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Analysis of a Non-standard Finite Element Method Based on Boundary Integral Operators

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ANALYSIS OF A NON-STANDARD FINITE ELEMENT METHOD BASED ON BOUNDARY INTEGRAL OPERATORS

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Abstract. We present and analyze a non-standard finite element method based on element-local boundary integral operators that permits polyhedral element shapes as well as meshes with hanging nodes. The method employs elementwise PDE-harmonic trial functions and can thus be interpreted as a local Trefftz method. The construction principle requires the explicit knowledge of the fundamental solution of the partial differential operator, but only locally, i.e. in every polyhedral element. This allows us to solve PDEs with elementwise constant coefficients. In this paper we consider the diffusion equation as a model problem, but the method can be generalized to convection-diffusion-reaction problems and to systems of PDEs like the linear elasticity system with elementwise constant coefficients. We provide a rigorous error analysis of the method under quite general assumptions on the geometric properties of the elements. Numerical results confirm our theoretical estimates.

1. Introduction

In some important practical applications one wants to discretize partial differential equations (PDEs) or systems of PDEs on polyhedral meshes without further decomposition of the polyhedra into simplices. For instance, in reservoir simulation, polyhedral elements appear naturally. Their use also gives great freedom in automatic mesh manipulation: elements can be split, joined and manipulated freely without the need to maintain a particular element topology. For instance, this freedom is advantageous in adaptive mesh refinement: straightforward subdivision of individual elements usually results in hanging nodes that are often eliminated by introducing additional edges/faces to retain conformity. This can be avoided if one can compute directly on polyhedral meshes with hanging nodes.

One established approach for this kind of problems is the family of so-called mimetic finite difference (MFD) methods. They are based on the construction of discrete spaces and operators which mimic properties of the continuous problem. MFD schemes for polygonal or polyhedral meshes have been proposed by Kuznetsov, Lipnikov, and Shashkov [17] as well as Brezzi, Lipnikov, and Simoncini [5]. A convergence analysis has been provided by Brezzi, Lipnikov, and Shashkov [4]. The realization of these methods requires the construction of

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a mesh-dependent inner product on a space of discrete velocities, which can be difficult for general polyhedral meshes.

Another approach that allows general meshes is the class of discontinuous Galerkin (DG) methods which have been intensively developed during the last decade, see e.g. [2]. As an example for a DG method on polyhedral meshes (albeit for nonlinear convection-diffusion problems), we refer to the work by Dolejší, Feistauer, and Sobotíková [11]. A DG approach generally necessitates the duplication of degrees of freedom across neighboring elements and thus an increase in the number of unknowns.

In this paper we analyze a discretization method for polyhedral meshes which has been proposed by Copeland, Langer and Pusch [8]. The method employs local boundary integral operators and has its roots in the symmetric boundary element domain decomposition method proposed by Hsiao and Wendland [14]. The latter has been developed into an efficient solution technique on parallel computers in [6, 18].

In the scheme we discuss, as in the finite element method (FEM), the stiffness matrix of the system is assembled from local element matrices. However, on each polyhedral element the corresponding element matrix is generated using a boundary element method (BEM) approach. For this reason, we refer to the method as a BEM-based FEM, or BBFEM for short. Since we use a symmetric BEM discretization [9, 14], the element matrices and consequently also the global stiffness matrix are symmetric. While the numerical realization of the element matrices is not straightforward, existing implementations from established BEM software packages like OSTBEM [24] can be leveraged for this task.

In the special case of the Laplace problem on a purely simplicial mesh, the obtained stiffness matrix is identical to that of a standard FEM. However, since the local assembly procedure via boundary element techniques is applicable to general Lipschitz polyhedra, the BBFEM can treat a much larger class of meshes naturally. In this sense, it may be viewed as a generalization of the FEM. As soon as more general PDEs and/or meshes come into play, a major difference to the FEM is that the trial functions are not piecewise polynomial, but rather piecewise PDE-harmonic, i.e. fulfill the PDE locally in every element.

The main aim of this paper is to give a rigorous error analysis of the BBFEM. We note that the error estimates for the domain decomposition variant given in [13, 14] are not explicit in the shapes and diameters of the individual domains. They are thus not applicable to the present case where we are interested in families of meshes whose element diameters uniformly tend to zero. Furthermore, the estimates given in these works bound the error only on the boundaries of the elements and are thus inherently mesh-dependent. In order to establish the relationship to the FEM, we derive estimates for the energy norm of the error over the whole computational domain.

We approach the analysis using a Strang lemma for the discrete variational formulation. Then, we derive approximation results for Dirichlet and Neumann data on the boundaries of general polyhedral elements. Some mesh-dependent quantities are bounded using recent results on explicit constants for boundary integral operators [22].

The remainder of this paper is organized as follows. In Section 2 we derive the skeletal variational formulation that will be the starting point for the discretization. Section 3 introduces the BBFEM by incorporating appropriate approximations of the local Steklov-Poincaré operators and discretizing. The error analysis is performed in Section 4. Some numerical results are given in Section 5, and Section 6 gives a conclusion and outlook on further work. The proofs of some technical intermediate results are given in Appendix A.

2. A skeletal variational formulation

We consider elliptic boundary value problems of the form

$$-\operatorname{div}(a(x)\nabla u(x)) = f(x)$$

in a bounded domain, after prescribing suitable boundary conditions. Due to the nature of the construction, a fundamental solution for the differential operator has to be explicitly known, however only locally per element. In practice, this means that we can treat problems with piecewise constant coefficients, i.e. $a(x) \equiv a_i$ in the i-th element. Because we employ boundary element methods, incorporating an inhomogeneous right-hand side $f \not\equiv 0$ requires the evaluation of element-local Newton potentials.

For the sake of simplicity, our presentation focuses on the Laplace equation with pure Dirichlet boundary conditions,

$$\begin{aligned} -\Delta u &= 0 \quad \text{in } \Omega, \\ u &= g \quad \text{on } \Gamma = \partial\Omega, \end{aligned}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain, $d = 2$ or 3, and g is the given Dirichlet data. The variational formulation of the above boundary value problem reads as follows: for given Dirichlet data $g \in H^{1/2}(\Gamma)$, find $u \in H^1(\Omega)$ such that

$$u|_\Gamma = g, \qquad \int_\Omega \nabla u \cdot \nabla v \, dx = 0 \qquad \forall v \in H_0^1(\Omega). \tag{1}$$

For a definition of the usual Sobolev spaces $H^1(\Omega)$ and $H^{1/2}(\Gamma)$, see e.g. [1].

Finite element methods typically use formulation (1) as their starting point. In our approach, however, we first introduce a mesh and derive a skeletal reformulation of (1). Later on, we will restrict to discrete trial spaces.

Consider a family of non-overlapping decompositions $(T_i)_{i=1}^N$ of Ω,

$$\overline{\Omega} = \bigcup_{i=1}^N \overline{T}_i, \qquad T_i \cap T_j = \emptyset \quad \forall i \neq j.$$

We assume that each *element* T_i is a Lipschitz polygon/polyhedron whose boundary $\Gamma_i = \partial T_i$ is composed of $(d-1)$-simplices, i.e., line segments in two dimensions and triangles in three dimensions. In the following, we refer to these boundary simplices as *facets*. We assume that the mesh is *conforming* in the sense that the intersection of the closure of two different boundary facets of any two elements is either empty, a vertex, or a facet edge (in three dimensions). A mesh with hanging nodes can be made conforming by integrating the hanging nodes as vertices into neighboring elements.

We call such a decomposition $(T_i)_{i=1}^N$ a *mesh* of Ω. In the following we will frequently refer to the *local mesh sizes* $h_i := \operatorname{diam} T_i$ and the *global mesh size* $h := \max_i h_i$. In this work, we are interested in families of such meshes where the element diameters h_i uniformly tend to zero, while the number of facets of every element remains uniformly bounded by a small constant. Within this framework we can treat typical element shapes like triangles or quadrilaterals in two dimensions, tetrahedra, hexahedra, prisms or pyramids in three dimensions, as well as other, less standard shapes. In particular, we do not necessarily assume convexity of the elements. We also retain the freedom to mix all these types of elements within one mesh; see Figure 1 for an example. Finally, we do not require the meshes within the family to be nested.

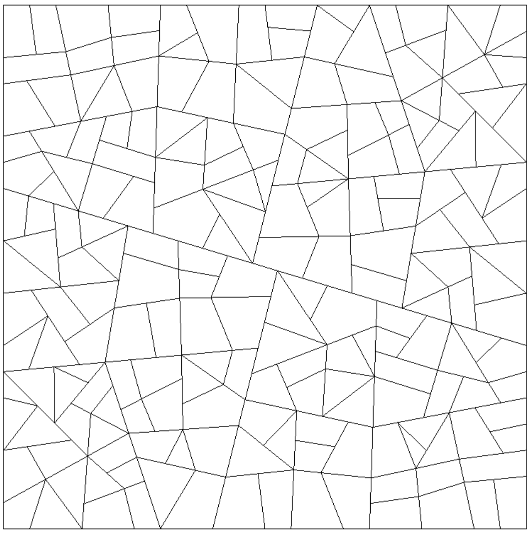

FIGURE 1. A heterogeneous polygonal mesh.

We define a restricted trial space by requiring that the trial functions fulfill the homogeneous form of the PDE locally in every element, while being globally continuous. For the Laplace equation, this means locally harmonic trial functions,

$$\begin{aligned} V_{\mathcal{H}} &:= \{v \in H^1(\Omega) : v|_{T_i} \in \mathcal{H}(T_i) \quad \forall i = 1, \dots, N\}, \\ V_{\mathcal{H},0} &:= V_{\mathcal{H}} \cap H_0^1(\Omega), \end{aligned}$$

with the space $\mathcal{H}(T_i)$ of harmonic functions on the element T_i defined by

$$\mathcal{H}(T_i) := \left\{ u \in H^1(T_i) : \int_{T_i} \nabla u \cdot \nabla v_0 \, dx = 0 \quad \forall v_0 \in H_0^1(T_i) \right\}.$$

Following McLean [20, Lemma 4.3], we define the *Neumann trace operator* $\gamma_i^1 : \mathcal{H}(T_i) \to H^{-1/2}(\Gamma_i)$ by the relation

$$\langle \gamma_i^1 u, w \rangle_{\Gamma_i} = \int_{T_i} \nabla u \cdot \nabla \widetilde{w} \, dx \qquad \forall w \in H^{1/2}(\Gamma_i),$$

where $\widetilde{w} \in H^1(T_i)$ is an arbitrary extension of w into T_i and $\langle \cdot, \cdot \rangle_{\Gamma_i}$ denotes the duality product between $H^{-1/2}(\Gamma_i)$ and $H^{1/2}(\Gamma_i)$. It follows from the definition of $\mathcal{H}(T_i)$ that the Neumann trace $\gamma_i^1 u$ does not depend on the actual choice of $\widetilde{w}$. In other words, if we denote by $\gamma_i^0 : H^1(T_i) \to H^{1/2}(\Gamma_i)$ the usual Dirichlet trace operator, then we have for any $u \in \mathcal{H}(T_i)$

$$\langle \gamma_i^1 u, \gamma_i^0 v \rangle_{\Gamma_i} = \int_{T_i} \nabla u \cdot \nabla v \, dx \qquad \forall v \in H^1(T_i). \tag{2}$$

We recognize this as Green's first identity for harmonic functions. This also shows that, in case of sufficient regularity, $\gamma_i^1 = n_i \cdot \nabla$ with the outward normal vector n_i on Γ_i.

Noting that $V_{\mathcal{H}} \subset H^1(\Omega)$ and $V_{\mathcal{H},0} \subset H_0^1(\Omega)$, we state a restricted version of the variational problem (1) as follows: find $u \in V_{\mathcal{H}}$ which satisfies

$$u|_\Gamma = g, \qquad \int_\Omega \nabla u \cdot \nabla v \, dx = 0 \qquad \forall v \in V_{\mathcal{H},0}. \tag{3}$$

Owing to $V_{\mathcal{H}} \subset H^1(\Omega)$, the usual boundedness and coercivity properties of the bilinear form in (1) carry over to (3). It follows that (3) is a well-posed variational problem. Furthermore, the two formulations are equivalent since the solution $u \in H^1(\Omega)$ of (1) lies in $V_{\mathcal{H}}$. This is easily seen by choosing, for arbitrary but fixed $i \in \{1, \dots N\}$, an arbitrary function $v_i \in H_0^1(T_i)$, extending it by zero to $v \in H_0^1(\Omega)$, and testing in (1) with this particular choice of v.

Green's identity (2) allows us to rewrite the variational problem (3) as follows: we seek $u \in V_{\mathcal{H},g} := \{u \in V_{\mathcal{H}} : u|_\Gamma = g\}$ satisfying

$$\sum_{i=1}^{N} \langle \gamma_i^1 u,\, \gamma_i^0 v \rangle_{\Gamma_i} \;=\; 0 \qquad \forall v \in V_{\mathcal{H},0}. \tag{4}$$

The only values of u occurring in this formulation are the Neumann traces on the element boundaries. This gives rise to the idea of representing u solely via its values on the *skeleton* $\Gamma_S = \bigcup_{i=1}^N \Gamma_i$.

Let $\mathcal{H}_i : H^{1/2}(\Gamma_i) \to \mathcal{H}(T_i)$ denote the local harmonic extension operator for the element T_i. It maps $g_i \in H^{1/2}(\Gamma_i)$ to the solution $u_i \in H^1(T_i)$ of the local variational problem

$$\gamma_i^0 u_i = g_i, \qquad \int_{T_i} \nabla u_i \cdot \nabla v_i \, dx \;=\; 0 \qquad \forall v_i \in H_0^1(T_i).$$

It is easy to see that $\mathcal{H}_i$ is bijective, with its inverse given by γ_i^0. Now, denoting by $H^{1/2}(\Gamma_S)$ the trace space of $H^1(\Omega)$ onto the skeleton, we introduce the *skeletal harmonic extension operator*

$$\begin{aligned} &\mathcal{H}_S : H^{1/2}(\Gamma_S) \to V_{\mathcal{H}}, \\ &\qquad (\mathcal{H}_S v)|_{T_i} = \mathcal{H}_i(v|_{\Gamma_i}) \quad \forall i \in \{1, \dots, N\}. \end{aligned} \tag{5}$$

From the above, we can infer that $\mathcal{H}_S$ is a bijection between $H^{1/2}(\Gamma_S)$ and $V_{\mathcal{H}}$, its inverse being the *skeletal Dirichlet trace operator* $\gamma_S : H^1(\Omega) \to H^{1/2}(\Gamma_S)$. Similarly, with the subspace W_0 and the manifold W_g given by, respectively,

$$W_0 \;:=\; \{v \in H^{1/2}(\Gamma_S) : v|_\Gamma = 0\}, \quad W_g \;:=\; \{v \in H^{1/2}(\Gamma_S) : v|_\Gamma = g\},$$

the operator $\mathcal{H}_S$ is a bijection between W_0 and $V_{\mathcal{H},0}$ as well as between W_g and $V_{\mathcal{H},g}$. In other words, we can represent any piecewise harmonic function $v \in V_{\mathcal{H},0}$ uniquely as $\mathcal{H}_S v_S$ with some skeletal function $v_S \in W_0$, and $u \in V_{\mathcal{H},g}$ as $\mathcal{H}_S u_S$ with some $u_S \in W_g$. If we define the local *Dirichlet-to-Neumann maps*

$$\begin{aligned} S_i : H^{1/2}(\Gamma_i) &\to H^{-1/2}(\Gamma_i), \\ v &\mapsto \gamma_i^1(\mathcal{H}_i v) \end{aligned} \tag{6}$$

and introduce the short-hand notation $v_i := v_S|_{\Gamma_i}$, we can rewrite the formulation (4) as seeking $u = \mathcal{H}_S u_S$ with a skeletal function $u_S \in W_g$ satisfying

$$\sum_{i=1}^{N} \langle S_i u_i,\, v_i \rangle_{\Gamma_i} \;=\; 0 \qquad \forall v_S \in W_0. \tag{7}$$

Since (7) is nothing but an equivalent rewriting of (3), which in turn we have above demonstrated to be equivalent to the standard variational formulation (1), we have proved the following proposition.

Proposition 2.1. *Let $g \in H^{1/2}(\Gamma)$ be given. The variational formulations to find $u \in H^1(\Omega)$ with $u|_\Gamma = g$ such that*

$$\int_\Omega \nabla u \cdot \nabla v \, dx \;=\; 0 \qquad \forall v \in H_0^1(\Omega),$$

and $u_S \in H^{1/2}(\Gamma_S)$ with $u_S|_\Gamma = g$ such that

$$\sum_{i=1}^N \langle S_i u_i, \, v_i \rangle_{\Gamma_i} \;=\; 0 \qquad \forall v_S \in W_0,$$

where $u_i = u_S|_{\Gamma_i}$, $v_i = v_S|_{\Gamma_i}$, are both well-posed. They are equivalent in the sense that their unique solutions u and u_S are related by

$$u_S = \gamma_S u, \qquad u = \mathcal{H}_S u_S.$$

Remark. *For brevity, we will drop the subscript S for skeletal functions in the remainder of this work and instead denote functions defined within the domain by the subscript Ω.*

3. A BEM-based finite element method

In this section we derive the BBFEM discretization of the skeletal variational formulation (7). Since we work with skeletal functions spaces which only incorporate boundary values of the involved functions on every element, it is natural to use a representation of the Dirichlet-to-Neumann map S_i in terms of boundary integral operators. We use symmetric approximations of the local Steklov-Poincaré operators in order to obtain a symmetric stiffness matrix.

3.1. **Boundary integral operators.**

We can only give a brief summary of some standard results on boundary integral operators here and refer the reader to, e.g., [15, 20, 23] for further details.

For $x, y \in \mathbb{R}^d$, let

$$U^*(x,y) \;:=\; \begin{cases} -\frac{1}{2\pi} \log|x-y| & \text{if } d=2, \\ \frac{1}{4\pi} |x-y|^{-1} & \text{if } d=3, \end{cases}$$

denote the *fundamental solution* of the Laplace operator. Following, e.g., McLean [20] or Steinbach [26], we introduce the boundary integral operators

$$V_i : H^{-1/2}(\Gamma_i) \to H^{1/2}(\Gamma_i), \quad K_i : H^{1/2}(\Gamma_i) \to H^{1/2}(\Gamma_i),$$
$$K_i' : H^{-1/2}(\Gamma_i) \to H^{-1/2}(\Gamma_i), \quad D_i : H^{1/2}(\Gamma_i) \to H^{-1/2}(\Gamma_i).$$

They are called, in turn, the *single layer potential*, *double layer potential*, *adjoint double layer potential*, and *hypersingular* operators. For sufficiently regular functions, they have the integral representations

$$(V_i v)(y) \;=\; \int_{\Gamma_i} U^*(x,y) v(x) \, ds_x, \quad (K_i u)(y) \;=\; \int_{\Gamma_i} \frac{\partial U^*}{\partial n_x}(x,y) u(x) \, ds_x,$$
$$(D_i u)(y) \;=\; -\frac{\partial}{\partial n_y} \int_{\Gamma_i} \frac{\partial U^*}{\partial n_x}(x,y) \big(u(x) - u(y)\big) \, ds_x.$$

In the present setting, V_i and D_i are self-adjoint operators, whereas K_i and K_i' are adjoint to each other. The bilinear form $\langle \cdot, \, V_i \, \cdot \rangle$ induced by the single layer potential operator can be shown to be coercive on $H^{-1/2}(\Gamma_i)$; in two dimensions, this requires the additional technical condition that the diameter of the domain T_i be less than one.

We also introduce the subspaces

$$\begin{aligned} H_*^{-1/2}(\Gamma_i) &:= \{w \in H^{-1/2}(\Gamma_i) : \langle w,\, 1\rangle_{\Gamma_i} = 0\}, \\ H_*^{1/2}(\Gamma_i) &:= \{v \in H^{1/2}(\Gamma_i) : \langle V_i^{-1}v,\, 1\rangle_{\Gamma_i} = 0\} \;=\; \mathrm{Im}_{V_i}(H_*^{-1/2}(\Gamma_i)). \end{aligned}$$

The bilinear form induced by D_i is coercive on $H_*^{1/2}(\Gamma_i)$. Furthermore, on $H_*^{1/2}(\Gamma_i)$, we have the contraction property [26]

$$(1 - c_{K,i})\|v\|_{V_i^{-1}} \;\le\; \|(\tfrac{1}{2}I + K_i)v\|_{V_i^{-1}} \;\le\; c_{K,i}\|v\|_{V_i^{-1}} \quad \forall v \in H_*^{1/2}(\Gamma_i),$$

with the contraction constants

$$c_{0,i} \;:=\; \inf_{v \in H_*^{1/2}(\Gamma_i)} \frac{\langle D_i v,\, v\rangle_{\Gamma_i}}{\langle V_i^{-1}v,\, v\rangle_{\Gamma_i}} \;\in\; (0, \tfrac{1}{4}), \quad c_{K,i} \;:=\; \tfrac{1}{2} + \sqrt{\tfrac{1}{4} - c_{0,i}} \;\in\; (\tfrac{1}{2}, 1).$$

Above, $\|v\|_{V_i^{-1}} = \sqrt{\langle V_i^{-1}v,\, v\rangle}$. Here and in the following we implicitly exclude $v = 0$ in infima and suprema of the above form.

Following [20, 26], the Dirichlet-to-Neumann map S_i defined in (6) is identical to the *Steklov-Poincaré operator* given by

$$S_i \;=\; V_i^{-1}(\tfrac{1}{2}I + K_i).$$

From the contraction properties of $(\frac{1}{2}I + K_i)$ above, one easily derives the following estimates using the Cauchy-Schwarz inequality (cf. [10, 21]):

$$(1 - c_{K,i})\langle V_i^{-1}v,\, v\rangle_{\Gamma_i} \;\le\; \langle S_i v,\, v\rangle_{\Gamma_i} \;\le\; c_{K,i}\langle V_i^{-1}v,\, v\rangle_{\Gamma_i} \quad \forall v \in H_*^{1/2}(\Gamma_i).$$

The constant functions form the kernel of both $(\frac{1}{2}I + K_i)$ and S_i, and for every $v \in H^{1/2}(\Gamma_i)$ there is a unique splitting $v = v_* + v_0$ with v_0 constant and $v_* \in H_*^{1/2}(\Gamma_i)$. Making use of these facts, we can derive the following inequality that we will make use of later:

$$\begin{aligned} \|(\tfrac{1}{2}I + K_i)v\|_{V_i^{-1}} \;&=\; \|(\tfrac{1}{2}I + K_i)v_*\|_{V_i^{-1}} \\ &\le\; c_{K,i}\|v_*\|_{V_i^{-1}} \;\le\; \frac{c_{K,i}}{\sqrt{1 - c_{K,i}}}\,|v_*|_{S_i} \;=\; \frac{c_{K,i}}{\sqrt{1 - c_{K,i}}}\,|v|_{S_i}. \end{aligned} \tag{8}$$

Above we have used the seminorm $|v|_{S_i} = \sqrt{\langle S_i v,\, v\rangle}$.

3.2. Approximation of the Steklov-Poincaré operator.

The Steklov-Poincaré operator S_i has the non-symmetric and symmetric representations

$$S_i u_i \;=\; V_i^{-1}(\tfrac{1}{2}I + K_i)u_i \;=\; D_i u_i + (\tfrac{1}{2}I + K_i')V_i^{-1}(\tfrac{1}{2}I + K_i)u_i.$$

Both representations are of course self-adjoint in the continuous setting. However, discretizing the first one yields a non-symmetric matrix, and the second one does not immediately permit a Galerkin discretization due to the occurrence of V_i^{-1}. To obtain a symmetric discretization, we first rewrite S_i as

$$S_i u_i \;=\; D_i u_i + (\tfrac{1}{2}I + K_i')w_i(u_i)$$

with $w_i(u_i) = V_i^{-1}(\frac{1}{2}I + K_i)u_i = S_i u_i \in H^{-1/2}(\Gamma_i)$. Let now $w_{h,i}(u_i) \in Z_{h,i}$ be the Galerkin projection of $w_i(u_i)$ onto some finite-dimensional space $Z_{h,i} \subset H^{-1/2}(\Gamma_i)$. That is, $w_{h,i}(u_i)$ is determined locally on Γ_i by the variational problem

$$\langle z_{h,i},\, V_i w_{h,i}(u_i)\rangle_{\Gamma_i} \;=\; \langle z_{h,i},\, (\tfrac{1}{2}I + K_i)u_i\rangle_{\Gamma_i} \qquad \forall\, z_{h,i} \in Z_{h,i}. \tag{9}$$

The outer symmetric BEM approximation of S_i is then defined as

$$\begin{aligned} \widetilde{S}_i : H^{1/2}(\Gamma_i) &\to H^{-1/2}(\Gamma_i), \\ u_i &\mapsto D_i u_i + (\tfrac{1}{2}I + K_i')w_{h,i}(u_i), \end{aligned}$$

see, e.g., [9, 25]. One natural choice for $Z_{h,i}$ is the space of piecewise (per boundary facet) constant functions on Γ_i, which we stick to here.

We observe that for all $u_i,\, v_i \in H^{1/2}(\Gamma_i)$,

$$\begin{aligned} \langle \widetilde{S}_i u_i,\, v_i\rangle &= \langle D_i u_i,\, v_i\rangle + \langle (\tfrac{1}{2}I + K_i')w_{i,h}(u_i),\, v_i\rangle \\ &= \langle D_i u_i,\, v_i\rangle + \langle w_{i,h}(u_i),\, (\tfrac{1}{2}I + K_i)v_i\rangle \\ &= \langle D_i u_i,\, v_i\rangle + \langle w_{i,h}(v_i),\, V_i w_{i,h}(u_i)\rangle, \end{aligned}$$

where the last expression is clearly symmetric with respect to u_i and v_i. This shows that $\widetilde{S}_i$ is indeed a self-adjoint operator, and this property carries over directly to its (now natural) Galerkin discretization.

The symmetric approximation of the Steklov-Poincaré operator fulfills the spectral equivalence relation (cf. [21, 25])

$$\frac{c_{0,i}}{c_{K,i}}\langle S_i v_i,\, v_i\rangle_{\Gamma_i} \;\le\; \langle \widetilde{S}_i v_i,\, v_i\rangle_{\Gamma_i} \;\le\; \langle S_i v_i,\, v_i\rangle_{\Gamma_i} \quad \forall v_i \in H^{1/2}(\Gamma_i). \tag{10}$$

Note that the bilinear forms induced by both S_i and $\widetilde{S}_i$ are positive semidefinite and symmetric and hence satisfy a Cauchy-Schwarz inequality.

3.3. **Discretization.** Let us restate the skeletal variational formulation (7) derived in Section 2. It is always possible to extend the given Dirichlet data $g \in H^{1/2}(\Gamma)$ to the skeleton. Therefore, without loss of generality, we assume $g \in H^{1/2}(\Gamma_S)$. After homogenization with this g, we seek $u \in W := W_0 = \{v \in H^{1/2}(\Gamma_S) : v|_\Gamma = 0\}$ such that

$$a(u, v) \;=\; \langle F,\, v\rangle \qquad \forall v \in W \tag{11}$$

with the symmetric bilinear form and the linear functional

$$a(u, v) \;:=\; \sum_{i=1}^{N} \langle S_i u_i,\, v_i\rangle_{\Gamma_i}, \qquad \langle F,\, v\rangle \;:=\; \sum_{i=1}^{N} \langle -S_i g_i,\, v_i\rangle_{\Gamma_i} \;=\; -a(g, v).$$

The solution of the boundary value problem is then given by $\mathcal{H}_S(u_g)$, where we denote by $u_g := u + g$ the skeletal solution incorporating boundary conditions.

Approximating S_i by $\widetilde{S}_i$, we get an approximate bilinear form and linear functional, respectively, as

$$\widetilde{a}(u, v) \;:=\; \sum_{i=1}^{N} \langle \widetilde{S}_i u_i,\, v_i\rangle_{\Gamma_i}, \qquad \langle \widetilde{F},\, v\rangle \;:=\; \sum_{i=1}^{N} \langle -\widetilde{S}_i g_i,\, v_i\rangle_{\Gamma_i} = -\widetilde{a}(g, v).$$

As a finite-dimensional trial space $W_h \subset W$, we choose the space of piecewise linear (per facet of Γ_S) and continuous functions on the skeleton. This yields the discretized variational formulation: find $u_h \in W_h$ such that

$$\widetilde{a}(u_h, v_h) \;=\; \langle \widetilde{F},\, v_h\rangle \qquad \forall v_h \in W_h. \tag{12}$$

As basis functions for W_h, we choose the skeletal nodal basis functions which are one in a designated vertex of the skeleton and zero in all others while being piecewise linear on the skeletal facets. To assemble the stiffness matrix corresponding to (12), we only need a means of computing the local stiffness matrices arising from $\widetilde{S}_i$. The resulting linear system is symmetric and positive definite.

It is interesting to note that, in the case of a purely simplicial mesh,

- the locally harmonic trial functions are just the piecewise linear functions,
- the space $Z_{h,i}$ of piecewise constant boundary functions can represent the Neumann derivatives of the piecewise linear functions exactly,
- the local Galerkin projections of the Neumann derivative are thus just the identity, i.e. $w_{h,i} = w_i$ and therefore also $\widetilde{S}_i = S_i$.

This means that in this special case, the scheme can be realized exactly and is equivalent to a standard nodal FEM with piecewise linear trial functions. Indeed, the resulting stiffness matrices from the BBFEM and this standard FEM are then identical.

4. Error analysis

The aim of this section is to derive rigorous error estimates for the numerical scheme described by (12). Recall that the discretization of the variational formulation (7) proceeded in two steps: we chose a finite-dimensional trial space $W_h \subset W$, and, to make the scheme computable, we chose an approximation $\widetilde{S}_i$ of the Dirichlet-to-Neumann map S_i. While the first step leads to a standard Galerkin method which is easily analyzed using the Céa lemma, the second step introduces a consistency error which demands analysis by a Strang lemma.

4.1. **Norms.** In order to derive error estimates, we first need appropriate norms for the involved boundary function spaces. Because we use harmonic extensions heavily, the natural norms to work with are those defined in terms of the extension operators $\mathcal{H}_i$. Thus, we equip the local trace spaces $H^{1/2}(\Gamma_i)$ with the seminorm and norm

$$|v_i|_{H^{1/2}(\Gamma_i)} \;:=\; |\mathcal{H}_i v_i|_{H^1(T_i)} \;=\; \inf_{\substack{\phi \in H^1(T_i)\\ \gamma_i^0 \phi = v_i}} |\phi|_{H^1(T_i)},$$

$$\|v_i\|^2_{H^{1/2}(\Gamma_i)} \;:=\; \frac{1}{\operatorname{diam}(T_i)^2} \|\mathcal{H}_i v_i\|^2_{L_2(T_i)} + |\mathcal{H}_i v_i|^2_{H^1(T_i)}.$$

The norm $\|\cdot\|_{H^{1/2}(\Gamma_i)}$ induces as usual an associated dual norm $\|\cdot\|_{H^{-1/2}(\Gamma_i)}$ on the dual space of $H^{1/2}(\Gamma_i)$.

We observe that, for all $v_i \in H^{1/2}(\Gamma_i)$,

$$\begin{aligned} \langle S_i v_i,\, v_i\rangle_{\Gamma_i} \;&=\; \langle \gamma_i^1(\mathcal{H}_i v_i),\, \gamma_i^0(\mathcal{H}_i v_i)\rangle_{\Gamma_i} \\ &\overset{(2)}{=} \int_{T_i} \nabla(\mathcal{H}_i v_i) \cdot \nabla(\mathcal{H}_i v_i)\, dx \;=\; |\mathcal{H}_i v_i|^2_{H^1(T_i)} \;=\; |v_i|^2_{H^{1/2}(\Gamma_i)}. \end{aligned} \tag{13}$$

On $W = \{v \in H^{1/2}(\Gamma_S) : v|_\Gamma = 0\}$, we define the skeletal energy norm by

$$|\!|\!| v |\!|\!|_S \;:=\; \Big(\sum_{i=1}^N |v_i|^2_{H^{1/2}(\Gamma_i)}\Big)^{1/2} \;=\; \Big(\sum_{i=1}^N |\mathcal{H}_i v_i|^2_{H^1(T_i)}\Big)^{1/2} \;=\; |\mathcal{H}_S v|_{H^1(\Omega)}.$$

On the space W, whose members satisfy homogeneous boundary conditions, this is indeed a full norm.

4.2. **Error of the inexact Galerkin scheme.** Our error analysis is based on the following variant of the first Strang lemma.

Lemma 4.1. *Let $X_h \subset X$ be Hilbert spaces with the norm $\|\cdot\|$. Assume that there are constants γ_1, γ_2, $\widetilde{\gamma}_1$, $\widetilde{\gamma}_2 > 0$ such that the bilinear forms $a(\cdot,\cdot)$, $\widetilde{a}(\cdot,\cdot) : X \times X \to \mathbb{R}$ satisfy*

$$\begin{aligned} \gamma_1 \|v\|^2 &\le a(v,v), & \widetilde{\gamma}_1 \|v\|^2 &\le \widetilde{a}(v,v) & \forall v \in X,\\ |a(v,w)| &\le \gamma_2 \|v\|\,\|w\|, & |\widetilde{a}(v,w)| &\le \widetilde{\gamma}_2 \|v\|\,\|w\| & \forall v, w \in X. \end{aligned}$$

Assume that $u \in X$ and $\widetilde{u}_h \in X_h$ solve

$$\begin{aligned} a(u,v) &= \langle F, v\rangle & \forall v \in X,\\ \widetilde{a}(\widetilde{u}_h, v_h) &= \langle \widetilde{F}, v_h\rangle & \forall v_h \in X_h, \end{aligned}$$

with the bounded linear functionals F, $\widetilde{F} \in X^*$. Then

$$\|u - \widetilde{u}_h\| \;\le\; C\Big(\inf_{v_h \in X_h} \|u - v_h\| \;+\; \sup_{w_h \in X_h} \frac{|\widetilde{a}(u, w_h) - \langle \widetilde{F}, w_h\rangle|}{\|w_h\|}\Big),$$

where $C = \max\Big\{\Big(1 + \frac{\widetilde{\gamma}_2}{\widetilde{\gamma}_1}\Big)\frac{\gamma_2}{\gamma_1}, \frac{1}{\widetilde{\gamma}_1}\Big\}$.

Proof. Let $u_h \in X_h$ be the solution of the variational problem

$$a(u_h, v_h) \;=\; \langle F, v_h\rangle \qquad \forall v_h \in X_h,$$

which exists and is uniquely defined due to the Lax-Milgram lemma. Observe that

$$\begin{aligned} \widetilde{\gamma}_1 \|u_h - \widetilde{u}_h\|^2 &\le \widetilde{a}(u_h - \widetilde{u}_h, u_h - \widetilde{u}_h)\\ &= \widetilde{a}(u_h - u, u_h - \widetilde{u}_h) + \widetilde{a}(u, u_h - \widetilde{u}_h) - \langle \widetilde{F}, u_h - \widetilde{u}_h\rangle\\ &\le \widetilde{\gamma}_2 \|u_h - u\|\|u_h - \widetilde{u}_h\| + |\widetilde{a}(u, u_h - \widetilde{u}_h) - \langle \widetilde{F}, u_h - \widetilde{u}_h\rangle|, \end{aligned}$$

and hence, by dividing by $\widetilde{\gamma}_1 \|u_h - \widetilde{u}_h\|$,

$$\begin{aligned} \|u_h - \widetilde{u}_h\| &\le \frac{\widetilde{\gamma}_2}{\widetilde{\gamma}_1}\|u_h - u\| + \frac{1}{\widetilde{\gamma}_1}\frac{|\widetilde{a}(u, u_h - \widetilde{u}_h) - \langle \widetilde{F}, u_h - \widetilde{u}_h\rangle|}{\|u_h - \widetilde{u}_h\|}\\ &\le \frac{\widetilde{\gamma}_2}{\widetilde{\gamma}_1}\|u_h - u\| + \frac{1}{\widetilde{\gamma}_1}\sup_{w_h \in X_h}\frac{|\widetilde{a}(u, w_h) - \langle \widetilde{F}, w_h\rangle|}{\|w_h\|}. \end{aligned}$$

Use of the triangle inequality and of the above estimate gives us

$$\begin{aligned} \|u - \widetilde{u}_h\| &\le \|u - u_h\| + \|u_h - \widetilde{u}_h\|\\ &\le \Big(1 + \frac{\widetilde{\gamma}_2}{\widetilde{\gamma}_1}\Big)\|u - u_h\| + \frac{1}{\widetilde{\gamma}_1}\sup_{w_h \in X_h}\frac{|\widetilde{a}(u, w_h) - \langle \widetilde{F}, w_h\rangle|}{\|w_h\|}. \end{aligned}$$

The desired statement follows by using Céa's lemma to estimate

$$\|u - u_h\| \;\le\; \frac{\gamma_2}{\gamma_1}\inf_{v_h \in X_h}\|u - v_h\|. \qquad \square$$

Using this abstract result, we can now prove a first Céa-type error estimate for our method.

Lemma 4.2. *Let $u \in W$ be the solution of* (11)*, and $u_h \in W_h$ the solution of* (12)*. Denote by $w_i(u_g) = S_i(u+g) \in H^{-1/2}(\Gamma_i)$ the skeletal Neumann data corresponding to the exact solution. Then we have the error estimate*

$$|\mathcal{H}_S(u-u_h)|_{H^1(\Omega)} = |||u-u_h|||_S \leq C\left\{\inf_{v_h\in W_h}|||u-v_h|||_S + \Big(\sum_{i=1}^N \inf_{z_{h,i}\in Z_{h,i}}\|w_i(u_g)-z_{h,i}\|_{V_i}^2\Big)^{1/2}\right\}, \quad (14)$$

where

$$C = \Big(1+\frac{1}{\underline{c}_S}\Big)\max\Big\{1, \frac{\overline{c}_K}{\sqrt{1-\overline{c}_K}}\Big\}$$

with the abbreviations $\overline{c}_K := \max_i c_{K,i} < 1$ for the largest contraction constant and $\underline{c}_S := \min_i \frac{c_{0,i}}{c_{K,i}} > 0$.

Proof. In the notation of Lemma 4.1, we use the Hilbert spaces $W_h \subset W$ with the norm $|||\cdot|||_S$. For the bilinear form $a(\cdot,\cdot)$ (cf. Section 3.3), identity (13) gives us the bounds $\gamma_1 = \gamma_2 = 1$. For the approximate bilinear form $\widetilde{a}(\cdot,\cdot)$, relation (10) yields the bounds $\widetilde{\gamma}_1 = \underline{c}_S$ and $\widetilde{\gamma}_2 = 1$. (The upper bounds follow from the spectral estimates via the Cauchy-Schwarz inequality, $\langle S_i v_i, w_i\rangle^2 \leq \langle S_i v_i, v_i\rangle\langle S_i w_i, w_i\rangle$.) Lemma 4.1 then implies the error estimate

$$|||u-u_h|||_S \leq C_1\left(\inf_{v_h\in W_h}|||u-v_h|||_S + \sup_{v_h\in W_h}\frac{|\widetilde{a}(u_g,v_h)|}{|||v_h|||_S}\right), \quad (15)$$

where $C_1 = 1+\frac{1}{\underline{c}_S}$. We now estimate the consistency error. Note first that $a(u_g,v)=0$ for all $v \in W$. Hence, $|\widetilde{a}(u_g,v_h)| = |a(u_g,v_h)-\widetilde{a}(u_g,v_h)|$, and we see that

$$\begin{aligned} a(u_g,v_h)-\widetilde{a}(u_g,v_h) &= \sum_{i=1}^N\Big(\langle S_i(u_i+g_i), v_{h,i}\rangle_{\Gamma_i} - \langle \widetilde{S}_i(u_i+g_i), v_{h,i}\rangle_{\Gamma_i}\Big)\\ &= \sum_{i=1}^N \langle(\tfrac12 I+K_i')(w_i(u_g)-w_{h,i}(u_g)), v_{h,i}\rangle_{\Gamma_i}\\ &= \sum_{i=1}^N \langle(\tfrac12 I+K_i)v_{h,i}, w_i(u_g)-w_{h,i}(u_g)\rangle_{\Gamma_i}, \end{aligned}$$

where $w_{h,i}(u_g)$ is determined by relation (9). In order to bound the local consistency error on each element boundary Γ_i, we use that

$$\sup_{v\in H^{1/2}(\Gamma_i)}\frac{\langle w, v\rangle_{\Gamma_i}}{\|v\|_{V_i^{-1}}} = \|w\|_{V_i},$$

which is easily obtained by standard techniques. In other words, $\|\cdot\|_{V_i}$ is the associated dual norm to $\|\cdot\|_{V_i^{-1}}$. Hence,

$$\begin{aligned} &\langle(\tfrac12 I+K_i)v_{h,i}, w_i(u_g)-w_{h,i}(u_g)\rangle_{\Gamma_i}\\ &\quad\leq \|(\tfrac12 I+K_i)v_{h,i}\|_{V_i^{-1}}\,\|w_i(u_g)-w_{h,i}(u_g)\|_{V_i}\\ &\quad\leq \frac{c_{K,i}}{\sqrt{1-c_{K,i}}}\,|v_{h,i}|_{H^{1/2}(\Gamma_i)}\,\|w_i(u_g)-w_{h,i}(u_g)\|_{V_i}, \end{aligned} \quad (16)$$

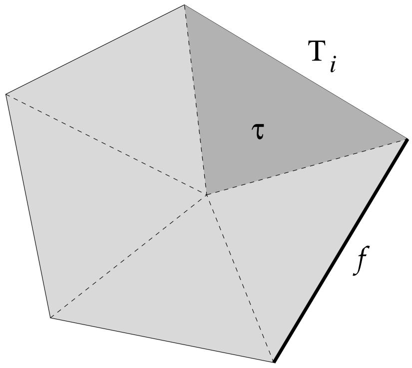

FIGURE 2. Sketch of a pentagonal element T_i with auxiliary triangulation Ξ_i, one of its constituting simplices $\tau \in \Xi_i$, and a boundary facet $f \in \mathcal{F}_i$.

where in the last line we have used inequality (8) and the fact that $|\cdot|_{S_i} = |\cdot|_{H^{1/2}(\Gamma_i)}$.

Consider now the remaining rightmost term in (16). By the defining relations $V_i w_i(u_g) = (\frac{1}{2}I + K_i)(u_i + g_i)$ for $w_i(u_g)$ and (9) for $w_{h,i}(u_g)$, we have the Galerkin orthogonality

$$\langle V_i(w_i(u_g) - w_{h,i}(u_g)),\, z_{h,i}\rangle \;=\; 0 \qquad \forall z_{h,i} \in Z_{h,i}.$$

By a simple application of Céa's lemma, we therefore get

$$\|w_i(u_g) - w_{h,i}(u_g)\|_{V_i} \;=\; \inf_{z_{h,i} \in Z_{h,i}} \|w_i(u_g) - z_{h,i}\|_{V_i}.$$

Combining these results with (15), we obtain the desired statement easily from the Cauchy-Schwarz inequality in $\mathbb{R}^N$. □

The error estimate (14) contains the constants $\overline{c}_K$ and $\underline{c}_S$. We have not yet clarified their dependence on the mesh (i.e., on the shapes of the elements), and will do so in the next section. Furthermore, estimating the error in terms of the Dirichlet and Neumann errors on the skeleton is not desirable since these terms are inherently mesh-dependent. The remainder of our error analysis is concerned with estimating the expressions on the right-hand side of (14) only in terms of the exact solution and certain regularity parameters of the mesh.

In the sequel we restrict ourselves to the three-dimensional case.

4.3. **Geometric assumptions on the mesh.** We assume that every element T_i has an auxiliary conforming triangulation Ξ_i consisting of mutually disjoint tetrahedra, $\overline{T}_i = \bigcup_{\tau \in \Xi_i} \overline{\tau}$. By $\mathcal{F}_i$, we denote the collection of all triangular faces f of tetrahedra $\tau \in \Xi_i$ which lie on the element boundary Γ_i. See Figure 2 for a sketch (in two dimensions). We assume that the triangulations of any two neighboring elements T_i and T_j are *matching* in the sense that, for facets $f_i \in \mathcal{F}_i$ and $f_j \in \mathcal{F}_j$ such that $f_i \neq f_j$, their intersection $\overline{f}_i \cap \overline{f}_j$ is either empty, a vertex, or an edge.

We emphasize that these local triangulations are a purely analytical device and not required for the numerical realization.

Definition 4.1. *The tetrahedral triangulation* Ξ_i *is called* regular *if and only if there exist positive constants* $\underline{c}_1$, $\overline{c}_1$, $\underline{c}_2$, *and* $\overline{c}_2$ *such that for all tetrahedra* $\tau \in \Xi$ *we have*

$$\underline{c}_1(\operatorname{diam}\tau)^3 \;\leq\; |\det J_\tau| \;\leq\; \overline{c}_1(\operatorname{diam}\tau)^3, \tag{17}$$

$$\|J_\tau\|_{\ell_2} \;\leq\; \overline{c}_2 \operatorname{diam}\tau, \tag{18}$$

$$\|J_\tau^{-1}\|_{\ell_2} \;\leq\; (\underline{c}_2 \operatorname{diam}\tau)^{-1}, \tag{19}$$

where J_τ *is the Jacobian of the affine mapping from the unit tetrahedron to* τ, *and* $\|A\|_{\ell_2} = \sqrt{\lambda_{\max}(A^\top A)}$ *denotes the spectral matrix norm.*

For some auxiliary results that will be given later on, we need the following shape regularity assumptions on the mesh.

Assumption 4.1. *We assume that the polyhedral mesh* $(T_i)_{i=1}^N$ *satisfies the following conditions.*

- *There is a small integer* $N_{\mathcal{F}}$ *uniformly bounding the number of boundary triangles per element,* $|\mathcal{F}_i| \leq N_{\mathcal{F}}$.
- *Every element* T_i *has a conforming triangulation* Ξ_i *which is regular with uniform constants* $\underline{c}_1$, $\overline{c}_1$, $\underline{c}_2$, *and* $\overline{c}_2 > 0$, *independent of the index* i.

In finite element analysis, one usually obtains uniform constants by transforming domain and surface integrals to reference elements. This way, estimates depend only on mesh regularity parameters as well as on some true constants stemming from inequalities on the reference elements.

For general polyhedral meshes, such a technique is not yet known. In particular, we cannot express the constants $c_{0,i}$ by transformation to reference elements. In order to nonetheless get uniform bounds, we make use of shape-explicit bounds on the constants $c_{0,i}$ that Pechstein [22] has recently obtained. The construction therein uses the following parameter introduced by Jones [16].

Definition 4.2 (Uniform domain [16])**.** *A bounded and connected set* $D \subset \mathbb{R}^d$ *is called a* uniform domain *if there exists a constant* $C_U(D)$ *such that any pair of points* $x_1 \in D$ *and* $x_2 \in D$ *can be joined by a rectifiable curve* $\gamma(t) : [0, 1] \to D$ *with* $\gamma(0) = x_1$ *and* $\gamma(1) = x_2$, *such that the Euclidean arc length of* γ *is bounded by* $C_U(D)\,|x_1 - x_2|$ *and*

$$\min_{i=1,2} |x_i - \gamma(t)| \;\leq\; C_U(D)\operatorname{dist}(\gamma(t), \partial D) \qquad \forall t \in [0, 1].$$

Any Lipschitz domain is also a uniform domain. In the following, for any Lipschitz domain D, we call the smallest constant $C_U(D)$ that complies with Definition 4.2 the Jones parameter of D.

The second parameter that we use is the constant in Poincaré's inequality. Let D be a uniform domain, then let $C_P(D)$ be the best constant such that

$$\inf_{c\in\mathbb{R}} \|u - c\|_{L_2(D)} \;\leq\; C_P(D)\operatorname{diam}(D)\,|u|_{H^1(D)} \qquad \forall u \in H^1(D). \tag{20}$$

Combining a famous result by Maz'ya [19] and Federer and Fleming [12] with an auxiliary result by Kim (see [22, Lemma 3.4]), the constant $C_P(D)$ can be tracked back to the constant in an isoperimetric inequality. For convex domains D, one can even show that $C_P(D) \leq 1/\pi$, cf. [3]. Estimates for shar-shaped domains can be found in [27].

Since each individual element T_i is Lipschitz, the Jones parameter $C_U(T_i)$ and the constant $C_P(T_i)$ in Poincaré's inequality are both bounded.

Lemma 4.3 ([22]). *For each element T_i we fix a ball B_i enclosing T_i with*

$$B_i \supset \overline{T_i}, \qquad \operatorname{dist}(\partial B_i, \partial T_i) \;\geq\; \tfrac{1}{2}\operatorname{diam}(T_i), \tag{21}$$

and let the Jones parameter $C_U(B_i \setminus \overline{T}_i)$ and Poincaré's constant $C_P(B_i \setminus \overline{T}_i)$ be bounded. Then, there exists a positive constant $\widetilde{c}_{0,i}$ depending solely on $C_U(T_i)$, $C_P(T_i)$, $C_U(B_i \setminus \overline{T}_i)$ and $C_P(B_i \setminus \overline{T}_i)$ (or on upper bounds of these constants) such that

$$c_{0,i} \;\geq\; \widetilde{c}_{0,i} \;>\; 0.$$

In order to get a uniform bound for the constants $c_{0,i}$, we fix a ball B_i enclosing each element T_i and fulfilling (21), and we need the following assumption.

Assumption 4.2. *We assume that there are constants $C_U^* > 0$ and $C_P^* > 0$ such that, for all $i \in \{1, \dots, N\}$,*

$$\begin{aligned} C_U(T_i) \;&\leq\; C_U^*, \qquad & C_U(B_i \setminus \overline{T}_i) \;&\leq\; C_U^*, \\ C_P(T_i) \;&\leq\; C_P^*, \qquad & C_P(B_i \setminus \overline{T}_i) \;&\leq\; C_P^*. \end{aligned}$$

Due to Lemma 4.3, if Assumption 4.2 holds, then each of the constants $c_{0,i}$ is bounded away from zero by an expression which depends only on C_U^* and C_P^*. This also allows us to bound $c_{K,i}$ away from one, as it is given in terms of $c_{0,i}$.

Furthermore, as shown in the same work [22], if Assumption 4.2 is satisfied, we have the bound

$$\|z_i\|_{V_i} \;\leq\; C_V^* \|z_i\|_{H^{-1/2}(\Gamma_i)} \qquad \forall z_i \in H^{-1/2}(\Gamma_i), \tag{22}$$

with a constant C_V^* that is again uniformly bounded.

Remark. *Due to the technical reasons detailed above, we have to use two (different) regularity assumptions on the mesh. We believe that there is significant redundancy between Assumption 4.1 and Assumption 4.2, but so far we have not succeeded in proving a relationship between them.*

4.4. **Approximation error in the Dirichlet data.** Under the assumption of full H^2-regularity of the exact solution, we easily get the following result on skeletal approximation of the Dirichlet data by standard finite element approximation techniques on the auxiliary triangulation Ξ_i.

Theorem 4.4. *Let the mesh $(T_i)_{i=1}^N$ satisfy Assumption 4.1. Let $u_\Omega \in H^2(\Omega)$ be the exact solution of the domain variational formulation* (1)*, and $u \in W$ the solution of* (11)*. Assume furthermore that the given Dirichlet data $g \in H^{1/2}(\Gamma_S)$ is piecewise linear. Then we have*

$$\inf_{v_h \in W_h} \|u - v_h\|_S \;\leq\; C \Big(\sum_{i=1}^{N} h_i^2 \, |u_\Omega|^2_{H^2(T_i)} \Big)^{1/2} \;\leq\; C\, h \, |u_\Omega|_{H^2(\Omega)}, \tag{23}$$

where the constant C depends only on the regularity parameters from Assumption 4.1.

Proof. Due to Ξ_i being a conforming triangulation of T_i and the assumption of the element triangulations being matching across element boundaries, $\Xi = \bigcup_i \Xi_i$ describes a conforming regular triangulation of Ω. Let $V_h \subset H^1(\Omega)$ denote a standard finite element space of piecewise linear, globally continuous functions over Ξ. Choose $\phi_h \in V_h$ with $\phi_h|_\Gamma = g$ arbitrarily and set

$$\Phi_h := \gamma_S(\phi_h) - g \in W_h.$$

With this we estimate

$$\inf_{v_h \in W_h} \|\!|u - v_h|\!\|_S^2 \leq \|\!|u - \Phi_h|\!\|_S^2 = \sum_{i=1}^{N} |\mathcal{H}_i(u - \Phi_h)|^2_{H^1(T_i)}.$$

Note now that

$$\gamma_S(u_\Omega - \phi_h) = u + g - (\Phi_h + g) = u - \Phi_h,$$

and hence, by the energy-minimizing property of the harmonic extension,

$$|\mathcal{H}_i(u - \Phi_h)|_{H^1(T_i)} \leq |u_\Omega - \phi_h|_{H^1(T_i)} \qquad \forall i \in \{1, \dots, N\}.$$

Since ϕ_h was chosen arbitrarily, we obtain

$$\inf_{v_h \in W_h} \|\!|u - v_h|\!\|_S \leq \inf_{\substack{\phi_h \in V_h \\ \phi_h|_\Gamma = g}} |u_\Omega - \phi_h|_{H^1(\Omega)}.$$

We can thus apply standard approximation results for finite element spaces, see e.g. Ciarlet [7], to obtain the desired statement. ☐

4.5. **Approximation error in the Neumann data.** For technical reasons, we need the Sobolev-Slobodeckii seminorm in addition to the harmonic extension norm we have worked with so far. For every boundary face $f \in \mathcal{F}_i$, we define

$$|u|^2_{H^{1/2}_{\sim}(f)} := \int_f \int_f \frac{[u(x) - u(y)]^2}{|x - y|^3}\, ds_x\, ds_y, \tag{24}$$

which gives rise to the piecewise Sobolev-Slobodeckii seminorm on Γ_i,

$$|u|^2_{H^{1/2}_{\sim \mathrm{pw}}(\Gamma_i)} := \sum_{f \in \mathcal{F}_i} |u|^2_{H^{1/2}_{\sim}(f)}.$$

For approximating the Neumann data, we use the space of piecewise constant functions on Γ_i,

$$Z_{h,i} := \{v \in L_2(\Gamma_i) : v|_f \equiv \text{const.} \quad \forall f \in \mathcal{F}_i\}.$$

We introduce the L_2-projector $Q_{h,i} : L_2(\Gamma_i) \to Z_{h,i}$ via the unique solution of the variational problem for a given $u \in L_2(\Gamma_i)$,

$$\langle Q_{h,i} u,\, v_h \rangle_{L_2(\Gamma_i)} = \langle u,\, v_h \rangle_{L_2(\Gamma_i)} \qquad \forall v_h \in Z_{h,i}.$$

The projector $Q_{h,i}$ permits the following interpolation error estimate.

Theorem 4.5. *Let T_i be an element from a mesh fulfilling Assumption 4.1. Then, for all $w \in H^{1/2}_{\mathrm{pw}}(\Gamma_i)$, we have the error estimate*

$$\|w - Q_{h,i} w\|_{H^{-1/2}(\Gamma_i)} \leq C\, h_i\, |w|_{H^{1/2}_{\sim \mathrm{pw}}(\Gamma_i)}, \tag{25}$$

where the constant C depends solely on the constants from Assumption 4.1.

Proof. Postponed to Section A.4.

Additionally, we need the following Neumann trace inequality.

Theorem 4.6 (Neumann trace inequality). *Let T_i be an element from a mesh fulfilling Assumption 4.1. Then, for all $u \in H^2(T_i)$,*

$$|\gamma_i^1 u|_{H^{1/2}_{\sim\mathrm{pw}}(\Gamma_i)} \;\le\; C\,|u|_{H^2(T_i)},$$

where the constant C depends solely on the constants from Assumption 4.1.

Proof. Postponed to Section A.2.

With this, we have the tools at hand to prove the following approximation result for the Neumann data.

Theorem 4.7. *Let the mesh $(T_i)_{i=1}^N$ satisfy Assumption 4.1 and Assumption 4.2. Let $u_\Omega \in H^2(\Omega)$ be the exact solution of the domain variational formulation (1), $u \in W$ the solution of (11), and $w_i(u_g) = S_i(u_i + g_i)$ the exact local Neumann data on Γ_i. Then,*

$$\inf_{z_{h,i}\in Z_{h,i}} \|w_i(u_g) - z_{h,i}\|_{V_i} \;\le\; C\,h_i\,|u_\Omega|_{H^2(T_i)}$$

where the constant C depends solely on the regularity parameters from Assumption 4.1 and Assumption 4.2.

Proof. Due to Proposition 2.1, $w_i(u_g) = S_i(u_i+g_i) = \gamma_i^1 u_\Omega \in H^{1/2}_{\mathrm{pw}}(\Gamma_i)$. Using relation (22), Theorem 4.5, and Theorem 4.6, we estimate

$$\begin{aligned}
\inf_{z_{h,i}\in Z_{h,i}} \|w_i(u_g) - z_{h,i}\|_{V_i} &\le \|w_i(u_g) - Q_{h,i} w_i(u_g)\|_{V_i} \\
&\overset{(22)}{\le} C_V^*\,\|w_i(u_g) - Q_{h,i} w_i(u_g)\|_{H^{-1/2}(\Gamma_i)} \\
&\overset{\text{Thm.4.5}}{\le} C\,h_i\,|w_i(u_g)|_{H^{1/2}_{\sim\mathrm{pw}}(\Gamma_i)} \\
&= C\,h_i\,|\gamma_i^1 u_\Omega|_{H^{1/2}_{\sim\mathrm{pw}}(\Gamma_i)} \\
&\overset{\text{Thm.4.6}}{\le} C\,h_i\,|u_\Omega|_{H^2(T_i)}.
\end{aligned}$$

□

4.6. Final error estimate.

Theorem 4.8. *Let the mesh $(T_i)_{i=1}^N$ satisfy Assumption 4.1 and Assumption 4.2. Assume further that the given Dirichlet data g is piecewise linear. If $u_\Omega \in H^2(\Omega)$ is the exact solution of the variational formulation (1), and $u_h \in W_h$ is the solution of the discrete skeletal formulation (12), we have the error estimate*

$$|u_\Omega - \mathcal{H}_S(u_h+g)|_{H^1(\Omega)} \;\le\; C\Big(\sum_{i=1}^N h_i^2\,|u_\Omega|^2_{H^2(T_i)}\Big)^{1/2} \;\le\; C\,h\,|u_\Omega|_{H^2(\Omega)},$$

where the constant C depends solely on the regularity parameters from Assumption 4.1 and Assumption 4.2.

Proof. Note first that $u_\Omega = \mathcal{H}_S(u+g)$ and thus $u_\Omega - \mathcal{H}_S(u_h+g) = \mathcal{H}_S(u-u_h)$. From Lemma 4.2, we have

$$|\mathcal{H}_S(u-u_h)|_{H^1(\Omega)} \;\le\; C\left\{\inf_{v_h\in W_h} |\!|\!|u - v_h|\!|\!|_S + \Big(\sum_{i=1}^N \inf_{z_{h,i}\in Z_{h,i}} \|w_i(u) - z_{h,i}\|^2_{V_i}\Big)^{1/2}\right\}$$

with

$$C = \Big(1 + \frac{1}{\underline{c}_S}\Big) \max\Big\{1, \frac{\overline{c}_K}{\sqrt{1-\overline{c}_K}}\Big\}.$$

Due to Lemma 4.3, C can be bounded in terms of the regularity parameters.

Theorem 4.4 yields the Dirichlet approximation property

$$\inf_{v_h \in W_h} \|u - v_h\|_S \;\leq\; C \Big(\sum_{i=1}^{N} h_i^2 \, |u_\Omega|^2_{H^2(T_i)} \Big)^{1/2}.$$

The remaining terms can be treated using the Neumann approximation property from Theorem 4.7:

$$\inf_{z_{h,i} \in Z_{h,i}} \|w_i(u_g) - z_{h,i}\|_{V_i} \;\leq\; C\, h_i \, |u_\Omega|_{H^2(T_i)}.$$

□

5. Numerical results

To verify our theoretical results, we have implemented the BBFEM and performed several numerical tests. The implementation was done in C++ and builds upon the parmax framework by Pechstein and Copeland (see `http://www.numa.uni-linz.ac.at/P19255/software`). For the computation of the boundary element matrix entries, we use the approach of the ostbem library [24]: the inner (collocation) integral is computed analytically, while the outer integral is approximated by a 7-point quadrature. For the solution of the resulting symmetric positive definite linear system, we use a non-preconditioned CG method.

As a model problem, we choose the pure Dirichlet Laplace equation on the unit cube, $\Omega = (0,1)^3$:

$$\begin{aligned} -\Delta u &= 0 \qquad \text{in } \Omega, \\ u &= g \qquad \text{on } \partial\Omega. \end{aligned}$$

In all tests, we prescribe the exact solution $u(x,y,z) = \exp(x)\cos(y)(1+z)$.

We perform computations on two different mesh configurations. The first one is a standard regular tetrahedral mesh obtained by uniform refinement of a coarse mesh. The second one is derived from the first one by unifying some pairs of adjacent tetrahedra. This results in meshes consisting of both tetrahedra and polyhedra having 5 vertices, 9 edges and 6 faces. Some of the latter may be non-convex. Because our method places its degrees of freedom in element vertices, this unification procedure does not change the number of unknowns.

For computing the L_2-error, we use the representation formula from the theory of boundary integral operators to evaluate the solution at some inner points of the elements and perform quadrature. For computing the H^1-error, we estimate the gradient as a piecewise constant quantity from the computed Neumann data and again perform quadrature.

The results are shown in Table 1, where Table 1(a) gives the results for the tetrahedral meshes, while Table 1(b) gives the results for the mixed meshes. In each table, the first column gives the mesh size (here calculated as the maximum edge length). The second and third columns give the error in the H^1-seminorm and the L_2-norm, respectively. The final columns give the number of tetrahedra and polyhedra in each mesh.

In both cases, the H^1-error decays with $\mathcal{O}(h)$, as Theorem 4.8 predicts. Also, the L_2-error decays with $\mathcal{O}(h^2)$ in both experiments. Figure 3 visualizes these results graphically. As can be seen, the errors for the tetrahedral and mixed meshes are virtually undistinguishable.

(A) Results with tetrahedral mesh.

mesh size h	H^1-error	L^2-error	#tets
0.866025	0.923507	0.0879679	48
0.433013	0.459565	0.0223147	384
0.216506	0.226186	0.00549834	3,072
0.108253	0.109806	0.00131165	24,576
0.0541266	0.0537825	0.000315016	196,608
0.0270633	0.0264988	7.62441e-05	1,572,864

(B) Results with mixed mesh.

mesh size h	H^1-error	L^2-error	#tets	#polys
0.866025	0.867685	0.0842554	40	4
0.433013	0.433557	0.0214242	258	63
0.216506	0.214188	0.00522372	2,044	514
0.108253	0.103955	0.00124863	15,822	4,377
0.0541266	0.0508436	0.000304395	125,350	35,629
0.0270633	0.0251327	7.76704e-05	996,390	288,237

TABLE 1. Numerical results

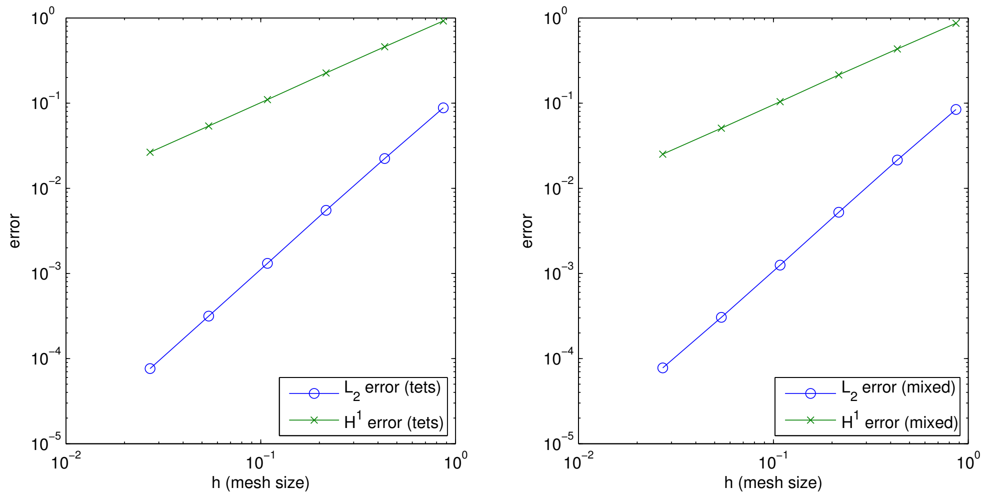

FIGURE 3. L_2- and H^1-error for tetrahedral and mixed mesh.

6. Conclusion and outlook

We have described in detail a discretization method for elliptic PDEs on polyhedral meshes introduced by Copeland, Langer and Pusch [8] and analyzed it in the special case of the 3D Laplace equation. To our knowledge, our main result, Theorem 4.8, is the first rigorous error estimate for a method of this type. Our numerical tests confirm the convergence rates which the theory suggests.

Due to the inconsistency introduced by approximating the local Dirichlet-to-Neumann maps S_i, the usual Aubin-Nitsche duality argument is not applicable. It is therefore an open question how to obtain L_2 error estimates, although all numerical experiments so far seem to indicate that convergence in the L_2-norm is optimal.

Our aim for further work is to investigate the BBFEM for solving diffusion-convection-reaction problems of the form

$$-\mathrm{div}(A(x)\nabla u(x)) + b(x)\cdot\nabla u(x) + c(x)u(x) = f(x)$$

with piecewise constant coefficient functions

$$A:\mathbb{R}^d \to \mathbb{R}^{d\times d}, \quad b:\mathbb{R}^d \to \mathbb{R}^d, \quad c:\mathbb{R}^d \to \mathbb{R}.$$

For this case, fundamental solutions are explicitly known [23, 20] and our method can be applied to the discretization of diffusion-convection-reaction problems with piecewise constant coefficient functions.

Appendix A. Proofs of some element-local properties

In the proof of our error estimates, we—perhaps surprisingly—found that among the greatest technical challenges was obtaining approximation properties for piecewise constant boundary functions which are valid on the quite general polyhedral elements we consider. This appendix serves to provide some technical results which we have used without proof in the main part of the article. Specifically, our aim here is to prove Theorem 4.5 and Theorem 4.6. Since all relevant properties can be analyzed locally, we simplify the notation by omitting the element index subscript in the following; e.g., we write T for an element T_i.

A.1. **Transformation properties.** Throughout this appendix, we assume that $T \subset \mathbb{R}^3$ is a polyhedral element from a mesh satisfying Assumption 4.1. That is, T has a regular triangulation Ξ with at most $N_{\mathcal{F}}$ boundary triangles $\mathcal{F}$. Note that for every boundary triangle $f \in \mathcal{F}$, there exists exactly one tetrahedron $\tau_f \in \Xi$ having f as one of its faces.

We write

$$\triangle_d \;:=\; \{(x_1,\dots,x_d)^\top \in \mathbb{R}^d : x_i > 0,\, x_1+\ldots+x_d < 1\}$$

for the unit simplex in $\mathbb{R}^d$. For any tetrahedron $\tau \in \Xi$, we fix an affine mapping $F_\tau : \mathbb{R}^3 \to \mathbb{R}^3$ such that $F_\tau(\triangle_3) = \tau$. The Jacobian of this mapping is denoted by $J_\tau = \nabla F_\tau \in \mathbb{R}^{3\times 3}$.

From the regularity conditions (18) and (19), we easily derive the property

$$\underline{c}_2(\mathrm{diam}\,\tau)\,|\xi| \;\le\; |J_\tau \xi| \;\le\; \overline{c}_2(\mathrm{diam}\,\tau)\,|\xi| \qquad \forall \xi \in \mathbb{R}^3, \tag{26}$$

which describes how lengths transform under F_τ.

In the following we show that regularity of Ξ implies regularity of $\mathcal{F}$.

Lemma A.1. *Let Ξ be a regular tetrahedral triangulation. Then for every triangular face $f \in \mathcal{F}$ and every tetrahedron $\tau = \tau_f \in \Xi$ with $f \subset \partial\tau$, we have*

$$\underline{c}_2 \mathrm{diam}\,\tau \;\le\; \mathrm{diam}\, f \;\le\; \mathrm{diam}\,\tau, \tag{27}$$

$$\frac{\underline{c}_1}{2\overline{c}_2}(\mathrm{diam}\,\tau)^2 \;\le\; |f| \;\le\; \frac{1}{2}(\mathrm{diam}\,\tau)^2, \tag{28}$$

where $|f|$ denotes the area of the triangle f.

Proof. The estimate $\operatorname{diam} f \leq \operatorname{diam} \tau$ is trivial as $\overline{f} \subset \overline{\tau}$. From this we easily get

$$|f| \;\leq\; \frac{1}{2}(\operatorname{diam} f)^2 \;\leq\; \frac{1}{2}(\operatorname{diam} \tau)^2,$$

and thus the upper bounds are proved.

For the lower bounds, let ξ_1 through ξ_4 denote the vertices of the unit tetrahedron $\triangle_3$. The vertices of τ are then given by $x_i = F_\tau(\xi_i)$, $i = 1, \ldots, 4$. Clearly, the diameter of f is the length of an edge, say (x_i, x_j), of τ. We have

$$\operatorname{diam} f \;=\; |x_i - x_j| \;=\; |F_\tau(\xi_i) - F_\tau(\xi_j)| \;=\; |J_\tau(\xi_i - \xi_j)| \;\overset{(26)}{\geq}\; \underline{c}_2 \operatorname{diam} \tau \, |\xi_i - \xi_j| \,.$$

Since $|\xi_i - \xi_j|$ is the length of an edge of the unit tetrahedron, it is clear that $|\xi_i - \xi_j| \geq 1$, which finishes the proof of (27).

For the lower area bound, let x_i, x_j, x_k be the vertices of f. With $y_1 := x_j - x_i$ and $y_2 := x_k - x_i$, the area of the triangle is given by $|f| = \frac{1}{2}\,|y_1 \times y_2|$. Furthermore, $\hat{f} := F_\tau^{-1}(f)$ is a face of $\triangle_3$, and we have $\left|\hat{f}\right| = \frac{1}{2}\,|\eta_1 \times \eta_2|$ with

$$\eta_1 \;=\; \xi_j - \xi_i \;=\; F_\tau^{-1}(x_j) - F_\tau^{-1}(x_i) \;=\; J_\tau^{-1}(x_j - x_i) = J_\tau^{-1} y_1,$$

and analogously $\eta_2 = J_\tau^{-1} y_2$. Thus we may estimate

$$\begin{aligned} \tfrac{1}{2} \;=\; |\hat{f}| \;=\; \tfrac{1}{2}\,|\eta_1 \times \eta_2| \;&=\; \tfrac{1}{2}\,\left|J_\tau^{-1} y_1 \times J_\tau^{-1} y_2\right| \\ &\overset{(*)}{=}\; \tfrac{1}{2}\,\left|\det J_\tau^{-1}\right| \left|J_\tau^{\top}(y_1 \times y_2)\right| \;\leq\; \tfrac{1}{2}\,\underline{c}_1^{-1}\,(\operatorname{diam}\tau)^{-3}\,\overline{c}_2\,(\operatorname{diam}\tau)\,2\,|f|\,, \end{aligned}$$

where we have used that $\det(J_\tau^{-1}) = (\det J_\tau)^{-1}$ and $\|J_\tau^\top\|_{\ell_2} = \|J_\tau\|_{\ell_2}$. The identity marked with $(*)$ stems from the following elementary property of the cross product that can easily be checked by direct calculation: for any non-singular matrix $A \in \mathbb{R}^{3\times 3}$,

$$Ay_1 \times Ay_2 \;=\; (\det A) A^{-\top}(y_1 \times y_2). \qquad \square$$

We also need some norm scaling relations for transforming functions to and from the unit tetrahedron.

Lemma A.2. *Let f be a face of a tetrahedron τ from a regular triangulation and $\hat{f} := F_\tau^{-1}(f)$ the corresponding triangle on the unit tetrahedron $\triangle_3$.*

Let $\phi \in H^{1/2}(f)$ and denote by $\hat{\phi} = \phi \circ F_\tau$ the pullback of ϕ to $\hat{f}$. Then,

$$|\phi|_{H_\sim^{1/2}(f)} \;\leq\; \underline{c}_2^{-3/2}\,(\operatorname{diam}\tau)^{1/2}\,|\hat{\phi}|_{H_\sim^{1/2}(\hat{f})} \tag{29}$$

with the Sobolev-Slobodeckii seminorm as defined in (24).

Let $u \in H^1(\tau)$ and denote by $\hat{u} = u \circ F_\tau$ the pullback of u to $\triangle_3$. Then,

$$\underline{c}_1^{1/2}\,\overline{c}_2^{-1}\,(\operatorname{diam}\tau)^{1/2}\,|\hat{u}|_{H^1(\triangle_3)} \;\leq\; |u|_{H^1(\tau)} \;\leq\; \overline{c}_1^{1/2}\,\underline{c}_2^{-1}\,(\operatorname{diam}\tau)^{1/2}\,|\hat{u}|_{H^1(\triangle_3)}. \tag{30}$$

Proof. Let $F_f, F_{\hat{f}} : \mathbb{R}^2 \to \mathbb{R}^3$ denote affine mappings such that $F_f(\triangle_2) = f$, $F_{\hat{f}}(\triangle_2) = \hat{f}$, and $F_f = F_\tau \circ F_{\hat{f}}$. Note that $\left|\frac{\partial F_f}{\partial x_1} \times \frac{\partial F_f}{\partial x_2}\right| = 2\,|f|$. For a suitable real-valued function ϕ defined on f, we see that

$$\begin{aligned}\int_f \phi(x)\,ds_x &= 2\,|f|\int_{\triangle_2}\phi(F_f(\xi))\,d\xi = 2\,|f|\int_{\triangle_2}\phi(F_\tau(F_{\hat f}(\xi)))\,d\xi \\ &= \frac{|f|}{|\hat f|}\int_{\hat f}\phi(F_\tau(x))\,ds_x = \frac{|f|}{|\hat f|}\int_{\hat f}\hat\phi(x)\,ds_x.\end{aligned} \tag{31}$$

For the Sobolev-Slobodeckii seminorm, the above identity gives us

$$\begin{aligned}|\phi|^2_{\underset{\sim}{H}^{1/2}(f)} &= \int_f\int_f \frac{|\phi(x)-\phi(y)|^2}{|x-y|^3}\,ds_x\,ds_y \\ &= \left(\frac{|f|}{|\hat f|}\right)^2 \int_{\hat f}\int_{\hat f}\frac{|\hat\phi(\xi)-\hat\phi(\eta)|^2}{|J_\tau(\xi-\eta)|^3}\,ds_\xi\,ds_\eta.\end{aligned}$$

Using the regularity relations (28) and (26) we obtain

$$|\phi|^2_{\underset{\sim}{H}^{1/2}(f)} \le \underline{c}_2^{-3}\left(\frac{(\operatorname{diam}\tau)^2}{2|\hat f|}\right)^2(\operatorname{diam}\tau)^{-3}\int_{\hat f}\int_{\hat f}\frac{|\hat\phi(\xi)-\hat\phi(\eta)|^2}{|\xi-\eta|^3}\,ds_\xi\,ds_\eta.$$

Noting finally that $|\hat f| \ge \frac{1}{2}$, we get (29).

The remaining statement (30) is shown by standard transformation arguments from finite element analysis, and we omit the proof. ☐

A.2. **Trace inequalities.** In this section we derive trace inequalities for T with constants which depend solely on the regularity parameters of its triangulation. First we consider a single tetrahedron τ with associated trace operator $\gamma_\tau : H^1(\tau) \to H^{1/2}(\partial\tau)$.

Lemma A.3. *For a tetrahedron τ from a regular triangulation and one of its faces, f, we have the Dirichlet trace inequality*

$$|\gamma_\tau u|_{\underset{\sim}{H}^{1/2}(f)} \le c_\gamma^\tau\,|u|_{H^1(\tau)} \qquad \forall u \in H^1(\tau) \tag{32}$$

with a trace constant $c_\gamma^\tau > 0$ which depends solely on the regularity parameters.

Proof. By a standard embedding argument, there exists a true constant $c_\gamma > 0$ such that for every face $\hat f$ of the unit tetrahedron $\triangle_3$, we have

$$|\gamma_{\triangle_3} u|_{\underset{\sim}{H}^{1/2}(\hat f)} \le c_\gamma\,|u|_{H^1(\triangle_3)} \qquad \forall u \in H^1(\triangle_3), \tag{33}$$

with the trace operator $\gamma_{\triangle_3} : H^1(\triangle_3) \to H^{1/2}(\partial\triangle_3)$. Using the transformation relations from Lemma A.2, we obtain

$$\begin{aligned}|\gamma_\tau u|_{\underset{\sim}{H}^{1/2}(f)} &\overset{(29)}{\le} \underline{c}_2^{-3/2}(\operatorname{diam}\tau)^{1/2}|\gamma_{\triangle_3}\hat u|_{\underset{\sim}{H}^{1/2}(\hat f)} \\ &\overset{(33)}{\le} c_\gamma\,\underline{c}_2^{-3/2}\,(\operatorname{diam}\tau)^{1/2}|\hat u|_{H^1(\triangle_3)} \\ &\overset{(30)}{\le} c_\gamma\,\underline{c}_1^{-1/2}\,\overline{c}_2\,\underline{c}_2^{-3/2}\,|u|_{H^1(\tau)}.\end{aligned}$$ ☐

This result extends straightforwardly to the piecewise Sobolev-Slobodeckii seminorm on the boundary of a polyhedral element.

Lemma A.4. *If the element T has a regular triangulation, then*

$$|\gamma_T u|_{H^{1/2}_{\sim\mathrm{pw}}(\partial T)} \;\leq\; 2\, c_\gamma^\tau\, |u|_{H^1(T)} \qquad \forall u \in H^1(T). \tag{34}$$

Proof. We fix $u \in H^1(T)$ and calculate

$$|\gamma_T u|^2_{H^{1/2}_{\sim\mathrm{pw}}(\partial T)} \;=\; \sum_{f\in\mathcal{F}} |\gamma_{\tau_f} u|^2_{H^{1/2}_\sim(f)} \;\overset{(32)}{\leq}\; (c_\gamma^\tau)^2 \sum_{f\in\mathcal{F}} |u|^2_{H^1(\tau_f)}.$$

Since every tetrahedron τ_f has four sides, every $\tau \in \Xi$ occurs at most four times in the rightmost sum. Thus we may further estimate

$$|\gamma_T u|^2_{H^{1/2}_{\sim\mathrm{pw}}(\partial T)} \;\leq\; 4\,(c_\gamma^\tau)^2 \sum_{\tau\in\Xi} |u|^2_{H^1(\tau)} \;=\; 4\,(c_\gamma^\tau)^2\, |u|^2_{H^1(T)}. \qquad \square$$

With this result we are able to prove the Neumann trace inequality used in our error estimates.

Proof of Theorem 4.6. On every boundary triangle $f \in \mathcal{F}$, there is a uniquely defined and constant outwards normal vector $n_f \in \mathbb{R}^3$ with $|n_f| = 1$. On a single face $f \in \mathcal{F}$ lying on the tetrahedron τ, by using the triangle inequality and then the Cauchy-Schwarz inequality, we get

$$\begin{aligned}
\big|\gamma_\tau^1 u\big|_{H^{1/2}_\sim(f)} \;&=\; \big|(\gamma_\tau \nabla u)\cdot n_f\big|_{H^{1/2}_\sim(f)} \;=\; \Big|\sum_{k=1}^{3} (\gamma_\tau \nabla u)_k\,(n_f)_k\Big|_{H^{1/2}_\sim(f)} \\
&\leq\; \sum_{k=1}^{3} |(n_f)_k|\;\big|(\gamma_\tau\nabla u)_k\big|_{H^{1/2}_\sim(f)} \;\leq\; |n_f|\,\Big(\sum_{k=1}^{3}\big|(\gamma_\tau\nabla u)_k\big|^2_{H^{1/2}_\sim(f)}\Big)^{1/2} \\
&=\; \Big(\sum_{k=1}^{3}\Big|\gamma_\tau \frac{\partial u}{\partial x_k}\Big|^2_{H^{1/2}_\sim(f)}\Big)^{1/2}.
\end{aligned}$$

With this we obtain that on the entire boundary,

$$\begin{aligned}
|\gamma_T^1 u|^2_{H^{1/2}_{\sim\mathrm{pw}}(\partial T)} \;&=\; \sum_{f\in\mathcal{F}} |\gamma_{\tau_f}^1 u|^2_{H^{1/2}_\sim(f)} \;\leq\; \sum_{f\in\mathcal{F}}\sum_{k=1}^{3}\Big|\gamma_{\tau_f}\frac{\partial u}{\partial x_k}\Big|^2_{H^{1/2}_\sim(f)} \\
&=\; \sum_{k=1}^{3}\Big|\gamma_T\frac{\partial u}{\partial x_k}\Big|^2_{H^{1/2}_{\sim\mathrm{pw}}(\partial T)} \;\overset{(34)}{\leq}\; 4\,(c_\gamma^\tau)^2\sum_{k=1}^{3}\Big|\frac{\partial u}{\partial x_k}\Big|^2_{H^1(T)} \;=\; 4\,(c_\gamma^\tau)^2\,|u|^2_{H^2(T)}. \qquad \square
\end{aligned}$$

A.3. **An auxiliary harmonic extension norm.** For our final approximation result, we will make use of a more general version of the norm defined via the harmonic extension, namely one which is defined on arbitrary parts of the surface. This first requires a generalization of the harmonic extension operator. For any Lipschitz domain D and some surface component $t \subseteq \partial D$ with positive measure, we define

$$\mathcal{H}_{t\to D} : H^{1/2}(t) \to H^1(D) :\; u \mapsto \underset{\substack{\phi\in H^1(D)\\ \phi|_t = u}}{\arg\min}\, |\phi|_{H^1(D)}.$$

The previously introduced harmonic extension operator may be seen as a special case of this definition: $\mathcal{H}_i = \mathcal{H}_{\partial T_i \to T_i}$. With this notation, we define a seminorm on $H^{1/2}(t)$ given by

$$|u|_{H^{1/2}(t,D)} := |\mathcal{H}_{t\to D} u|_{H^1(D)} = \inf_{\substack{\phi\in H^1(D)\\ \phi|_t = u}} |\phi|_{H^1(D)} \qquad \forall u \in H^{1/2}(t).$$

Again, this may be viewed as a generalization of $|\cdot|_{H^{1/2}(\partial D)} = |\cdot|_{H^{1/2}(\partial D,D)}$.

It is of interest to know how this seminorm relates to the previously introduced Sobolev-Slobodeckii seminorm. For our purposes, the following simple result will suffice.

Lemma A.5. *Let $\tau \in \Xi$ be a tetrahedron from a regular triangulation, and let $f \subset \partial\tau$ be one of its faces. For every $v \in H^{1/2}(f)$, we have*

$$|v|_{\underset{\sim}{H}^{1/2}(f)} \leq C\,|v|_{H^{1/2}(f,\tau)} \tag{35}$$

with a constant C that depends solely on the regularity parameters.

Proof. Using the trace inequality, we easily get

$$|v|_{\underset{\sim}{H}^{1/2}(f)} = |\gamma_\tau \mathcal{H}_{f\to\tau} v|_{\underset{\sim}{H}^{1/2}(f)} \overset{(32)}{\leq} c_\gamma^\tau\,|\mathcal{H}_{f\to\tau} v|_{H^1(\tau)} = c_\gamma^\tau |v|_{H^{1/2}(f,\tau)}. \qquad \square$$

The following lemma gives some indication of the monotonic behavior of the new seminorm when either the domain into which extends or the surface component on which it is defined is restricted.

Lemma A.6. *Let $D' \subset D$ be Lipschitz domains and $t' \subset t \subseteq \partial D' \cap \partial D$ surface components with positive measure. Then, for every $v \in H^{1/2}(t)$, we have*

$$|v|_{H^{1/2}(t,D')} \leq |v|_{H^{1/2}(t,D)}, \tag{36}$$

$$|v|_{H^{1/2}(t',D)} \leq |v|_{H^{1/2}(t,D)}. \tag{37}$$

Proof. We observe that

$$|\mathcal{H}_{t\to D'} v|_{H^1(D')} \leq |\mathcal{H}_{t\to D} v|_{H^1(D')} \leq |\mathcal{H}_{t\to D} v|_{H^1(D)},$$

where the first inequality holds because of the energy-minimizing property of the harmonic extension. This proves the first statement.

Because of $t' \subset t$, it is clear that

$$\{u \in H^1(D) : u|_{t'} = v\} \supseteq \{u \in H^1(D) : u|_t = v\},$$

and thus the minimum that is attained over the left set is smaller than that over the right one. This proves the second statement. $\square$

We now return to the polyhedral element T. For $u \in H^{1/2}_{\mathrm{pw}}(\partial T)$, we define the seminorm

$$|u|^2_{H^{1/2}_{\mathrm{pw}}(\partial T)} := \sum_{f\in\mathcal{F}} |u|^2_{H^{1/2}(f,\tau_f)}.$$

If $u \in H^{1/2}(\partial T)$, then by applying (36) and (37) we immediately obtain

$$|u|_{H^{1/2}_{\mathrm{pw}}(\partial T)} \leq \sqrt{N_{\mathcal{F}}}\,|u|_{H^{1/2}(\partial T,T)} = \sqrt{N_{\mathcal{F}}}\,|u|_{H^{1/2}(\partial T)}. \tag{38}$$

A.4. **Approximation properties.** We now study approximation properties for piecewise constant boundary functions on ∂T. The final aim of this section is the proof of Theorem 4.5. We follow quite closely the approach by Steinbach [26].

Recall the L_2-projector Q_h into the space of piecewise constant functions Z_h on ∂T introduced in Section 4.3. It is easy to see that the values of the projection are given by

$$(Q_h u)|_f \equiv \frac{1}{|f|} \int_f u(y)\, ds_y \qquad \text{for } f \in \mathcal{F}. \tag{39}$$

Lemma A.7. *Let Ξ be a regular triangulation of T and $f \in \mathcal{F}$ a boundary face. For $u \in H^{1/2}_{\mathrm{pw}}(\partial T)$, we have the error estimates*

$$\begin{aligned} \|u - Q_h u\|_{L_2(f)} &\le \sqrt{\frac{2\,\overline{c}_2}{\underline{c}_1}}\,(\operatorname{diam} f)^{1/2}\, |u|_{\underset{\sim}{H}^{1/2}(f)}, \\ \|u - Q_h u\|_{L_2(\partial T)} &\le C\,(\operatorname{diam} T)^{1/2}\, |u|_{\underset{\sim}{H}^{1/2}_{\mathrm{pw}}(\partial T)} \end{aligned} \tag{40}$$

with a constant C which depends solely on the regularity parameters.

Proof. Because of (39), we have

$$u(x) - Q_h u(x) = \frac{1}{|f|} \int_f [u(x) - u(y)]\, ds_y \qquad \text{for } x \in f.$$

Squaring this relation and using the Cauchy-Schwarz inequality yields

$$\begin{aligned} |u(x) - Q_h u(x)|^2 &= \frac{1}{|f|^2} \left(\int_f [u(x) - u(y)]\, ds_y \right)^2 \\ &= \frac{1}{|f|^2} \Big(\int_f \frac{[u(x) - u(y)]}{|x-y|^{3/2}}\, |x-y|^{3/2}\, ds_y \Big)^2 \\ &\le \frac{1}{|f|^2} \int_f \frac{[u(x) - u(y)]^2}{|x-y|^3}\, ds_y \int_f |x-y|^3\, ds_y \\ &\le (\operatorname{diam} f)^3\, \frac{1}{|f|} \int_f \frac{[u(x) - u(y)]^2}{|x-y|^3}\, ds_y. \end{aligned}$$

Estimating $|f|$ from below using the regularity condition (28) and integrating over f proves the first statement. The second statement follows by summing up over all $f \in \mathcal{F}$ and using that $\operatorname{diam} f \le \operatorname{diam} T$. ◻

With Lemma A.7, we can finally prove the approximation property used in our error estimates using an Aubin-Nitsche duality argument.

Proof of Theorem 4.5. By the definition of the dual norm and of the L_2-projection Q_h, and per the Cauchy-Schwarz inequality, we have

$$\begin{aligned} \|w - Q_h w\|_{H^{-1/2}(\partial T)} &= \sup_{v \in H^{1/2}(\partial T)} \frac{\langle w - Q_h w,\, v\rangle_{L_2(\partial T)}}{\|v\|_{H^{1/2}(\partial T)}} \\ &= \sup_{v \in H^{1/2}(\partial T)} \frac{\langle w - Q_h w,\, v - Q_h v\rangle_{L_2(\partial T)}}{\|v\|_{H^{1/2}(\partial T)}} \\ &\le \|w - Q_h w\|_{L_2(\partial T)} \sup_{v \in H^{1/2}(\partial T)} \frac{\|v - Q_h v\|_{L_2(\partial T)}}{\|v\|_{H^{1/2}(\partial T)}}. \end{aligned}$$

We estimate $\|w - Q_h w\|_{L_2(\partial T)}$ using (40). For $\|v - Q_h v\|_{L_2(\partial T)}$, we again use (40) and then estimate

$$\begin{aligned} \|v - Q_h v\|_{L_2(\partial T)} &\le C\,(\operatorname{diam} T)^{1/2}\, |v|_{\widetilde{H}^{1/2}_{\mathrm{pw}}(\partial T)} \\ &= C\,(\operatorname{diam} T)^{1/2} \Big(\sum_{f \in \mathcal{F}} |v|^2_{\widetilde{H}^{1/2}(f)} \Big)^{1/2} \overset{(35)}{\le} C\,(\operatorname{diam} T)^{1/2} \Big(\sum_{f \in \mathcal{F}} |v|^2_{H^{1/2}(f,\tau_f)} \Big)^{1/2} \\ &= C\,(\operatorname{diam} T)^{1/2}\, |v|_{H^{1/2}_{\mathrm{pw}}(\partial T)} \overset{(38)}{\le} C\,\sqrt{N_{\mathcal{F}}}\,(\operatorname{diam} T)^{1/2}\, |v|_{H^{1/2}(\partial T)}. \end{aligned}$$

Since we assumed that $N_{\mathcal{F}}$ is a uniform, small bound on the number of boundary triangles per element, we may subsume it into the generic constant C. Combined, these estimates yield the statement of Theorem 4.5. □

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