\Gamma_A} |\nabla_{\tau} u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} \\ &\leq 2 \operatorname{Re} \int_{\Omega} \phi \mathbf{y} \cdot \nabla \overline{u_{\phi}^*} + (d-2) |u_{\phi}^*|_{1,\Omega}^2 + 2k^2 \int_{\Gamma_A} |u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} + 2 \operatorname{Re} ik \left\{ \int_{\Gamma_A} u_{\phi}^* \mathbf{y}_{\tau} \cdot \nabla_{\tau} \overline{u_{\phi}^*} \right\} \\ &\leq 2 \operatorname{Re}(\phi, \mathbf{y} \cdot \nabla u_{\phi}^*) + (d-2) |u_{\phi}^*|_{1,\Omega}^2 + 2k^2 \int_{\Gamma_A} |u_{\phi}^*|^2 \mathbf{y} \cdot \mathbf{n} + 2k \int_{\Gamma_A} |u_{\phi}^*| |\nabla_{\tau} u_{\phi}^*| |\mathbf{y}_{\tau}|. \end{aligned}$$

At this point, since $\mathbf{y} \cdot \mathbf{n} > 0$ on Γ_A , we use the inequality

$$\begin{aligned} 2k|u_\phi^*| |\nabla_\tau u_\phi^*| |\mathbf{y}_\tau| &= 2k|u_\phi^*| |\nabla_\tau u_\phi^*| |\mathbf{y} \times \mathbf{n}| \\ &= 2 \left(k \frac{|\mathbf{y} \times \mathbf{n}|}{\sqrt{\mathbf{y} \cdot \mathbf{n}}} |u_\phi^*| \right) (|\nabla_\tau u_\phi^*| \sqrt{\mathbf{y} \cdot \mathbf{n}}) \\ &\leq k^2 \frac{|\mathbf{y} \times \mathbf{n}|^2}{\mathbf{y} \cdot \mathbf{n}} |u_\phi^*|^2 + |\nabla_\tau u_\phi^*|^2 \mathbf{y} \cdot \mathbf{n}, \end{aligned}$$

and infer that

$$\begin{aligned} dk^2 \|u_\phi^*\|_{0,\Omega}^2 &\leq 2 \operatorname{Re}(\phi, \mathbf{y} \cdot \nabla u_\phi^*) + (d-2) |u_\phi^*|_{1,\Omega}^2 + k^2 \int_{\Gamma_A} \left(2\mathbf{y} \cdot \mathbf{n} + \frac{|\mathbf{y} \times \mathbf{n}|^2}{\mathbf{y} \cdot \mathbf{n}} \right) |u_\phi^*|^2 \\ &\leq 2\lambda(\mathbf{x}_0) \|\phi\|_{0,\Omega} |u_\phi^*|_{1,\Omega} + (d-2) |u_\phi^*|_{1,\Omega}^2 + k^2 \mu(\mathbf{x}_0) \|u_\phi^*\|_{0,\Gamma_A}^2 \\ &\leq \lambda(\mathbf{x}_0)^2 \|\phi\|_{0,\Omega}^2 + (d-1) |u_\phi^*|_{1,\Omega}^2 + k^2 \mu(\mathbf{x}_0) \|u_\phi^*\|_{0,\Gamma_A}^2, \end{aligned}$$

where, recalling that $\mathbf{y} = \mathbf{x} - \mathbf{x}_0$, we have set

$$\lambda(\mathbf{x}_0) := \sup_{\mathbf{x} \in \Omega} |\mathbf{x} - \mathbf{x}_0|, \quad \mu(\mathbf{x}_0) := \sup_{\mathbf{x} \in \Gamma_A} \left(2(\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n} + \frac{|(\mathbf{x} - \mathbf{x}_0) \times \mathbf{n}|^2}{(\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{n}} \right).$$

Moreover, we have

$$|u_\phi^*|_{1,\Omega}^2 = \operatorname{Re} b(u_\phi^*, u_\phi^*) + k^2 \|u_\phi^*\|_{0,\Omega}^2 \leq \|\phi\|_{0,\Omega} \|u_\phi^*\|_{0,\Omega} + k^2 \|u_\phi^*\|_{0,\Omega}^2$$

and

$$k \|u_\phi^*\|_{0,\Gamma_A}^2 = -\operatorname{Im} b(u_\phi^*, u_\phi^*) \leq \|\phi\|_{0,\Omega} \|u_\phi^*\|_{0,\Omega}.$$

It follows that

$$k^2 \|u_\phi^*\|_{0,\Omega}^2 \leq \lambda(\mathbf{x}_0)^2 \|\phi\|_{0,\Omega}^2 + ((d-1) + k\mu(\mathbf{x}_0)) \|\phi\|_{0,\Omega} \|u_\phi^*\|_{0,\Omega}.$$

Lemma 3.2 with $a = k^2$, $b = (d-1) + k\mu(\mathbf{x}_0) \|\phi\|_{0,\Omega}$, and $c = \lambda(\mathbf{x}_0)^2 \|\phi\|_{0,\Omega}^2$ shows that

$$\begin{aligned} k^2 \|u_\phi^*\|_{0,\Omega} &\leq \left(\frac{(d-1) + k\mu(\mathbf{x}_0)}{2} + \sqrt{\left(\frac{(d-1) + k\mu(\mathbf{x}_0)}{2} \right)^2 + k^2 \lambda(\mathbf{x}_0)^2} \right) \|\phi\|_{0,\Omega} \\ &\leq ((d-1) + k(\lambda(\mathbf{x}_0) + \mu(\mathbf{x}_0))) \|\phi\|_{0,\Omega}. \end{aligned}$$

Then (5.1) follows since $C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) = \inf_{\mathbf{x}_0 \in \mathcal{O}_{\Gamma_D, \Gamma_A}} (1/h_\Omega)(\lambda(\mathbf{x}_0) + \mu(\mathbf{x}_0))$. \square

5.2. A bound on σ_{ba} for scattering by a non-trapping obstacle (Case 1a). We prove the bound (2.28) from Theorem 2.6. Observe first that

$$(5.2) \quad \sigma_{\text{ba}} = k \sup_{\phi \in L^2(\Omega) \setminus \{0\}} \inf_{v_h \in V_h} \frac{|u_\phi^* - v_h|_{1,\Omega}}{\|\phi\|_{0,\Omega}} \leq k \sup_{\phi \in L^2(\Omega) \setminus \{0\}} \frac{|u_\phi^*|_{1,\Omega}}{\|\phi\|_{0,\Omega}}.$$

Then, we consider an arbitrary $\phi \in L^2(\Omega)$ and the associated solution $u_\phi^* \in H_{\Gamma_D}^1(\Omega)$. Selecting the test function $v = u_\phi^*$ in (2.8) and considering the real part of the equality, we see that

$$|u_\phi^*|_{1,\Omega}^2 = \operatorname{Re}(\phi, u_\phi^*) + k^2 \|u_\phi^*\|_{0,\Omega}^2.$$

Hence, employing (5.1), we have

$$\begin{aligned} k^2 |u_\phi^*|_{1,\Omega}^2 &\leq \frac{k^2}{2\varepsilon} \|\phi\|_{0,\Omega}^2 + \frac{\varepsilon}{2k^2} k^4 \|u_\phi^*\|_{0,\Omega}^2 + k^4 \|u_\phi^*\|_{0,\Omega}^2 \\ &\leq \left(F(\varepsilon) + \left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0) kh_\Omega \right)^2 \right) \|\phi\|_{0,\Omega}^2 \end{aligned}$$

for all $\varepsilon > 0$ with

$$F(\varepsilon) = \frac{k^2}{2\varepsilon} + \frac{\varepsilon}{2k^2} \left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0) kh_\Omega \right)^2.$$

Then, considering the equation $F'(\varepsilon) = 0$, we see that the minimum of F is achieved for

$$\varepsilon_\star = \frac{k^2}{(d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0) kh_\Omega},$$

and

$$F(\varepsilon_\star) = \left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0) kh_\Omega \right).$$

We thus obtain that

$$k^2 |u_\phi^*|_{1,\Omega}^2 \leq \left\{ \left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0) kh_\Omega \right) + \left((d-1) + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D, \mathbf{x}_0) kh_\Omega \right)^2 \right\} \|\phi\|_{0,\Omega}^2,$$

for all $\phi \in L^2(\Omega)$, and (2.28) follows from (5.2).

5.3. A bound on σ_{ba} for wave propagation in free space (Case 1b). We prove here the estimate (2.29) of Theorem 2.6. We thus consider the case where $\Gamma_D = \emptyset$ and Ω is convex. In this case (see [15]), $u_\phi^* \in H^2(\Omega)$. Using (2.30), we observe that

$$(5.3) \quad \sigma_{\text{ba}} = k \sup_{\phi \in L^2(\Omega) \setminus \{0\}} \inf_{v_h \in V_h} \frac{|u_\phi^* - v_h|_{1,\Omega}}{\|\phi\|_{0,\Omega}} \leq k C_i(\kappa) \frac{h}{p^\beta} \sup_{\phi \in L^2(\Omega) \setminus \{0\}} \frac{|u_\phi^*|_{2,\Omega}}{\|\phi\|_{0,\Omega}}.$$

We can view u_ϕ^* as the unique solution to

$$(\nabla v, \nabla u_\phi^*) - ik(v, u_\phi^*)_{\Gamma_A} = (v, \widetilde{f}) \quad \forall v \in H_{\Gamma_D}^1(\Omega),$$

with $\widetilde{f} = \phi + k^2 u_\phi^*$. Then, Theorem 3.2 of [15] states that $u_\phi^* \in H^2(\Omega)$ with

$$|u_\phi^*|_{2,\Omega} \leq \|\widetilde{f}\|_{0,\Omega}.$$

Then, (5.1) shows that

$$|u_\phi^*|_{2,\Omega} \leq \left(d + C_{\text{stab}}(\widehat{\Omega}, \widehat{\Gamma}_D) kh_\Omega \right) \|\phi\|_{0,\Omega},$$

and (2.29) follows from (5.3).

6. NUMERICAL EXPERIMENTS

We present here two numerical experiments illustrating Theorems 2.3, 2.5, and 2.6.

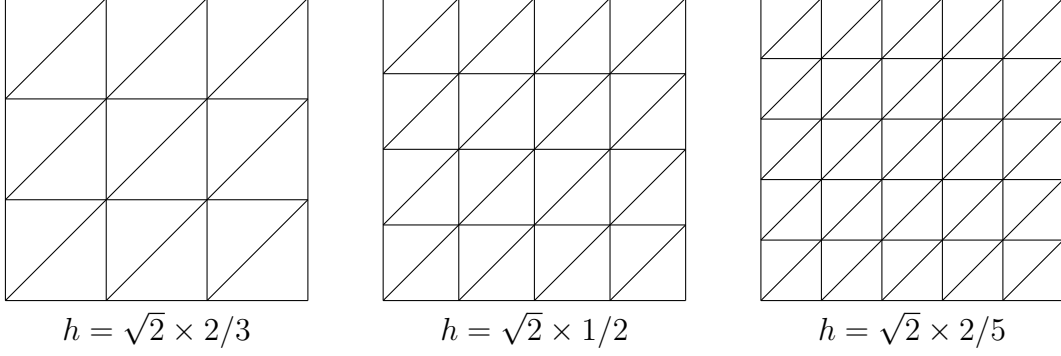


FIGURE 2. Cartesian meshes for the plane wave problem of Section 6.1

6.1. Plane wave in free space. We consider problem (1.1) in the square $\Omega = (-1, 1)^2$ with $\Gamma_D = \emptyset$ and $\Gamma_A = \partial\Omega$. We fix the angle $\nu := \pi/3$, set $\mathbf{d} := (\cos \nu, \sin \nu)$, and define the plane wave $\xi_\nu(\mathbf{x}) := e^{ik\mathbf{d}\cdot\mathbf{x}}$, $\mathbf{x} \in \bar{\Omega}$. We remark that ξ_ν is a homogeneous solution. The problem is thus to find u such that

$$(6.1) \quad \begin{cases} -k^2 u - \Delta u = 0 & \text{in } \Omega, \\ \nabla u \cdot \mathbf{n} - ik u = g & \text{on } \partial\Omega, \end{cases}$$

where $g = \nabla \xi_\nu \cdot \mathbf{n} - ik \xi_\nu$ on $\partial\Omega$. The unique solution is the plane wave $u = \xi_\nu$.

We consider different values of the wavenumber k . In each case, we discretize problem (6.1) with meshes based on Cartesian grids (see Figure 2) with different sizes h . For all meshes and wavenumbers, we compute the relative estimators

$$E_{\text{est}} := 100 \cdot \frac{\eta}{\|u\|_{1,k,\Omega}}, \quad \tilde{E}_{\text{est}} := c_{\text{up}} E_{\text{est}},$$

where, following (2.22) of Theorem 2.3 and (2.29) of Theorem 2.6 (here $d = 2$, $\beta = 0$)

$$(6.2) \quad c_{\text{up}} := \sqrt{\left(\frac{1}{2} + \sqrt{\frac{1}{4} + (c_{\text{ba}})^2}\right)^2 + \left(\frac{1}{2} + \sqrt{\frac{1}{4} + (c_{\text{ba}})^2}\right)^2 + (c_{\text{ba}})^2},$$

$$c_{\text{ba}} := c_i (2 + c_{\text{stab}} k h_\Omega) k h$$

with

$$h_\Omega = 2\sqrt{2}, \quad c_{\text{stab}} := \frac{3 + \sqrt{2}}{2\sqrt{2}}, \quad c_i := \frac{0.493}{\sqrt{2}},$$

see Remarks 2.7 and 2.8. \tilde{E}_{est} is the relative form of the guaranteed upper bound (2.21), where C_{up} is only taken as $\sqrt{2} + \tilde{\theta}_1(\sigma_{\text{ba}})$; E_{est} is the relative form of the constant-free equilibrated error estimator η without the prefactor c_{up} and is relevant in the asymptotical regime. Furthermore, as the analytical solution is known, we also introduce the relative errors

$$E_{\text{fem}} := 100 \cdot \frac{\|u - u_h\|_{1,k,\Omega}}{\|u\|_{1,k,\Omega}}, \quad E_{\text{ba}} := 100 \cdot \frac{\|u - \pi_h u\|_{1,k,\Omega}}{\|u\|_{1,k,\Omega}},$$

where the best approximation $\pi_h u \in V_h$ to u is numerically computed by solving

$$k^2(\pi_h u, v_h) + k(\pi_h u, v_h)_{\Gamma_A} + (\nabla(\pi_h u), \nabla v_h) = k^2(u, v_h) + k(u, v_h)_{\Gamma_A} + (\nabla u, \nabla v_h)$$

for all $v_h \in V_h$. The behavior of E_{fem} , E_{ba} , E_{est} , and \tilde{E}_{est} for polynomial degrees $p = 1, 2,$ and 4 is respectively presented in Figures 3, 4, and 5. In addition, Tables 1, 2, and 3 present the efficiency of the asymptotical and guaranteed relative estimators E_{est} and \tilde{E}_{est} (which coincide with those of η and $c_{\text{up}}\eta$).

We see that by either decreasing the mesh size h or increasing the polynomial degree p , the relative estimator E_{est} approaches the relative error E_{fem} , with the effectivity index tending to one. More precisely, E_{est} seems to approach rather rapidly the best approximation error E_{ba} , which itself behaves like the finite element error E_{fem} in the asymptotic regime $\sigma_{\text{ba}} \leq 1$ and tends to it for $\sigma_{\text{ba}} \rightarrow 0$. The asymptotical estimator E_{est} is efficient as long as there are sufficiently many degrees of freedom per wavelength, see (2.25); actually $E_{\text{est}} \leq E_{\text{fem}}$ in all the results presented. Unfortunately, E_{est} can severely underestimate E_{fem} ; moreover, this does not seem to be completely predictable, see in particular the column for $k = 60\pi$ in Table 2, where the effectivity index drops to 0.07 on a rather refined mesh. The corresponding curve is in the bottom-right panel of Figure 4. We see that the experiment with very low efficiency (3rd from the right) takes place in the resolved regime (after the best-approximation starts to converge) but before the asymptotic regime (where the best-approximation and the finite element error meet in the last experiment on the right). This highlights the fact that the asymptotical estimator cannot be trusted in the preasymptotic regime.

The relative estimator \tilde{E}_{est} introduced in this work indeed gives a guaranteed upper bound on the finite element error E_{fem} in all situations. Its effectivity index can reach high values but it decreases rather swiftly with mesh refinement for \mathcal{P}_1 elements, see Table 1. Unfortunately, we were not able to design the upper bound (2.29) on σ_{ba} to be sharp for $p > 1$: we only employ it with $\beta = 0$ which means that c_{ba} does not decrease with increasing p (cf. the optimal asymptotic behavior of σ_{ba} with respect to both h and p in (1.3)). Consequently, the effectivity indices of \tilde{E}_{est} are relatively poor for higher order elements in Tables 2 and 3, and, moreover, only improve with decreasing the mesh size h but not with increasing the polynomial degree p . We also see from Table 1 when $k = \pi$ that asymptotically, the effectivity index of the guaranteed estimator \tilde{E}_{est} is close to $\sqrt{2} \simeq 1.41$, which is in agreement with (2.22). Recall that theoretically, this is remedied by the use of the constant $1 + \tilde{\theta}_2(\sigma_{\text{ba}}, \tilde{\sigma}_{\text{ba}})$ in (2.23). In practice, however, we do not have a computable estimate on $\tilde{\sigma}_{\text{ba}}$.

6.2. Scattering by a non-trapping obstacle. We now consider the scattering of a plane wave by an obstacle. This problem consists in finding u such that

$$\begin{cases} -k^2 u - \Delta u = 0 & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \nabla u \cdot \mathbf{n} - iku = g & \text{on } \Gamma_A, \end{cases}$$

	$k = \pi$		$k = 4\pi$		$k = 10\pi$		$k = 20\pi$	
h	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$
$2\sqrt{2}/8$	0.78	7.38	0.36	45.55	0.28	219.62	0.16	502.52
$2\sqrt{2}/16$	0.94	4.80	0.27	17.18	0.36	137.48	0.21	314.17
$2\sqrt{2}/32$	1.01	3.01	0.31	10.07	0.30	57.24	0.35	265.17
$2\sqrt{2}/64$	1.02	2.05	0.52	8.48	0.19	18.42	0.29	112.57
$2\sqrt{2}/128$	1.03	1.64	0.77	6.65	0.20	9.84	0.19	36.61
$2\sqrt{2}/256$	1.03	1.51	0.94	4.43	0.36	8.89	0.12	11.60
$2\sqrt{2}/512$	1.03	1.47	1.01	2.81	0.61	7.79	0.19	9.27
$2\sqrt{2}/1024$	1.03	1.46	1.02	1.96	0.85	5.76	0.36	8.81
$2\sqrt{2}/2048$	1.03	1.46	1.03	1.61	0.97	3.70	0.61	7.76

TABLE 1. Effectivity indices of the asymptotical and guaranteed error estimators in the plane wave test case of Section 6.1 with \mathcal{P}_1 elements

	$k = 10\pi$		$k = 20\pi$		$k = 40\pi$		$k = 60\pi$	
h	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$
$2\sqrt{2}/32$	0.19	46.58	0.22	213.82	0.46	1753.21	0.12	1014.61
$2\sqrt{2}/64$	0.55	66.32	0.11	54.52	0.22	424.74	0.15	658.57
$2\sqrt{2}/128$	0.93	56.13	0.32	75.82	0.10	91.05	0.17	359.92
$2\sqrt{2}/256$	1.00	30.36	0.79	94.49	0.17	79.18	0.07	70.88
$2\sqrt{2}/512$	1.00	15.57	0.98	58.91	0.55	129.81	0.19	102.77
$2\sqrt{2}/1024$	1.00	8.12	1.00	30.30	0.93	111.08	0.61	162.98

TABLE 2. Effectivity indices of the asymptotical and guaranteed error estimators in the plane wave test case of Section 6.1 with \mathcal{P}_2 elements

	$k = 10\pi$		$k = 20\pi$		$k = 40\pi$		$k = 60\pi$	
h	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$	E_{est}	$\widetilde{E}_{\text{est}}$
$2\sqrt{2}/32$	0.95	227.91	0.24	224.79	0.10	376.03	0.30	2548.49
$2\sqrt{2}/64$	0.99	119.14	0.92	438.82	0.12	234.70	0.11	451.99
$2\sqrt{2}/128$	1.00	60.35	0.99	236.00	0.83	787.63	0.23	486.20
$2\sqrt{2}/256$	1.00	30.54	1.00	119.27	0.99	469.50	0.94	1000.73
$2\sqrt{2}/512$	1.00	15.58	1.00	60.06	1.00	237.14	1.00	530.32

TABLE 3. Effectivity indices of the asymptotical and guaranteed error estimators in the plane wave test case of Section 6.1 with \mathcal{P}_4 elements

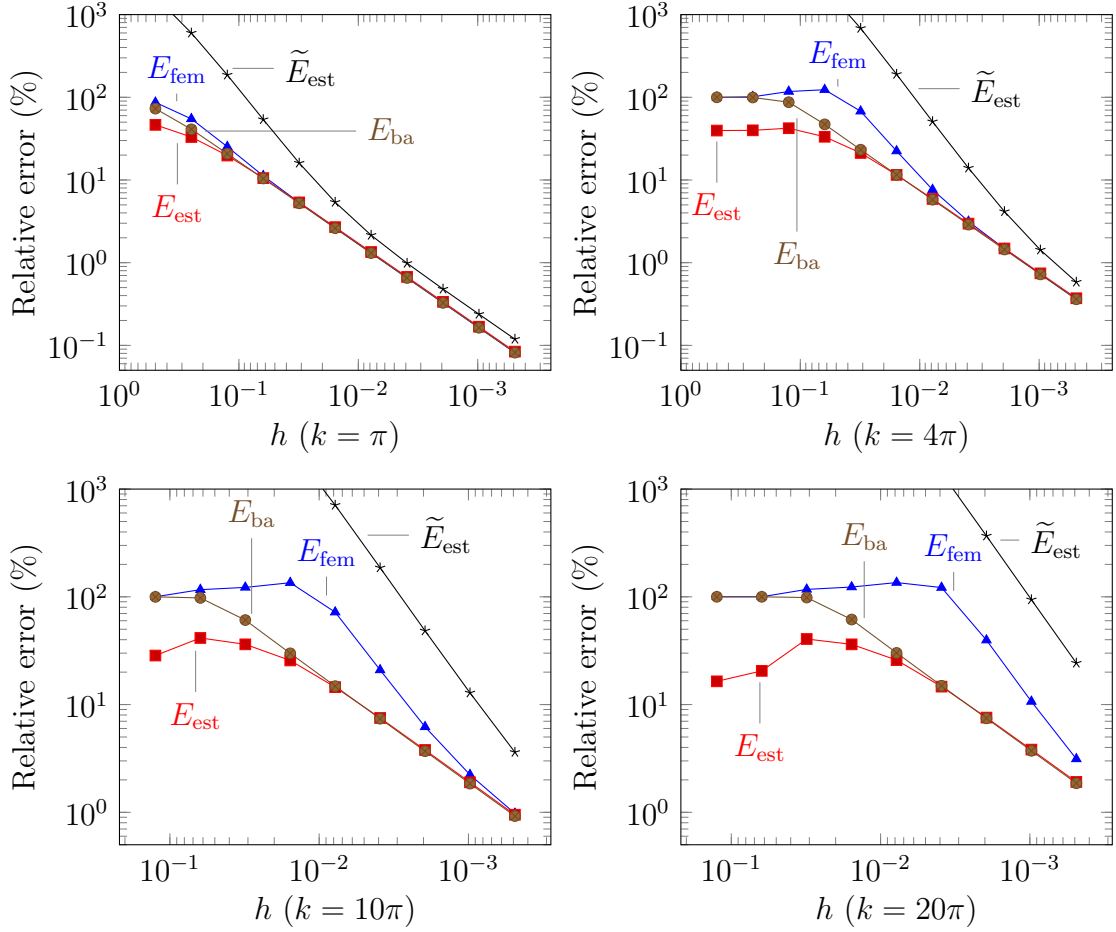


FIGURE 3. Behaviors of the estimated and analytical errors for the plane wave test case of Section 6.1 with \mathcal{P}_1 elements

where again $g = \nabla \xi_\nu \cdot \mathbf{n} - ik\xi_\nu$ with ξ_ν given in Section 6.1. The computational domain is constructed such that $\Omega = \Omega_0 \setminus \overline{D}$, $\Gamma_D = \partial D$, and $\Gamma_A = \partial\Omega_0$, where $\Omega_0 = (-1, 1)^2$ and

$$D = \left\{ \mathbf{x} \in \Omega \mid 2|\mathbf{x}_1| - \frac{1}{2} < \mathbf{x}_2 < |\mathbf{x}_1| \right\},$$

see the left panel of Figure 6. We see that we have $\mathbf{x} \cdot \mathbf{n} \leq 0$ on Γ_D and $\mathbf{x} \cdot \mathbf{n} > 0$ on Γ_A , so that this setting enters Case 1a) of Theorem 2.6 with $\mathbf{x}_0 = (0, 0)$.

We select the wavenumbers $k = 2\pi$ and 10π and employ polynomials of degree $p = 1, 2$, and 3 . As the analytical solution of the problem is not available, we employ an accurate numerical solution as a reference. Specifically, for each mesh \mathcal{T}_h , we employ the approximation $u \simeq \tilde{u}_h$ for the comparison, where \tilde{u}_h is computed using the mesh \mathcal{T}_h with \mathcal{P}_6 finite elements.

We consider a simple procedure based on the software platform `mmg` [26] in order to generate unstructured adaptive meshes. We start with the initial mesh depicted in the right

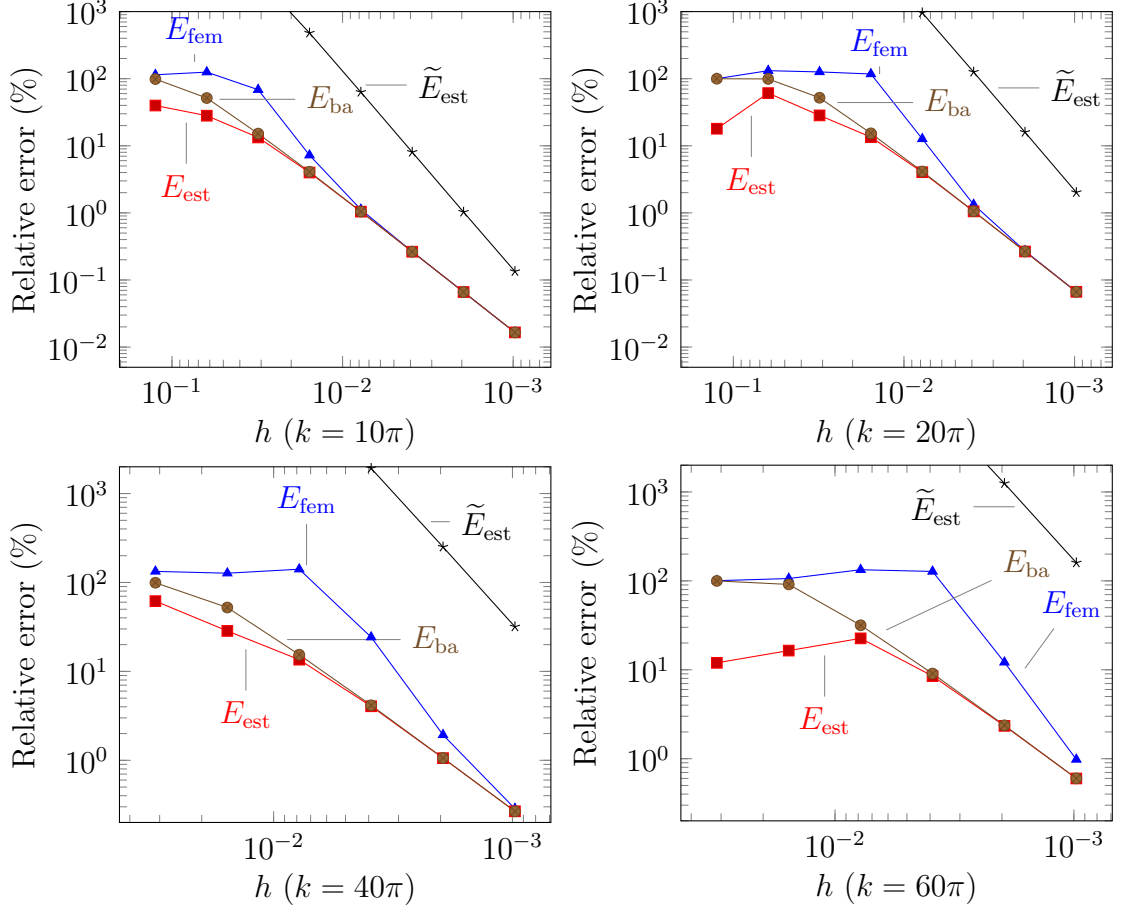


FIGURE 4. Behaviors of the estimated and analytical errors for the plane wave test case of Section 6.1 with \mathcal{P}_2 elements

panel of Figure 6. The software `mmg` allows one to impose a map of maximal allowed mesh sizes (or metric). This map is specified by defining values on the vertices of a previously introduced mesh. Thus, at each iteration, after solving the problem on the mesh \mathcal{T}_h and computing the corresponding estimators η_K , we produce a metric to generate the mesh of the next iteration. We start by defining a new maximal mesh size h_K^* for each element. This is done by sorting the elements in decreasing values of η_K , setting $h_K^* := h_K/2$ for the $|\mathcal{T}_h|/10$ first elements, and defining $h_K^* := 1.1h_K$ for the last $|\mathcal{T}_h|/10$ elements (we set $h_K^* = h_K$ for the remaining elements). Then, the maximal mesh size value at the vertex $\mathbf{a} \in \mathcal{V}_h$ is specified as $h_{\mathbf{a}}^* := \min_{K \in \mathcal{T}_h^{\mathbf{a}}} h_K^*$. Examples of meshes produced by this algorithm can be seen in Figure 9. We point out that the object of our study is not to analyze the performance of this very simple adaptive algorithm (actually, we start with an initial mesh that is already adapted), but only to analyze the performance of the estimator on a prototypical family of adaptive meshes.

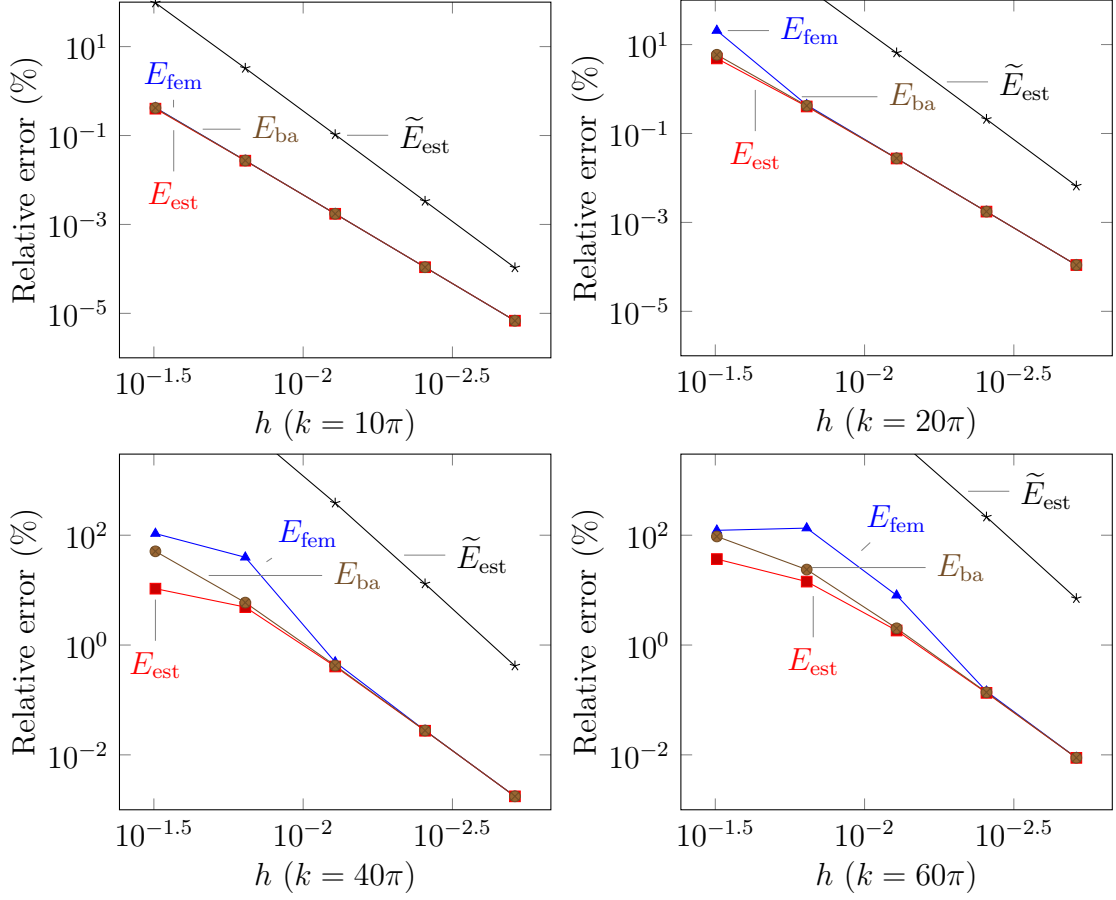


FIGURE 5. Behaviors of the estimated and analytical errors for the plane wave test case of Section 6.1 with \mathcal{P}_4 elements

Figures 7 and 8 represent the relative analytical and estimated errors

$$E_{\text{fem}} := 100 \cdot \frac{\|\tilde{u}_h - u_h\|_{1,k,\Omega}}{\|\tilde{u}_h\|_{1,k,\Omega}}, \quad E_{\text{est}} := 100 \cdot \frac{\eta}{\|\tilde{u}_h\|_{1,k,\Omega}}$$

in the different stages of the adaptive procedure for both $k = 2\pi$ and $k = 10\pi$ and for all \mathcal{P}_1 , \mathcal{P}_2 , and \mathcal{P}_3 elements. All the observations made in the example of Section 6.1 still hold true here, even though the meshes are now unstructured and feature elements of significantly different sizes. The relative estimators E_{est} are in particular a much better match to the approximate relative errors E_{fem} for \mathcal{P}_3 elements than for \mathcal{P}_1 and \mathcal{P}_2 elements in the $k = 10\pi$ case.

Following (2.22) in Theorem 2.3, Case 1a) of Theorem 2.6, and Remark 2.7, we can also define

$$\tilde{E}_{\text{est}} := c_{\text{up}} E_{\text{est}}$$

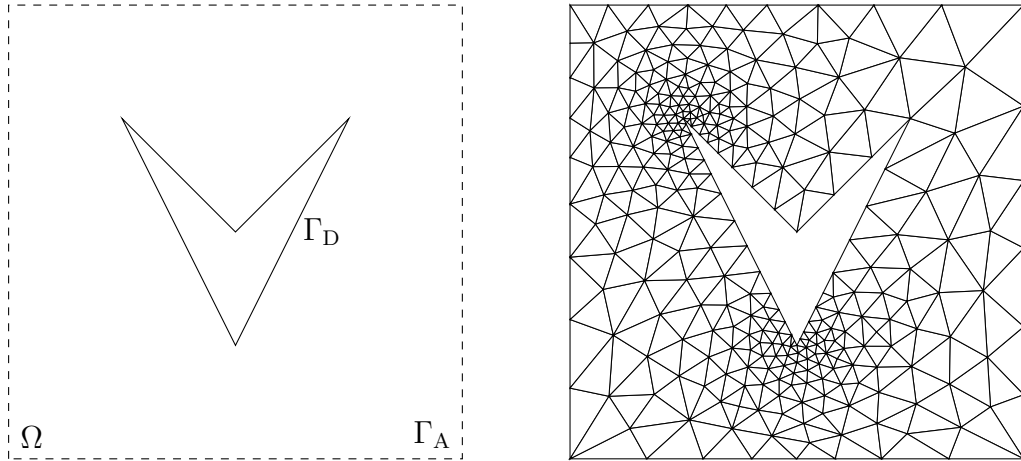


FIGURE 6. Scattering problem of Section 6.2: domain settings (left) and the initial mesh (right)

with c_{up} given by (6.2) and

$$c_{\text{ba}} := \left((1 + c_{\text{stab}} k h_{\Omega}) + (1 + c_{\text{stab}} k h_{\Omega})^2 \right)^{\frac{1}{2}}, \quad c_{\text{stab}} := \frac{3 + \sqrt{2}}{2\sqrt{2}}, \quad h_{\Omega} = 2\sqrt{2},$$

where we have employed the point $\mathbf{x}_0 = \mathbf{0}$ in Remark 2.7. We remark that here c_{up} only depends on k and does not improve with the mesh size h (nor with the polynomial degree p). We compute $c_{\text{up}} = 42.05$ for $k = 2\pi$, and $c_{\text{up}} = 198.94$ for $k = 10\pi$. We observe that with this definition, \tilde{E}_{est} indeed constitutes a guaranteed upper bound for all meshes, wavenumbers, and polynomial degrees considered in this example. However, as the overestimation factor for E_{est} is about 1 asymptotically, the overestimation factor for \tilde{E}_{est} will be about 40 and 200 for $k = 2\pi$ and $k = 10\pi$, respectively, which might unfortunately be too large for being useful in applications.

Finally, Figure 9 depicts the local estimators η_K compared to the actual errors $e_K = \|\tilde{u}_h - u_h\|_{1,k,K}$ (evaluated using the reference numerical solution \tilde{u}_h) on a sequence of adapted meshes for $k = 10\pi$ and \mathcal{P}_3 elements. We see that the estimators η_K provide a very good representation of the error distribution, even if the wavenumber is relatively high and the mesh is unstructured, with a significant ratio between the largest and the smallest element sizes. This result illustrates the local efficiency of the proposed estimator as stated in (2.24). The solution corresponding to the finest mesh is depicted in Figure 10.

7. CONCLUSIONS

We have proposed a novel a posteriori estimator for the Helmholtz problem with mixed boundary conditions in two and three space dimensions. The estimator is based on equilibrated flux reconstruction that relies on the solution of patchwise mixed finite element problems. We have shown that our estimator is locally efficient and p -robust in the resolved

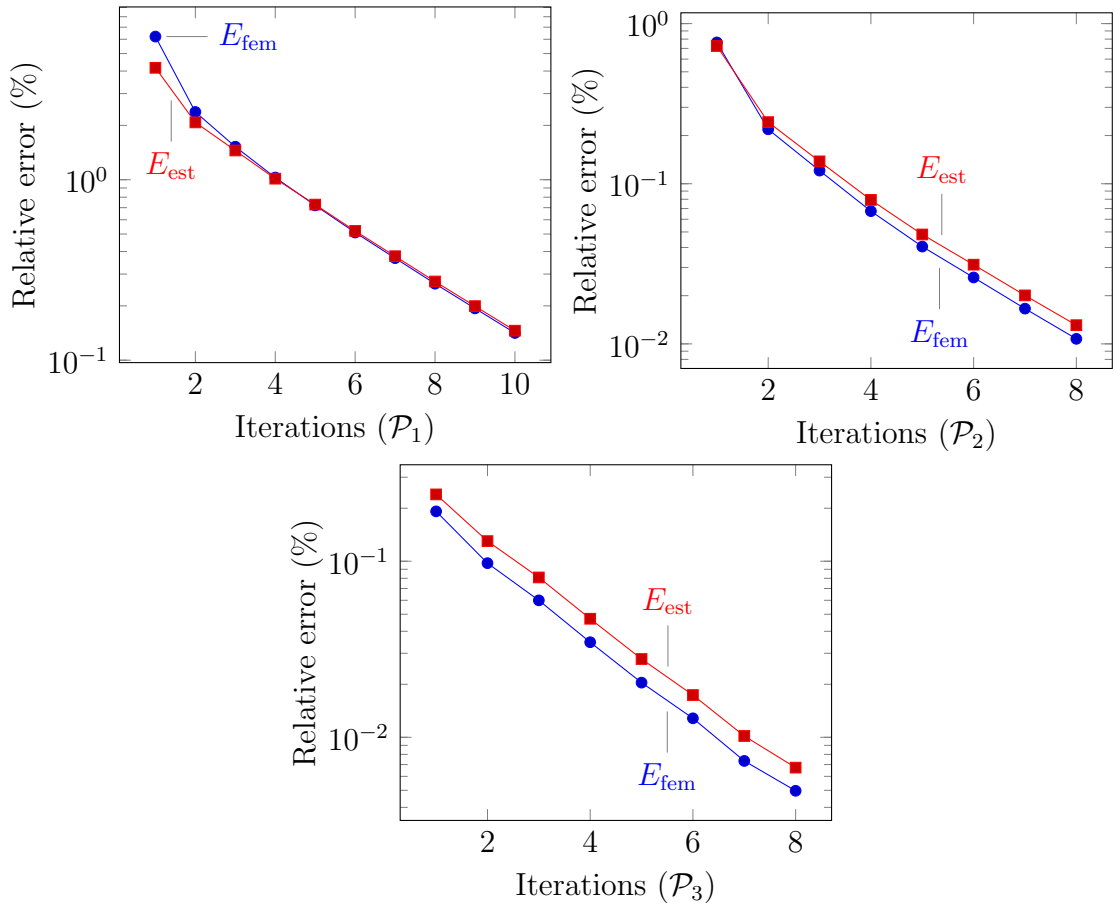


FIGURE 7. Behaviors of the estimated and analytical errors in the adaptive procedure for the scattering problem of Section 6.2 with $k = 2\pi$

regime where $\frac{kh}{p}$ is sufficiently small. The proposed estimator is also reliable, and the upper bound contains the (in general unknown) approximation factors σ_{ba} and/or $\tilde{\sigma}_{ba}$. We have shown that asymptotically, $\sigma_{ba}, \tilde{\sigma}_{ba} \rightarrow 0$, so that our upper bound becomes unknown-constant-free in the limit. In addition, we have demonstrated that the conditions of “ σ_{ba} and $\tilde{\sigma}_{ba}$ being small” correspond to the asymptotic regime in which the finite element solution is quasi-optimal. Hence, the proposed estimator is locally efficient, p -robust, and unknown-constant-free in the asymptotic regime.

In addition, we have provided computable upper bounds for σ_{ba} in particular settings of interest, including scattering by non-trapping obstacles and wave propagation in free space. For such configurations, our upper bounds thus additionally become guaranteed and fully computable with no unknown constant and no assumptions on the mesh size, the polynomial degree, or the wavenumber, though an important overestimation can appear in particular on rough meshes. The presented numerical experiments illustrate our findings and suggest that the proposed estimators are additionally asymptotically exact.

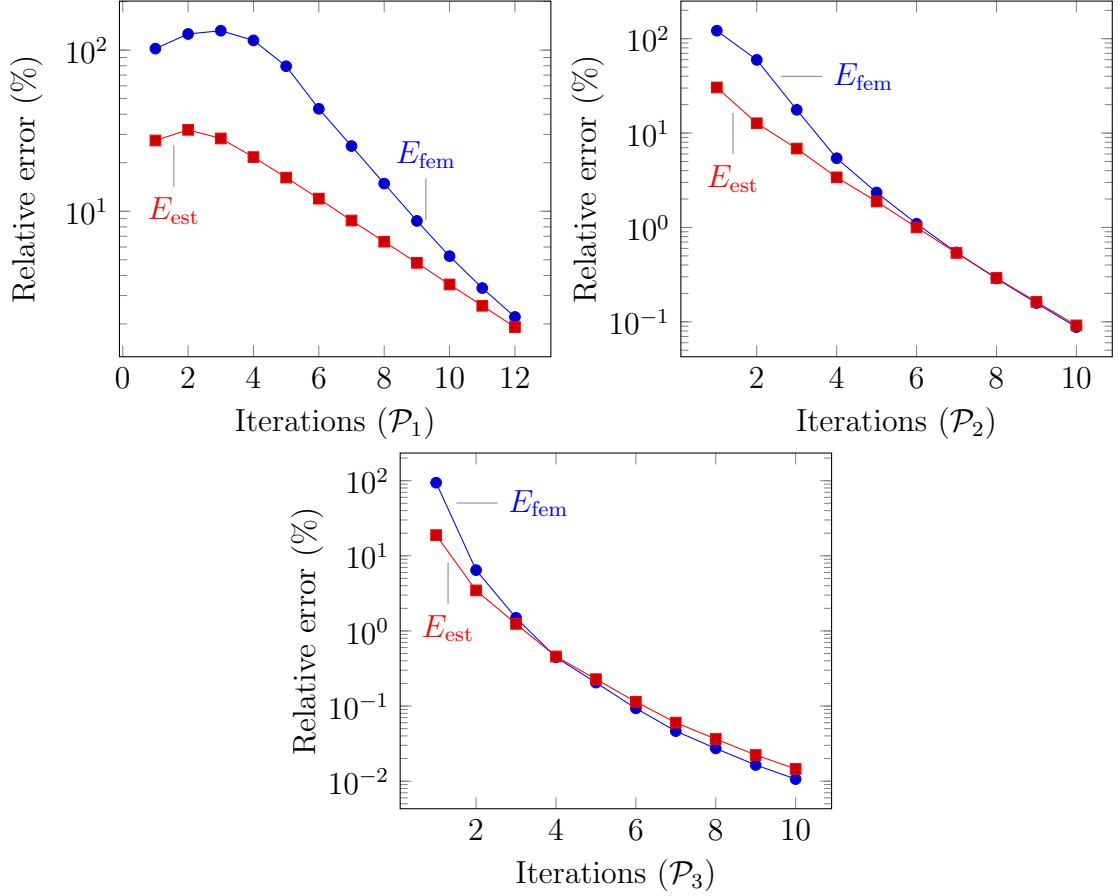


FIGURE 8. Behaviors of the estimated and analytical errors in the adaptive procedure for the scattering problem of Section 6.2 with $k = 10\pi$

APPENDIX A. ESTIMATE ON THE BEST-APPROXIMATION CONSTANT FOR BOUNDARY DATA

In this appendix, we analyze the behavior of the quantity $\tilde{\sigma}_{ba}$ defined in (2.10) in terms of σ_{ba} defined in (2.7). For the sake of simplicity, in this section, the notation $C(\hat{\Omega}, \hat{\Gamma}_D)$ denotes a generic constant that only depends on the geometry of Ω and Γ_D but may vary from one occurrence to the other. In addition $C_{qi}(\kappa)$ is a “quasi-interpolation” constant that only depends on the mesh shape-regularity parameter κ [34, 42].

The results derived in this appendix rely on the following regularity assumption.

Assumption A.1 (Additional regularity). *Let $\phi \in L^2(\Omega)$. We assume that if $u \in H^1(\Omega)$ satisfies*

$$\begin{cases} -\Delta u = \phi & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \nabla u \cdot \mathbf{n} = 0 & \text{on } \Gamma_A, \end{cases}$$

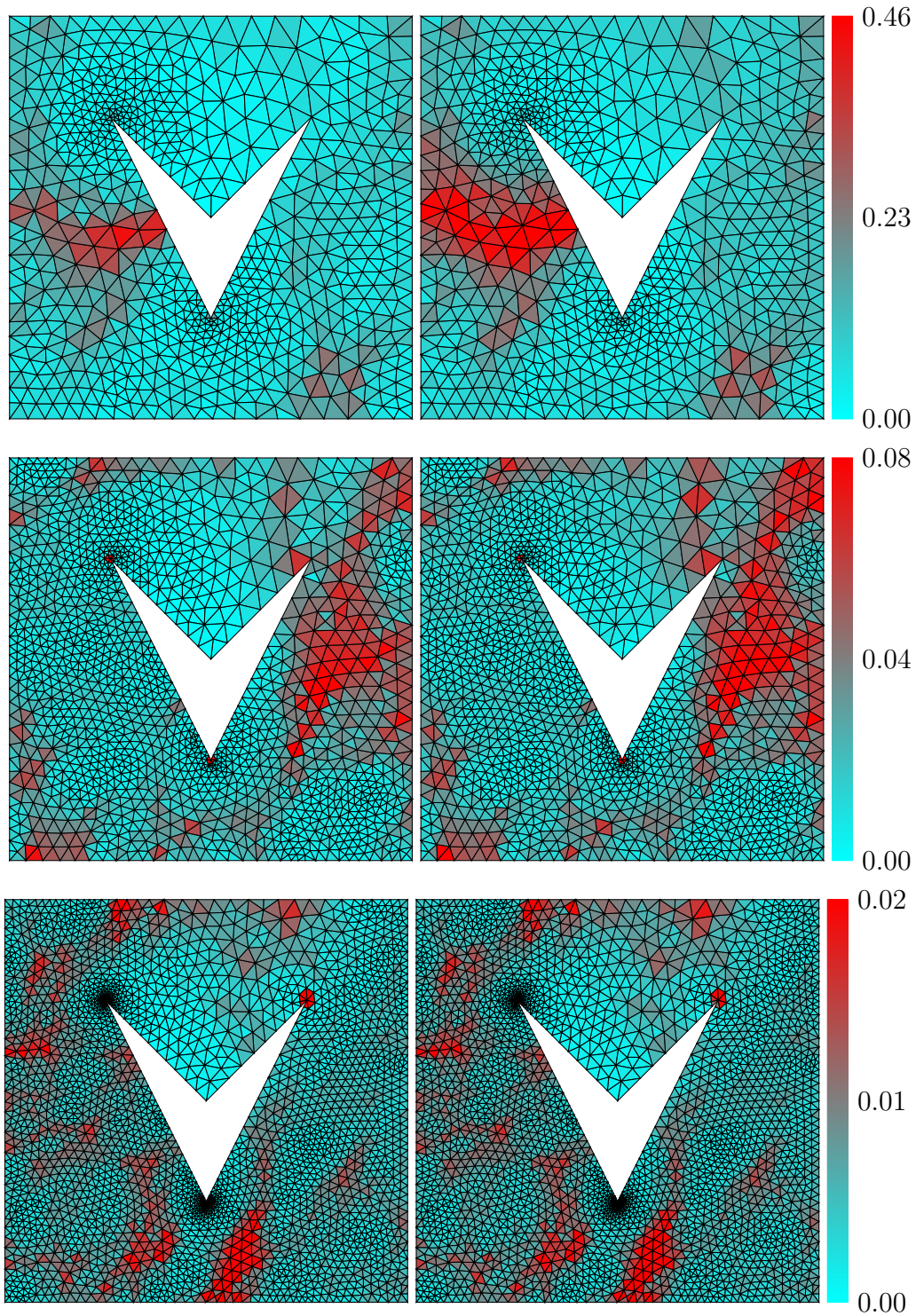


FIGURE 9. Estimators η_K (left) and elementwise errors $\|\tilde{u}_h - u_h\|_{1,k,K}$ (right) for the scattering problem of Section 6.2 for $k = 10\pi$ with \mathcal{P}_3 elements

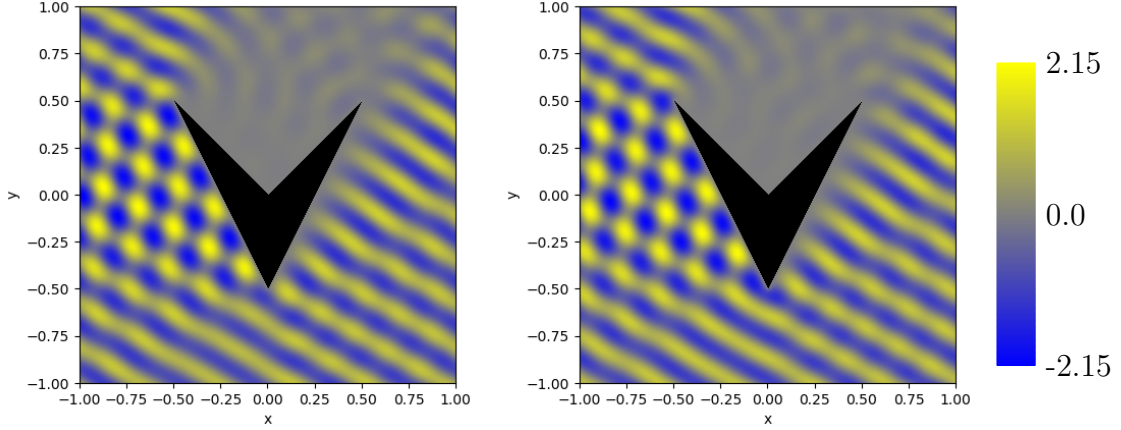


FIGURE 10. Scattering problem of Section 6.2: real (left) and imaginary (right) parts of the solution for $k = 10\pi$ with \mathcal{P}_6 elements

then $u \in H^2(\tilde{\Omega})$ with

$$|u|_{2,\tilde{\Omega}} \leq C(\hat{\Omega}, \hat{\Gamma}_D) \|\phi\|_{0,\Omega},$$

where $\tilde{\Omega} \subset \Omega$ is a neighborhood of Γ_A (i.e., $\tilde{\Omega}$ is an open subset of Ω and Γ_A is a subset of the closure of $\tilde{\Omega}$) and the constant $C(\hat{\Omega}, \hat{\Gamma}_D)$ depends on the shape of Ω and the splitting of its boundary into Γ_D and Γ_A but not on its diameter h_Ω . Furthermore, we assume that if $\psi \in L^2(\Gamma_A)$ and $u \in H^1(\Omega)$ solves

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \nabla u \cdot \mathbf{n} = \psi & \text{on } \Gamma_A, \end{cases}$$

then $u \in H^{\frac{3}{2}}(\tilde{\Omega})$ with

$$|u|_{\frac{3}{2},\tilde{\Omega}} \leq C(\hat{\Omega}, \hat{\Gamma}_D) \|\psi\|_{0,\Gamma_A}.$$

Assumption A.1 is not an important restriction. Indeed, it is typically satisfied in applications, as the boundary Γ_A is artificially designed to enclose the region of interest. For instance, Γ_A is usually selected as the boundary of a convex polytope for scattering problems, so that Assumption A.1 holds (see [15] and [21, Lemma 1]). In the case of cavity problems, Γ_A is typically planar, and Assumption A.1 holds if the solid angle between Γ_A and Γ_D is less than or equal to $\pi/2$ (we can perform an odd reflexion across the Dirichlet boundary, and recover a situation similar to the scattering problem, see [15]). As a result, Assumption A.1 is satisfied in all the configurations depicted in Figure 1.

Our next step is to devise a lifting operator \mathcal{L} that transforms the boundary right-hand side on Γ_A , say ψ , appearing in the definition (2.10) of $\tilde{\sigma}_{\text{ba}}$ into a volume right-hand side $\mathcal{L}\psi$. We remark that there exists a function $\chi \in C^\infty(\bar{\Omega})$ such that $0 \leq \chi \leq 1$ in $\bar{\Omega}$, $\chi = 0$ outside $\tilde{\Omega}$, and $\chi = 1$ in a neighborhood on Γ_A . In addition, a simple scaling argument

shows that we can choose χ such that

$$|\chi|_{j,\infty,\Omega} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) h_\Omega^{-j}$$

for all $j \in \mathbb{N}$.

Lemma A.2 (Boundary lifting operator). *Let Assumption A.1 hold. For all $\psi \in L^2(\Gamma_A)$, we define \mathcal{L}_ψ as the unique element of $H_{\Gamma_D}^1(\Omega)$ such that*

$$(A.1) \quad a(w, \mathcal{L}_\psi) = (w, \psi)_{\Gamma_A}$$

for all $w \in H_{\Gamma_D}^1(\Omega)$, where

$$a(w, \mathcal{L}_\psi) := k^2(w, \mathcal{L}_\psi) - ik(w, \mathcal{L}_\psi)_{\Gamma_A} + (\nabla w, \nabla \mathcal{L}_\psi).$$

Then we have

$$(A.2) \quad k \|\mathcal{L}_\psi\|_{0,\Gamma_A} \leq \|\psi\|_{0,\Gamma_A},$$

$$(A.3) \quad k^2 \|\mathcal{L}_\psi\|_{0,\Omega}^2 + |\mathcal{L}_\psi|_{1,\Omega}^2 \leq \frac{1}{k} \|\psi\|_{0,\Gamma_A}^2.$$

In addition, we have

$$(A.4) \quad k^{\frac{1}{2}} \inf_{v_h \in V_h} |\chi \mathcal{L}_\psi - v_h|_{1,\Omega} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) C_{\text{qi}}(\kappa) \left(\left(\frac{kh}{p} \right)^{\frac{1}{2}} + \frac{kh}{p} \right) \|\psi\|_{0,\Gamma_A},$$

where the last term is present only if Γ_D has positive surface measure.

Proof. We first pick $w = \mathcal{L}_\psi$ as a test function in (A.1). Taking the imaginary part yields

$$k \|\mathcal{L}_\psi\|_{0,\Gamma_A}^2 = -\text{Im}(\mathcal{L}_\psi, \psi)_{\Gamma_A} \leq \|\psi\|_{0,\Gamma_A} \|\mathcal{L}_\psi\|_{0,\Gamma_A},$$

and (A.2) follows. Now, we take the real part and use the above bound to obtain

$$k^2 \|\mathcal{L}_\psi\|_{0,\Omega}^2 + |\mathcal{L}_\psi|_{1,\Omega}^2 = \text{Re}(\mathcal{L}_\psi, \psi)_{\Gamma_A} \leq \frac{1}{k} \|\psi\|_{0,\Gamma_A}^2.$$

This yields (A.3). Finally, we observe that we can see \mathcal{L}_ψ as the unique element of $H_{\Gamma_D}^1(\Omega)$ such that

$$(\nabla w, \nabla \mathcal{L}_\psi) = -k^2(w, \mathcal{L}_\psi) + (w, \psi + ik\mathcal{L}_\psi)_{\Gamma_A}$$

for all $w \in H_{\Gamma_D}^1(\Omega)$.

At this point, we distinguish the case where Γ_D is of zero measure or not. If $|\Gamma_D| = 0$, then Assumption A.1 together with classical arguments (see [32]) away from Γ_A show that

$$\begin{aligned} \|\mathcal{L}_\psi\|_{\frac{3}{2},\Omega} &\leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \left(k^2 \|\mathcal{L}_\psi\|_{\frac{1}{2},\Omega} + \|\psi\|_{0,\Gamma_A} + k \|\mathcal{L}_\psi\|_{0,\Gamma_A} \right) \\ &\leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \left(k^2 \sqrt{\|\mathcal{L}_\psi\|_{0,\Omega} \|\mathcal{L}_\psi\|_{1,\Omega}} + \|\psi\|_{0,\Gamma_A} + k \|\mathcal{L}_\psi\|_{0,\Gamma_A} \right), \end{aligned}$$

and we conclude with (A.2) and (A.3) that

$$\|\chi \mathcal{L}_\psi\|_{\frac{3}{2},\Omega} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \|\mathcal{L}_\psi\|_{\frac{3}{2},\Omega} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \|\psi\|_{0,\Gamma_A}.$$

Then, (A.4) follows from standard approximation theory [34, 42].

On the other hand, when $|\Gamma_D| \neq 0$, we split $\mathcal{L}_\psi = \phi_2 + \phi_{\frac{3}{2}}$ where $\phi_2, \phi_{\frac{3}{2}} \in H_{\Gamma_D}^1(\Omega)$ are uniquely defined by

$$(\nabla w, \nabla \phi_2) = -k^2(w, \mathcal{L}_\psi), \quad (\nabla w, \nabla \phi_{\frac{3}{2}}) = (w, \psi + ik\mathcal{L}_\psi)_{\Gamma_A}$$

for all $w \in H_{\Gamma_D}^1(\Omega)$. Picking the test function $w = \phi_2$, it follows that

$$|\phi_2|_{1,\Omega}^2 \leq k^2 \|\mathcal{L}_\psi\|_{0,\Omega} \|\phi_2\|_{0,\Omega} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) k^{\frac{1}{2}} h_\Omega \|\psi\|_{0,\Gamma_A} |\phi_2|_{1,\Omega},$$

where we used the Poincaré inequality to handle $\|\phi_2\|_{0,\Omega}$ and (A.2) to estimate $k\|\mathcal{L}_\psi\|_{0,\Omega}$. Similarly, employing a multiplicative trace inequality which combined with the Poincaré inequality yields $\|\phi_{\frac{3}{2}}\|_{0,\Gamma_A} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) h_\Omega^{\frac{1}{2}} |\phi_{\frac{3}{2}}|_{1,\Omega}$, we infer that

$$|\phi_{\frac{3}{2}}|_{1,\Omega}^2 \leq \|\psi + ik\mathcal{L}_\psi\|_{0,\Gamma_A} \|\phi_{\frac{3}{2}}\|_{0,\Gamma_A} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) h_\Omega^{\frac{1}{2}} \|\psi\|_{0,\Gamma_A} |\phi_{\frac{3}{2}}|_{1,\Omega}.$$

Then, invoking Assumption A.1, we have

$$|\phi_2|_{2,\widetilde{\Omega}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) k^2 \|\mathcal{L}_\psi\|_{0,\Omega} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) k^{\frac{1}{2}} \|\psi\|_{0,\Gamma_A},$$

and

$$|\phi_{\frac{3}{2}}|_{\frac{3}{2},\widetilde{\Omega}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \|\psi + ik\mathcal{L}_\psi\|_{0,\Gamma_A} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \|\psi\|_{0,\Gamma_A}.$$

Thus, since $\text{supp } \chi \subset \widetilde{\Omega}$ and invoking once again the Poincaré inequality, we infer that

$$\begin{aligned} |\chi\phi_2|_{2,\Omega} &\leq \|\chi\|_{0,\Omega} |\phi_2|_{2,\widetilde{\Omega}} + |\chi|_{1,\Omega} |\phi_2|_{1,\Omega} + |\chi|_{2,\Omega} \|\phi_2\|_{0,\Omega} \\ &\leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \left(|\phi_2|_{2,\widetilde{\Omega}} + h_\Omega^{-1} |\phi_2|_{1,\Omega} \right) \\ &\leq C(\widehat{\Omega}, \widehat{\Gamma}_D) k^{\frac{1}{2}} \|\psi\|_{0,\Gamma_A}, \end{aligned}$$

and similar arguments show that

$$|\chi\phi_{\frac{3}{2}}|_{\frac{3}{2},\widetilde{\Omega}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) \|\psi\|_{0,\Gamma_A}.$$

At this point, (A.4) follows from standard approximation theory [34, 42]. \square

Having introduced our lifting operator, we are ready to establish the main result of this appendix which proves the claim (A.6).

Proposition A.3 (Bound on $\widetilde{\sigma}_{\text{ba}}$). *Let Assumption A.1 hold. Then*

$$\widetilde{\sigma}_{\text{ba}} \leq C(\widehat{\Omega}, \widehat{\Gamma}_D) C_{\text{qi}}(\kappa) \left(\left(\frac{kh}{p} \right)^{\frac{1}{2}} + \frac{kh}{p} \right) + \left(C(\widehat{\Omega}, \widehat{\Gamma}_D) \frac{1}{kh_\Omega} \left(1 + \frac{1}{kh_\Omega} \right) + 2 \right) \sigma_{\text{ba}}.$$

Proof. We consider an arbitrary element $\psi \in L^2(\Gamma_A)$ and define u_ψ^* as the unique element of $H_{\Gamma_D}^1(\Omega)$ such that $b(w, u_\psi^*) = (w, \psi)_{\Gamma_A}$ for all $w \in H_{\Gamma_D}^1(\Omega)$. Then, defining $\mathcal{L}_\psi \in H_{\Gamma_D}^1(\Omega)$

following Lemma A.2, we have

$$\begin{aligned}
& b(w, \chi \mathcal{L}_\psi) \\
&= -k^2(w, \chi \mathcal{L}_\psi) - ik(w, \chi \mathcal{L}_\psi)_{\Gamma_A} + (\nabla w, \nabla(\chi \mathcal{L}_\psi)) \\
&= k^2(\chi w, \mathcal{L}_\psi) - ik(\chi w, \mathcal{L}_\psi)_{\Gamma_A} + (\nabla(\chi w), \nabla \mathcal{L}_\psi) \\
&\quad + (\nabla w, \nabla(\chi \mathcal{L}_\psi)) - (\nabla(\chi w), \nabla \mathcal{L}_\psi) - 2k^2(\chi w, \mathcal{L}_\psi) \\
&= a(\chi w, \mathcal{L}_\psi) + (\nabla w, \mathcal{L}_\psi \nabla \chi) - (w \nabla \chi, \nabla \mathcal{L}_\psi) - 2k^2(\chi w, \mathcal{L}_\psi) \\
&= (\chi w, \psi)_{\Gamma_A} + (\nabla w, \mathcal{L}_\psi \nabla \chi) - (w \nabla \chi, \nabla \mathcal{L}_\psi) - 2k^2(\chi w, \mathcal{L}_\psi) \\
&= (w, \psi)_{\Gamma_A} + (w, \mathcal{L}_\psi \nabla \chi \cdot \mathbf{n})_{\partial\Omega} - (w, \nabla \cdot (\mathcal{L}_\psi \nabla \chi)) - (w, \nabla \chi \cdot \nabla \mathcal{L}_\psi) - 2k^2(w, \chi \mathcal{L}_\psi) \\
&= (w, \psi)_{\Gamma_A} - (w, \nabla \cdot (\mathcal{L}_\psi \nabla \chi) + \nabla \chi \cdot \nabla \mathcal{L}_\psi + 2k^2 \chi \mathcal{L}_\psi),
\end{aligned}$$

where we used the fact that $\nabla \chi \cdot \mathbf{n} = 0$ on Γ_A , as $\chi = 1$ in a neighborhood of Γ_A , and that $w = 0$ on Γ_D so that $(w, \mathcal{L}_\psi \nabla \chi \cdot \mathbf{n})_{\partial\Omega} = 0$. It follows that

$$b(w, u_\psi^* - \chi \mathcal{L}_\psi) = (w, \tilde{f}),$$

with $\tilde{f} = \nabla \cdot (\mathcal{L}_\psi \nabla \chi) + \nabla \chi \cdot \nabla \mathcal{L}_\psi + 2k^2 \chi \mathcal{L}_\psi$. In particular, we have $\tilde{f} \in L^2(\Omega)$, and using (A.3), we infer that

$$(A.5) \quad \|\tilde{f}\|_{0,\Omega} \leq \left(C(\widehat{\Omega}, \widehat{\Gamma}_D) \frac{1}{h_\Omega} \left(1 + \frac{1}{kh_\Omega} \right) k^{-\frac{1}{2}} + 2k^{\frac{1}{2}} \right) \|\psi\|_{0,\Gamma_A}.$$

Then, we have

$$\begin{aligned}
k^{\frac{1}{2}} \left(\inf_{v_h \in V_h} |u_\psi^* - v_h|_{1,\Omega} \right) &\leq k^{\frac{1}{2}} \left(\inf_{y_h \in V_h} |(u_\psi^* - \chi \mathcal{L}_\psi) - y_h|_{1,\Omega} + \inf_{w_h \in V_h} |\chi \mathcal{L}_\psi - w_h|_{1,\Omega} \right) \\
&\leq k^{-\frac{1}{2}} \sigma_{\text{ba}} \|\tilde{f}\|_{0,\Omega} + k^{\frac{1}{2}} \inf_{w_h \in V_h} |\chi \mathcal{L}_\psi - w_h|_{1,\Omega},
\end{aligned}$$

where the first bound stems by taking the function $v_h = y_h + w_h$ where $y_h \in V_h$ and $w_h \in V_h$ realize the two infimums in the right-hand side. Using (A.5) and Lemma A.2, we see that

$$\begin{aligned}
k^{\frac{1}{2}} \left(\inf_{v_h \in V_h} |u_\psi^* - v_h|_{1,\Omega} \right) &\leq \left(C(\widehat{\Omega}, \widehat{\Gamma}_D) \frac{1}{kh_\Omega} \left(1 + \frac{1}{kh_\Omega} \right) + 2 \right) \sigma_{\text{ba}} \|\psi\|_{0,\Gamma_A} \\
&\quad + C(\widehat{\Omega}, \widehat{\Gamma}_D) C_{\text{qi}}(\kappa) \left(\frac{kh}{p} + \left(\frac{kh}{p} \right)^{\frac{1}{2}} \right) \|\psi\|_{0,\Gamma_A},
\end{aligned}$$

and we conclude by taking the supremum over $\psi \in L^2(\Gamma_A)$. \square

Corollary A.4 (Asymptotic regime). *Under Assumption A.1, we have*

$$(A.6) \quad 1 + \tilde{\theta}_2(\sigma_{\text{ba}}, \tilde{\sigma}_{\text{ba}}) \leq 1 + \tilde{\theta}_3 \left(\sigma_{\text{ba}}, \frac{kh}{p} \right),$$

where $\tilde{\theta}_3$ is a decreasing function of its two arguments such that $\lim_{t,t' \rightarrow 0} \tilde{\theta}_3(t, t') = 0$.

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