

On the coupling of VEM and BEM in two and three dimensions*

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Dedicated to Professor Dr. George C. Hsiao on the occasion of his 85th birthday

Abstract

This paper introduces and analyzes the combined use of the virtual element method (VEM) and the boundary element method (BEM) to numerically solve linear transmission problems in 2D and 3D. As a model we consider an elliptic equation in divergence form holding in an annular domain coupled with the Laplace equation in the corresponding unbounded exterior region, together with transmission conditions on the interface and a suitable radiation condition at infinity. We employ the usual primal formulation in the bounded region, and combine it, by means of the Costabel & Han approach, with the boundary integral equation method in the exterior domain. As a consequence, and besides the original unknown of the model, its normal derivative in 2D, and both its normal derivative and its trace in the 3D case, are introduced as auxiliary non-virtual unknowns. Moreover, for the latter case, a new and more suitable variational formulation for the coupling is introduced. In turn, the main ingredients required by the discrete analyses include the virtual element subspaces for the domain unknowns, explicit polynomial subspaces for the boundary unknowns, and suitable projection and interpolation operators that allow to define the corresponding discrete bilinear forms. In particular, two VEM/BEM schemes are proposed in the three-dimensional case, one of them mimicking the non-symmetric interior penalty discontinuous Galerkin method. Then, as for the continuous formulations, the classical Lax-Milgram lemma is employed to derive the well-posedness of our coupled VEM-BEM scheme. Finally, a priori error estimates in the energy and weaker norms, and corresponding rates of convergence for the solution as well as for a fully computable projection of the virtual component of it, are provided.

Key words: virtual element method, boundary element method, coupling, transmission problem, error estimates

Mathematics subject classifications (2000): 65N38, 65N99, 65N12, 65N15

1 Introduction

The numerical solution of diverse linear and nonlinear boundary value problems in continuum mechanics by means of the virtual element method (VEM) has become a very active and promising research subject during the last few years. The VEM approach, which can be interpreted as an extension of the classical finite element technique to general polygonal and polyhedral meshes, as well

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as a generalization of the mimetic finite difference method to arbitrary degrees of accuracy and continuity properties, was first introduced and analyzed in [4] for a primal formulation of the Poisson problem. The idea underlying the VEM philosophy is twofold. On one hand, the discrete spaces are defined on meshes made of polygonal or polyhedral elements, and the corresponding basis functions are not known explicitly (which explains the concept *virtual* utilized), but only the degrees of freedom defining them uniquely on each element are required to implement the method. These degrees of freedom normally have to do with polynomial moments within each element and with traces and normal traces, both polynomial as well, on the boundaries of them. On the other hand, suitable projection operators and stabilizing terms are employed to define approximated bilinear forms that mimic the original ones and that provide still consistency and stability of the resulting discrete scheme. Among the several advantages of VEM, and besides the simplicity of the respective coding and the quality of the numerical results provided, we highlight the fact that the meshes are formed by nonoverlapping convex or nonconvex elements that can be of very general shape.

For a sample of the diverse developments and applications of VEM so far, including linear elasticity problems in 2D and 3D, the linear plate bending problem, the incorporation of further global regularity into the discrete solution, practical aspects of the computational implementation, the two-dimensional Steklov eigenvalue problem, and the acoustic vibration problem, we refer to [5], [6], [12], [13], [17], [33], and [51]. Additionally, the virtual element methods have also been extensively utilized in fluid mechanics. In particular, stream function-based, divergence free, and non-conforming virtual element methods for the classical velocity-pressure formulation of the Stokes equations have been developed in [2], [10], and [23], respectively, whereas a primal virtual element approach for the Darcy and Brinkman models is proposed in [56]. In turn, regarding the Navier-Stokes equations, we first mention [11], where a family of virtual element methods for the two-dimensional case is proposed, thus yielding the first work applying VEM to solve that nonlinear model. Furthermore, other contributions involving the application of VEM in fluid mechanics have mainly concentrated in the use of dual-mixed variational formulations, particularly pseudostress-based ones, which all go back to the basic principles of the mixed virtual element method established in [15]. In this regard, we refer to [20], [21], [22], [39] and [40], where mixed virtual element schemes for the Stokes equation, the linear and nonlinear Brinkman problems, the nonlinear Stokes equation arising from quasi-Newtonian Stokes flows, and the Navier-Stokes equations, have been introduced and analyzed. In particular, we highlight that the main novelty of [40] lies on the simultaneous use of virtual element subspaces for \mathbf{H}^1 and $\mathbb{H}(\mathbf{div})$ to approximate the velocity and pseudostress unknowns, respectively. Also, we stress that most of the aforementioned works have made extensive use of the exact computations of the L^2 -projections onto suitable spaces of polynomials, as explained in [1], [8] and [9].

On the other hand, boundary element method (BEM) is the name given to the Galerkin scheme of the classical boundary integral equation method, which consists of using the associated fundamental solutions to transform boundary value problems into equivalent equations holding only on the boundary of the underlying domain (see, e.g. [44] and [52] for further details). These equations are usually formed by boundary integral operators whose kernels depend on the aforementioned fundamental solutions, and whose densities are given by the Cauchy data of the solution of the original boundary value problem. Now, besides the use of BEM alone, we highlight that its combination with other procedures such as finite element method (FEM) or discontinuous Galerkin methods, which aims mainly to solve transmission problems, has been frequently utilized for many years in diverse applications. In particular, the most popular ways of coupling FEM and BEM are the Johnson & Nédélec and Costabel & Han procedures (cf. [16], [29], [42], [45], and [57]), which use the Green representation of the solution in the corresponding region. Initially, and during a couple of decades, the applicability of the former, being based on a single boundary integral equation and the Fredholm theory (as suggested by the compactness of a boundary integral operator involved), was restricted basically to transmission problems involving the Laplace operator. For other elliptic equations, such as the Lamé system, the

above-mentioned compactness did not hold and hence the technique could not be employed.

The above difficulty motivated the approaches by Costabel and Han in [29] and [42], respectively, which were both based on the addition of a boundary integral equation for the normal derivative (or traction in the case of elasticity). As a consequence, the former yielded a symmetric and non-positive definite scheme, whereas the latter, on the contrary, gave rise to a non-symmetric but elliptic system. However, since the only difference between them is the sign of a common integral identity, one simply refers to either one of them as the Costabel & Han method. In turn, the aforementioned drawback of the Johnson & Nédélec coupling method, was surprisingly solved in [53] (see also [55], [38] and [54]), where it was established that actually all Galerkin schemes for this approach are stable, thus expanding its use to other elliptic equations and to arbitrary polygonal/polyhedral regions. In addition, the corresponding extension to the coupling of mixed-FEM and BEM on Lipschitz-continuous domains was successfully developed later on in [48], and the particular application of the latter to the three dimensional exterior Stokes problem was analyzed in [36] and [37]. Further contributions dealing with the application of the Johnson & Nédélec and Costabel & Han coupling procedures to solve 2D and 3D problems, including nonlinear models, fluid-solid interaction, eddy current problems, coupling with mixed-FEM, non-conforming FEM, local discontinuous Galerkin, and hybridizable discontinuous Galerkin methods, can be found in [3], [18], [19], [24], [25], [28], [30], [34], [35], [41], [43], [47], [49], [50], and the references therein.

According to the above discussion, and in order to continue extending the applicability of VEM, as well as to continue developing the ability of BEM to be coupled with other numerical procedures, our purpose in this paper is to introduce and analyze, up to our knowledge for the first time, the combined use of VEM and BEM for solving a model transmission problem in 2D and 3D. Another reason that makes attractive the coupling of VEM and BEM lies on the fact, as commented in the previous paragraphs, that the densities of the boundary integral operators involved in the formulation of BEM coincide with some of the degrees of freedom employed by VEM, which certainly generates a natural way of performing the coupling. Indeed, this coincidence will be particularly important in our 2D case below, and on the other hand, it will suggest a suitable modification of our approach for the 3D problem.

The rest of this work is organized as follows. In Section 2 we describe the model problem, and then establish the main results concerning the continuous formulation to be employed in two dimensions. Next, in Section 3 we introduce and analyze the coupling of VEM and BEM for this 2D case. This section is splitted into preliminary results on VEM, the VEM/BEM scheme itself, solvability analysis and error estimates in the energy norm, error estimates in the $L^2(\Omega)$ -norm, and a fully computable approximation of the virtual component of the solution, for which its corresponding rates of convergence are also provided. Finally, in Section 4 we consider the 3D case, for whose analysis we adopt basically the same structure of Section 3. However, and differently from the 2D case, we make use of a new variational formulation specially introduced for this purpose, and propose and analyze two associated VEM/BEM schemes, one of them being motivated by the non-symmetric interior penalty discontinuous Galerkin method.

We end this section with some notations to be employed throughout the paper. Given a real number $r \geq 0$ and a polyhedron $\mathcal{O} \subseteq \mathbb{R}^d$, ($d = 2, 3$), we denote the norms and seminorms of the usual Sobolev space $H^r(\mathcal{O})$ by $\|\cdot\|_{r,\mathcal{O}}$ and $|\cdot|_{r,\mathcal{O}}$ respectively (cf. [46]), and we use the convention $L^2(\mathcal{O}) := H^0(\mathcal{O})$. Also, we recall that, for any $t \in [-1, 1]$, the spaces $H^t(\partial\mathcal{O})$ have an intrinsic definition (by localization) on the Lipschitz surface $\partial\mathcal{O}$ due to their invariance under Lipschitz coordinate transformations. Moreover, for all $t \in (0, 1]$, $H^{-t}(\partial\mathcal{O})$ is the dual of $H^t(\partial\mathcal{O})$ with respect to the pivot space $L^2(\partial\mathcal{O})$. In addition, for nonnegative integers k , \mathcal{P}_k is the space of polynomials of degree $\leq k$ with the convention $\mathcal{P}_{-1} = \{0\}$. Then, given a domain $D \subseteq \mathbb{R}^d$, $d \in \{2, 3\}$, $\mathcal{P}_k(D)$ represents the restriction of \mathcal{P}_k to D .

2 The model problem

Let Ω_0 and \mathcal{O} be two simply connected and bounded polygonal/polyhedral domains with boundaries $\Gamma_0 := \partial\Omega_0$ and $\Gamma := \partial\mathcal{O}$. We assume that $\Omega_0 \subseteq \mathcal{O} \subseteq \mathbb{R}^d$, with $d = 2, 3$, and introduce the annular region $\Omega := \mathcal{O} \setminus \overline{\Omega_0}$ and the exterior domain $\mathcal{O}_e := \mathbb{R}^d \setminus \overline{\mathcal{O}}$ (see Figure 2.1 below). Then, we denote by \mathbf{n} the unit outward normal to Γ pointing towards \mathcal{O}_e , and consider the transmission problem

$$\begin{aligned}
 -\operatorname{div}(\kappa \nabla u) &= f && \text{in } \Omega, \\
 u &= 0 && \text{on } \Gamma_0, \\
 u &= u_e && \text{on } \Gamma, \\
 \kappa \frac{\partial u}{\partial \mathbf{n}} &= \frac{\partial u_e}{\partial \mathbf{n}} && \text{on } \Gamma, \\
 -\Delta u_e &= 0 && \text{in } \mathcal{O}_e, \\
 u_e(x) &= O\left(\frac{1}{|x|}\right) && \text{as } |x| \rightarrow \infty,
 \end{aligned} \tag{2.1}$$

where $f \in L^2(\Omega)$ and $\kappa \in L^\infty(\Omega)$ are given functions. Additionally, we assume that there exists a constant $\underline{\kappa} > 0$ such that

$$\underline{\kappa} \leq \kappa(x) \leq \bar{\kappa} := \|\kappa\|_{L^\infty(\Omega)} \quad \forall x \in \Omega.$$

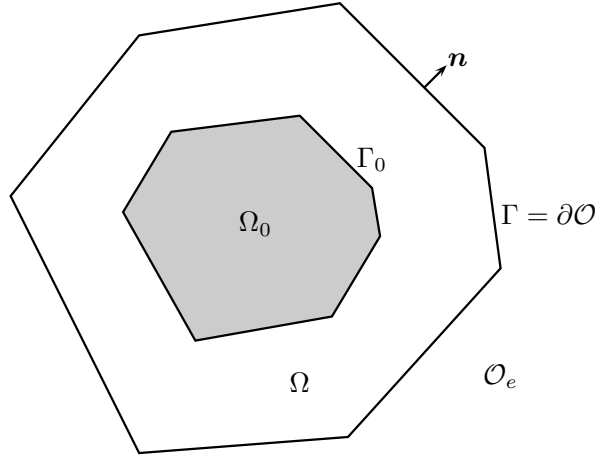


Figure 2.1: 2D geometry of the model problem.

In order to solve the transmission problem (2.1) by using only Ω as a computational domain, we follow the Costabel & Han approach (see [29], [42], [52] and the references therein), and compute the harmonic solution in the exterior domain \mathcal{O}_e by means of the integral representation formula

$$u_e(x) = \int_{\Gamma} \frac{\partial \mathbf{E}(|x-y|)}{\partial \mathbf{n}_y} \gamma u(y) ds_y - \int_{\Gamma} \mathbf{E}(|x-y|) \lambda(y) ds_y \quad \forall x \in \mathcal{O}_e, \tag{2.2}$$

where

$$\mathbf{E}(|x-y|) := \begin{cases} \frac{1}{4\pi} \frac{1}{|x-y|} & \text{if } d = 3 \\ -\frac{1}{2\pi} \log |x-y| & \text{if } d = 2 \end{cases}$$

is the fundamental solution of the Laplace operator, γ is the usual trace operator on Γ (acting either from Ω or \mathcal{O}_e), and $\gamma u = \gamma u_e$ and $\lambda := \kappa \nabla u \cdot \mathbf{n} = \frac{\partial u_e}{\partial \mathbf{n}}$ are the Cauchy data on this interface. Then,

employing the jump conditions on Γ of the two potentials in the right hand side of (2.2), we arrive at (cf. [44], [52])

$$\gamma u_e = \left(\frac{\text{id}}{2} + K\right)\gamma u - V\lambda \quad \text{on } \Gamma, \quad (2.3)$$

and

$$\frac{\partial u_e}{\partial \mathbf{n}} = -W\gamma u + \left(\frac{\text{id}}{2} - K^\mathfrak{t}\right)\lambda \quad \text{on } \Gamma, \quad (2.4)$$

where V , K , $K^\mathfrak{t}$ are the boundary integral operators representing the single, double and adjoint of the double layer, respectively, id is a generic identity operator, and W is the hypersingular operator. Moreover, replacing γu_e and $\frac{\partial u_e}{\partial \mathbf{n}}$ by γu and λ , respectively, (2.3) and (2.4) become

$$0 = \left(\frac{\text{id}}{2} - K\right)\gamma u + V\lambda \quad \text{on } \Gamma, \quad (2.5)$$

and

$$\lambda = -W\gamma u + \left(\frac{\text{id}}{2} - K^\mathfrak{t}\right)\lambda \quad \text{on } \Gamma. \quad (2.6)$$

From now on, $\langle \cdot, \cdot \rangle$ stands for the duality pairing between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$ with respect to the pivot space $L^2(\Gamma)$. Then, we introduce the subspaces

$$H_0^{1/2}(\Gamma) := \{\varphi \in H^{1/2}(\Gamma) : \langle 1, \varphi \rangle = 0\}$$

and

$$H_0^{-1/2}(\Gamma) := \{\mu \in H^{-1/2}(\Gamma) : \langle \mu, 1 \rangle = 0\},$$

and recall in the following lemma the main mapping properties of V , K , $K^\mathfrak{t}$, and W .

Lemma 2.1. *The operators*

$$\begin{aligned} V : H^{-1/2}(\Gamma) &\longrightarrow H^{1/2}(\Gamma), & K : H^{1/2}(\Gamma) &\longrightarrow H^{1/2}(\Gamma), \\ K^\mathfrak{t} : H^{-1/2}(\Gamma) &\longrightarrow H^{-1/2}(\Gamma), & W : H^{1/2}(\Gamma) &\longrightarrow H^{-1/2}(\Gamma), \end{aligned}$$

are continuous. Furthermore, there exist positive constants α_V , α_W such that

$$\langle \mu, V\mu \rangle \geq \alpha_V \|\mu\|_{-1/2, \Gamma}^2 \quad \begin{cases} \forall \mu \in H_0^{-1/2}(\Gamma), & \text{if } d = 2, \\ \forall \mu \in H^{-1/2}(\Gamma), & \text{if } d = 3, \end{cases} \quad (2.7)$$

and

$$\langle W\varphi, \varphi \rangle \geq \alpha_W \|\varphi\|_{1/2, \Gamma}^2 \quad \forall \varphi \in H_0^{1/2}(\Gamma). \quad (2.8)$$

Proof. See [52]. □

Then, introducing the spaces

$$X := \left\{v \in H^1(\Omega) : v|_{\Gamma_0} = 0\right\} \quad \text{and} \quad \mathbf{X} := X \times H_0^{-1/2}(\Gamma),$$

the variational formulation for the first four rows of (2.1) completed with the boundary integral equations (2.5) and (2.6), reads as follows: Find $(u, \lambda) \in \mathbf{X}$ such that

$$\begin{aligned} \int_{\Omega} \kappa \nabla u \cdot \nabla v + \langle W\gamma u, \gamma v \rangle - \langle \lambda, \left(\frac{\text{id}}{2} - K\right)\gamma v \rangle &= \int_{\Omega} f v & \forall v \in X, \\ \langle \mu, V\lambda \rangle + \langle \mu, \left(\frac{\text{id}}{2} - K\right)\gamma u \rangle &= 0 & \forall \mu \in H_0^{-1/2}(\Gamma). \end{aligned} \quad (2.9)$$

Equivalently, (2.9) can be rewritten as: Find $(u, \lambda) \in \mathbf{X}$ such that

$$\mathbf{A}((u, \lambda), (v, \mu)) = \mathbf{F}(v, \mu) := \int_{\Omega} f v \quad \forall (v, \mu) \in \mathbf{X}, \quad (2.10)$$

where

$$\begin{aligned} \mathbf{A}((u, \lambda), (v, \mu)) &:= a(u, v) + \langle W\gamma u, \gamma v \rangle + \langle \mu, V\lambda \rangle \\ &+ \langle \mu, (\frac{\text{id}}{2} - K)\gamma u \rangle - \langle \lambda, (\frac{\text{id}}{2} - K)\gamma v \rangle \end{aligned} \quad (2.11)$$

and

$$a(u, v) := \int_{\Omega} \kappa \nabla u \cdot \nabla v.$$

We deduce from Lemma 2.1 that there exist constants $M_0 > 0$ and $\alpha_0 > 0$ such that, for all $(u, \lambda), (v, \mu) \in \mathbf{X}$, there holds

$$\mathbf{A}((u, \lambda), (v, \mu)) \leq M_0 \|(u, \lambda)\| \|(v, \mu)\|$$

and

$$\mathbf{A}((v, \mu), (v, \mu)) \geq \alpha_0 \|(v, \mu)\|^2,$$

where

$$\|(v, \mu)\|^2 := \|v\|_{1, \Omega}^2 + \|\mu\|_{-1/2, \Gamma}^2.$$

stands for the square of the norm in the product space \mathbf{X} .

In this way, the well-posedness of problem (2.10) follows then directly from the foregoing estimates and the Lax-Milgram lemma.

We end this section by remarking that the transmission conditions imposed for the derivation of our continuous formulation are actually recovered from (2.10) and (2.2). In fact, we first notice that the second equation of (2.9) together with (2.3) yields $\gamma u = \gamma u_e$ on Γ . In turn, integrating by parts backwardly the field term of the first equation in (2.9), we deduce that $-\text{div}(k\nabla u) = f$ in Ω , and then that $\kappa \nabla u \cdot \mathbf{n} = -W\gamma u + (\frac{\text{id}}{2} - K^t)\lambda$, which, combined with (2.4), gives $\kappa \nabla u \cdot \mathbf{n} = \frac{\partial u_e}{\partial \mathbf{n}}$ on Γ . Then, knowing that u_e can also be represented with $\frac{\partial u_e}{\partial \mathbf{n}}$ instead of λ in (2.2), we deduce that $V\lambda = V \frac{\partial u_e}{\partial \mathbf{n}}$, and hence the ellipticity of V (cf. (2.7)) yields $\lambda = \frac{\partial u_e}{\partial \mathbf{n}} = \kappa \nabla u \cdot \mathbf{n}$.

3 The VEM/BEM coupling in two dimensions

3.1 Preliminaries

From now on we assume that there exists a polygonal partition $\cup_{i=1}^I \bar{\Omega}_i = \bar{\Omega}$ such that $f|_{\Omega_i} \in H^k(\Omega_i)$ and $\kappa|_{\Omega_i} \in W^{k+1, \infty}(\Omega_i)$, for $i = 1, \dots, I$. Then we let $\{\mathcal{F}_h\}_h$ be a family of partitions of $\bar{\Omega}$ constituted of connected polygons $F \in \mathcal{F}_h$ of diameter $h_F \leq h$, and assume that the meshes $\{\mathcal{F}_h\}_h$ are aligned with each Ω_i , $i = 1, \dots, I$. For each $F \in \mathcal{F}_h$ the boundary ∂F is subdivided into straight segments e , which are referred to in what follows as edges. In particular, we introduce the set

$$\mathcal{E}_h := \left\{ \text{edges of } \mathcal{F}_h : e \subseteq \Gamma \right\}.$$

In addition, we assume that the family $\{\mathcal{F}_h\}_h$ of meshes satisfy the following conditions: There exists $\rho \in (0, 1)$ such that

(A1) each F of $\{\mathcal{F}_h\}_h$ is star-shaped with respect to a disk D_F of radius ρh_F ,

(A2) for each F of $\{\mathcal{F}_h\}_h$ and for all edges $e \subseteq \partial F$ it holds $|e| \geq \rho h_F$.

Then, for each F of $\{\mathcal{F}_h\}_h$, we introduce the projection operator $\Pi_k^{\nabla, F} : \mathbf{H}^1(F) \rightarrow \mathcal{P}_k(F)$ uniquely characterized by (see [7])

$$\int_F \nabla(\Pi_k^{\nabla, F} v) \cdot \nabla p + \left(\int_{\partial F} \Pi_k^{\nabla, F} v \right) \left(\int_{\partial F} p \right) = \int_F \nabla v \cdot \nabla p + \left(\int_{\partial F} v \right) \left(\int_{\partial F} p \right) \quad (3.1)$$

for all $p \in \mathcal{P}_k(F)$. Moreover, we let Π_k^F be the $L^2(F)$ -orthogonal projection onto $\mathcal{P}_k(F)$ with vectorial counterpart $\mathbf{\Pi}_k^F : L^2(F)^2 \rightarrow \mathcal{P}_k(F)^2$, and following [1] we introduce, for $k \geq 1$, the local virtual element space

$$X_h^k(F) := \left\{ v \in \mathbf{H}^1(F) : v|_e \in \mathcal{P}_k(e), \forall e \subseteq \partial F, \Delta v \in \mathcal{P}_k(F), \quad \Pi_k^F v - \Pi_k^{\nabla, F} v \in \mathcal{P}_{k-2}(F) \right\}. \quad (3.2)$$

It can be shown (cf. [1]) that the degrees of freedom of $X_h^k(F)$ consist of:

- i) the values at the vertices of F ,
- ii) the moments of order $\leq k - 2$ on the edges of F , and
- iii) the moments of order $\leq k - 2$ on F .

We are then allowed to introduce the global virtual element space as

$$X_h^k := \left\{ v \in X : v|_F \in X_h^k(F) \quad \forall F \in \mathcal{F}_h \right\}.$$

On the other hand, for any integer $k \geq 0$, we denote by $\mathcal{P}_k(\mathcal{F}_h)$ the space of piecewise polynomials of degree $\leq k$ with respect to \mathcal{F}_h , and let $\Pi_k^{\mathcal{F}}$ be the global $L^2(\Omega)$ -orthogonal projection onto $\mathcal{P}_k(\mathcal{F}_h)$, which is assembled cellwise, i.e. $(\Pi_k^{\mathcal{F}} v)|_F := \Pi_k^F(v|_F)$ for all $F \in \mathcal{F}_h$ and for all $v \in L^2(\Omega)$. Similarly, for any $\mathbf{q} \in L^2(\Omega)^2$, $\mathbf{\Pi}_k^{\mathcal{F}} \mathbf{q}$ is defined by $(\mathbf{\Pi}_k^{\mathcal{F}} \mathbf{q})|_F = \mathbf{\Pi}_k^F(\mathbf{q}|_F)$ for all $F \in \mathcal{F}_h$. It is important to notice that $\mathcal{P}_k(F) \subseteq X_h^k(F)$ and that the projectors $\Pi_k^{\nabla, F} v$ and $\Pi_k^F v$ are computable for all $v \in X_h^k(F)$. Furthermore, it is also easy to check that $\mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla v$ is explicitly known for all $v \in X_h^k(F)$ (cf. [7]).

Hereafter, given any positive functions A_h and B_h of the mesh parameter h , the notation $A_h \lesssim B_h$ means that $A_h \leq C B_h$ with $C > 0$ independent of h , whereas $A_h \simeq B_h$ means that $A_h \lesssim B_h$ and $B_h \lesssim A_h$. Then, under the conditions on \mathcal{F}_h , the technique of averaged Taylor polynomials introduced in [32] permits to prove the following error estimates,

$$\|v - \Pi_k^F v\|_{0,F} + h_F \|v - \Pi_k^F v\|_{1,F} \lesssim h_F^{\ell+1} |v|_{\ell+1,F} \quad \forall \ell \in \{0, 1, \dots, k\}, \quad \forall v \in \mathbf{H}^{\ell+1}(F), \quad (3.3)$$

$$\|v - \Pi_k^{\nabla, F} v\|_{0,F} + h_F \|v - \Pi_k^{\nabla, F} v\|_{1,F} \lesssim h_F^{\ell+1} |v|_{\ell+1,F} \quad \forall \ell \in \{1, 2, \dots, k\}, \quad \forall v \in \mathbf{H}^{\ell+1}(F). \quad (3.4)$$

In turn, the local interpolation operator $I_k^F : \mathbf{H}^2(F) \rightarrow X_h^k(F)$ is defined by imposing that $v - I_k^F v$ has vanishing degrees of freedom, which satisfies (cf. [14, Lemma 2.23])

$$\|v - I_k^F v\|_{0,F} + h_F \|v - I_k^F v\|_{1,F} \lesssim h_F^{\ell+1} |v|_{\ell+1,F} \quad \forall \ell \in \{1, 2, \dots, k\}, \quad \forall v \in \mathbf{H}^{\ell+1}(F). \quad (3.5)$$

In addition, we denote by $I_k^{\mathcal{F}}$ the global virtual element interpolation operator, i.e., for each $v \in \mathcal{C}^0(\bar{\Omega})$, we set locally $(I_k^{\mathcal{F}} v)|_F = I_k^F(v|_F)$ for all $F \in \mathcal{F}_h$.

On the other hand, we will seek an approximation for λ in the non-virtual (but explicit) subspace

$$\Lambda_h^{k-1} := \left\{ \mu \in L^2(\Gamma) : \mu|_e \in P_{k-1}(e), \quad \forall e \in \mathcal{E}_h, \quad \int_{\Gamma} \mu = 0 \right\},$$

and denote by $\Pi_{k-1}^\mathcal{E}$ the $L^2(\Gamma)$ -orthogonal projection onto Λ_h^{k-1} . We let $\{\Gamma_j, j \in \{1, \dots, J\}\}$ be the set of segments constituting Γ , and for any $t \geq 0$ we consider the broken Sobolev space $H_b^t(\Gamma) := \prod_{j=1}^J H^t(\Gamma_j)$ endowed with the graph norm

$$\|\varphi\|_{t,b,\Gamma}^2 := \sum_{j=1}^J \|\varphi\|_{t,\Gamma_j}^2.$$

We recall the following classical approximation property.

Lemma 3.1. *Assume that $\mu \in H^{-1/2}(\Gamma) \cap H_b^r(\Gamma)$ for some $r \geq 0$. Then,*

$$\|\mu - \Pi_{k-1}^\mathcal{E} \mu\|_{-t,\Gamma} \lesssim h^{\min\{r,k\}+t} \|\mu\|_{r,b,\Gamma} \quad \forall t \in \{0, 1/2\}.$$

Proof. See [52, Theorem 4.3.20]. □

3.2 The VEM/BEM scheme

For all $F \in \mathcal{F}_h$ we let S_h^F be the symmetric bilinear form defined on $H^1(F) \times H^1(F)$ by

$$S_h^F(v, w) := h_F^{-1} \sum_{e \subseteq \partial F} \int_e \pi_k^e v \pi_k^e w \quad \forall v, w \in H^1(F), \quad (3.6)$$

where π_k^e is the $L^2(e)$ -projection onto $\mathcal{P}_k(e)$. It is shown in [14, Lemma 3.2] that

$$S_h^F(v, v) \simeq a^F(v, v) \quad \forall v \in X_h^k(F) \quad \text{such that} \quad \Pi_k^{\nabla, F} v = 0, \quad (3.7)$$

where a^F is the local version of a , that is

$$a^F(v, w) := \int_F \kappa \nabla v \cdot \nabla w \quad \forall v, w \in H^1(F). \quad (3.8)$$

It is important to notice that S_h^F is computable on $X_h^k(F) \times X_h^k(F)$ since $\pi_k^e v = v \in \mathcal{P}_k(e)$ for all $v \in X_h^k(F)$, and that, by symmetry, there holds

$$S_h^F(v, w) \leq S_h^F(v, v)^{1/2} S_h^F(w, w)^{1/2} \lesssim a^F(v, v)^{1/2} a^F(w, w)^{1/2}$$

for all $v, w \in X_h^k(F)$ satisfying $\Pi_k^{\nabla, F} v = \Pi_k^{\nabla, F} w = 0$. Next, for each $F \in \mathcal{F}_h$ we introduce

$$a_h^F(v, w) := \int_F \kappa \mathbf{\Pi}_{k-1}^F \nabla v \cdot \mathbf{\Pi}_{k-1}^F \nabla w + S_h^F(v - \Pi_k^{\nabla, F} v, w - \Pi_k^{\nabla, F} w), \quad (3.9)$$

and let a_h be the global extension of it, that is

$$a_h(v, w) = \sum_{F \in \mathcal{F}_h} a_h^F(v, w) \quad \forall v, w \in X_h^k. \quad (3.10)$$

We now stress, as shown in [7], that the first term defining a_h^F is also calculable on $X_h^k(F) \times X_h^k(F)$ even if κ is not a polynomial function. Indeed, using the fact that $\mathbf{\Pi}_{k-1}^F$ is self-adjoint and integrating by parts, we find that there holds

$$\begin{aligned} \int_F \kappa \mathbf{\Pi}_{k-1}^F \nabla v \cdot \mathbf{\Pi}_{k-1}^F \nabla w &= \int_F \mathbf{\Pi}_{k-1}^F (\kappa \mathbf{\Pi}_{k-1}^F \nabla v) \cdot \nabla w \\ &= - \int_F \operatorname{div} (\mathbf{\Pi}_{k-1}^F (\kappa \mathbf{\Pi}_{k-1}^F \nabla v)) w + \int_{\partial F} \mathbf{\Pi}_{k-1}^F (\kappa \mathbf{\Pi}_{k-1}^F \nabla v) \cdot \mathbf{n}_{\partial F} w \end{aligned}$$

for all $v, w \in X_h^k(F)$. Then, we notice that the first term on the right hand side of the foregoing identity is calculable thanks to the moments of w on F of order $\leq k-2$, whereas the second one is calculable as well since each factor of it is a known polynomial.

We now let $\mathbf{X}_h := X_h^k \times \Lambda_h^{k-1}$ and introduce the discrete version of problem (2.10): Find $(u_h, \lambda_h) \in \mathbf{X}_h$ such that

$$\mathbf{A}_h((u_h, \lambda_h), (v_h, \mu_h)) = \mathbf{F}_h(v_h, \mu_h) := \int_{\Omega} (\Pi_{k-1}^{\mathcal{F}} f) v_h \quad \forall (v_h, \mu_h) \in \mathbf{X}_h, \quad (3.11)$$

where

$$\begin{aligned} \mathbf{A}_h((u_h, \lambda_h), (v_h, \mu_h)) &:= a_h(u_h, v_h) + \langle W\gamma u_h, \gamma v_h \rangle + \langle \mu_h, V\lambda_h \rangle \\ &+ \langle \mu_h, (\frac{\text{id}}{2} - K)\gamma u_h \rangle - \langle \lambda_h, (\frac{\text{id}}{2} - K)\gamma v_h \rangle. \end{aligned} \quad (3.12)$$

3.3 Solvability and error estimates

We begin with the boundedness property of \mathbf{A}_h .

Lemma 3.2. *There hold*

$$|a_h^F(z, v)| \lesssim \|z\|_{1,F} \|v\|_{1,F} \quad \forall F \in \mathcal{F}_h, \quad \forall z, v \in \mathbf{H}^1(F), \quad (3.13)$$

and

$$|\mathbf{A}_h((z, \eta), (v, \mu))| \lesssim \|(z, \eta)\| \|(v, \mu)\| \quad \forall (z, \eta), (v, \mu) \in \mathbf{X}_h. \quad (3.14)$$

Proof. The local estimate (3.13) is basically consequence of the Cauchy-Schwarz inequality and the fact that (see [7])

$$S_h^F(z - \Pi_k^{\nabla, F} z, v - \Pi_k^{\nabla, F} v) \lesssim |z - \Pi_k^{\nabla, F} z|_{1,F} |v - \Pi_k^{\nabla, F} v|_{1,F} \lesssim |z|_{1,F} |v|_{1,F}, \quad (3.15)$$

whereas (3.14) follows from (3.13) and the mapping properties provided by Lemma 2.1. \square

Next, the following lemma recalls from [7] some useful estimates between a^F and a_h^F , which involve the local operators Π_k^F and I_k^F .

Lemma 3.3. *For each $F \in \mathcal{F}_h$ there hold*

$$|a^F(\Pi_k^F z, v_h) - a_h^F(\Pi_k^F z, v_h)| \lesssim h_F^k \|z\|_{k+1,F} \|v_h\|_{1,F} \quad \forall (z, v_h) \in \mathbf{H}^{k+1}(F) \times X_h^k(F), \quad (3.16)$$

$$|a^F(v_h, I_k^F z) - a_h^F(v_h, I_k^F z)| \lesssim h_F \|v_h\|_{1,F} \|z\|_{2,F} \quad \forall (z, v_h) \in \mathbf{H}^2(F) \times X_h^k(F), \quad (3.17)$$

and

$$|a^F(\Pi_k^F z, I_k^F v) - a_h^F(\Pi_k^F z, I_k^F v)| \lesssim h_F^{k+1} \|z\|_{k+1,F} \|v\|_{2,F} \quad \forall (z, v) \in \mathbf{H}^{k+1}(F) \times \mathbf{H}^2(F). \quad (3.18)$$

Proof. For (3.16) we refer to [7, Lemma 5.5], whereas (3.17) can be proved as explained in [7, Remark 5.1]. In turn, (3.18) follows by combining the proofs of (3.16) and (3.17). We omit further details. \square

We now establish the \mathbf{X}_h -ellipticity of the bilinear form \mathbf{A}_h .

Lemma 3.4. *There holds*

$$\mathbf{A}_h((v, \mu), (v, \mu)) \gtrsim \|(v, \mu)\|^2 \quad \forall (v, \mu) \in \mathbf{X}_h. \quad (3.19)$$

Proof. We first observe, by using (2.7) and (2.8), that for all $(v, \mu) \in \mathbf{X}_h$ we obtain

$$\mathbf{A}_h((v, \mu), (v, \mu)) = a_h(v, v) + \langle W\gamma v, \gamma v \rangle + \langle \mu, V\mu \rangle \geq a_h(v, v) + \alpha_V \|\mu\|_{-1/2, \Gamma}^2. \quad (3.20)$$

On the other hand, according to the definition of a_h^F (cf. (3.9)), noting that certainly there holds $\Pi_k^{\nabla, F}(v - \Pi_k^{\nabla, F}v) = 0$, and then employing (3.7) and the fact that

$$|v - \Pi_k^{\nabla, F}v|_{1, F} = \|\nabla v - \nabla \Pi_k^{\nabla, F}v\|_{0, F} \geq \|\nabla v - \Pi_{k-1}^F \nabla v\|_{0, F},$$

we deduce that

$$\begin{aligned} a_h^F(v, v) &\gtrsim \|\Pi_{k-1}^F \nabla v\|_{0, F}^2 + a^F(v - \Pi_k^{\nabla, F}v, v - \Pi_k^{\nabla, F}v) \\ &\gtrsim \left\{ \|\Pi_{k-1}^F \nabla v\|_{0, F}^2 + |v - \Pi_k^{\nabla, F}v|_{1, F}^2 \right\} \\ &\gtrsim \left\{ \|\Pi_{k-1}^F \nabla v\|_{0, F}^2 + \|\nabla v - \Pi_{k-1}^F \nabla v\|_{0, F}^2 \right\} \gtrsim |v|_{1, F}^2. \end{aligned} \quad (3.21)$$

In this way, the proof follows from the definition of a_h (cf. (3.10)), (3.20), and (3.21). \square

As a consequence of Lemmas 3.2 and 3.4, a straightforward application again of the Lax-Milgram lemma shows that (3.11) admits a unique solution $(u_h, \lambda_h) \in \mathbf{X}_h$. Moreover, we have the following a priori error estimate.

Theorem 3.1. *Under the assumption that $u \in X \cap \prod_{i=1}^I \mathbf{H}^2(\Omega_i)$, there holds*

$$\begin{aligned} \|(u, \lambda) - (u_h, \lambda_h)\| &\lesssim \|(u, \lambda) - (I_k^{\mathcal{F}}u, \Pi_{k-1}^{\mathcal{E}}\lambda)\| \\ &+ \sup_{w_h \in X_h^k} \frac{|a(u, w_h) - a_h(I_k^{\mathcal{F}}u, w_h)|}{\|w_h\|_{1, \Omega}} + \|f - \Pi_{k-1}^{\mathcal{F}}f\|_{0, \Omega}. \end{aligned} \quad (3.22)$$

Proof. We first observe from the definitions of \mathbf{F} and \mathbf{F}_h (cf. (2.10) and (3.11)) that

$$\sup_{\substack{(v_h, \mu_h) \in \mathbf{X}_h \\ (v_h, \mu_h) \neq \mathbf{0}}} \frac{|\mathbf{F}(v_h, \mu_h) - \mathbf{F}_h(v_h, \mu_h)|}{\|(v_h, \mu_h)\|} \leq \|f - \Pi_{k-1}^{\mathcal{F}}f\|_{0, \Omega}.$$

In turn, according to the definitions of \mathbf{A} and \mathbf{A}_h (cf. (2.11) and (3.12)) it readily follows that

$$\mathbf{A}((v_h, \mu_h), (w_h, \xi_h)) - \mathbf{A}_h((v_h, \mu_h), (w_h, \xi_h)) = a(v_h, w_h) - a_h(v_h, w_h)$$

for all $(v_h, \mu_h), (w_h, \xi_h) \in \mathbf{X}_h$. In addition, adding and subtracting u to the first component of a , and using the boundedness of this bilinear form, we obtain

$$|a(v_h, w_h) - a_h(v_h, w_h)| \lesssim \left\{ \|u - v_h\| \|w_h\|_{1, \Omega} + |a(u, w_h) - a_h(v_h, w_h)| \right\} \quad \forall v_h, w_h \in X_h^k.$$

Hence, bearing in mind the foregoing estimates, a straightforward application of the first Strang Lemma (cf. [27, Theorem 4.1.1]) to the context given by (2.10) and (3.11) gives

$$\begin{aligned} \|(u, \lambda) - (u_h, \lambda_h)\| &\lesssim \inf_{(v_h, \mu_h) \in \mathbf{X}_h} \left\{ \|(u, \lambda) - (v_h, \mu_h)\| \right. \\ &+ \left. \sup_{\substack{w_h \in X_h^k \\ w_h \neq \mathbf{0}}} \frac{|a(u, w_h) - a_h(v_h, w_h)|}{\|w_h\|_{1, \Omega}} \right\} + \|f - \Pi_{k-1}^{\mathcal{F}}f\|_{0, \Omega}. \end{aligned} \quad (3.23)$$

Next, since $X \cap \prod_{i=1}^I \mathbf{H}^2(\Omega_i) \subseteq \mathcal{C}^0(\bar{\Omega})$ and $\mathbf{H}_b^{1/2}(\Gamma) \subseteq \mathbf{L}^2(\Gamma)$, we deduce by hypotheses that $u \in \mathcal{C}^0(\bar{\Omega})$ and $\lambda = \kappa \nabla u \cdot \mathbf{n} \in \mathbf{L}^2(\Gamma)$, which implies that $I_k^{\mathcal{F}}u$ and $\Pi_{k-1}^{\mathcal{E}}\lambda$ are meaningful. In this way, taking in particular $(v_h, \mu_h) = (I_k^{\mathcal{F}}u, \Pi_{k-1}^{\mathcal{E}}\lambda) \in \mathbf{X}_h$ in (3.23) we arrive at (3.22) and conclude the proof. \square

We now aim to bound the supremum in (3.22). To this end, we begin by noticing that for each $w_h \in X_h^k$ we have

$$a(u, w_h) - a_h(I_k^{\mathcal{F}} u, w_h) = \sum_{F \in \mathcal{F}_h} \left\{ a^F(u, w_h) - a_h^F(I_k^F u, w_h) \right\}, \quad (3.24)$$

where each term of the sum in (3.24) can be decomposed as

$$\begin{aligned} a^F(u, w_h) - a_h^F(I_k^F u, w_h) &= a^F(u - \Pi_k^F u, w_h) \\ &+ a^F(\Pi_k^F u, w_h) - a_h^F(\Pi_k^F u, w_h) + a_h^F(\Pi_k^F u - I_k^F u, w_h). \end{aligned} \quad (3.25)$$

Then, employing the boundedness of a^F (cf. (3.8)) and a_h^F (cf. (3.13)), we obtain, respectively,

$$|a^F(u - \Pi_k^F u, w_h)| \lesssim \|u - \Pi_k^F u\|_{1,F} \|w_h\|_{1,F} \quad (3.26)$$

and

$$|a_h^F(\Pi_k^F u - I_k^F u, w_h)| \lesssim \left\{ \|u - I_k^F u\|_{1,F} + \|u - \Pi_k^F u\|_{1,F} \right\} \|w_h\|_{1,F}, \quad (3.27)$$

which, replaced back in (3.25) and then in (3.24), and after some algebraic manipulations, yields

$$\begin{aligned} \sup_{w_h \in X_h^k} \frac{|a(u, w_h) - a_h(I_k^{\mathcal{F}} u, w_h)|}{\|w_h\|_{1,\Omega}} &\lesssim \|u - I_k^{\mathcal{F}} u\|_{1,\Omega} + \left(\sum_{F \in \mathcal{F}_h} \|u - \Pi_k^F u\|_{1,F}^2 \right)^{1/2} \\ &+ \sup_{w_h \in X_h^k} \frac{\sum_{F \in \mathcal{F}_h} |a^F(\Pi_k^F u, w_h) - a_h^F(\Pi_k^F u, w_h)|}{\|w_h\|_{1,\Omega}}, \end{aligned} \quad (3.28)$$

where we also used that $\|u - I_k^{\mathcal{F}} u\|_{1,\Omega}^2 = \sum_{F \in \mathcal{F}_h} \|u - I_k^F u\|_{1,F}^2$. In this way, using (3.28) in (3.22), we find that

$$\begin{aligned} \|(u, \lambda) - (u_h, \lambda_h)\| &\lesssim \left\{ \|(u, \lambda) - (I_k^{\mathcal{F}} u, \Pi_{k-1}^{\mathcal{E}} \lambda)\| + \left(\sum_{F \in \mathcal{F}_h} \|u - \Pi_k^F u\|_{1,F}^2 \right)^{1/2} \right. \\ &\left. + \sup_{w_h \in X_h^k} \frac{\sum_{F \in \mathcal{F}_h} |a^F(\Pi_k^F u, w_h) - a_h^F(\Pi_k^F u, w_h)|}{\|w_h\|_{1,\Omega}} + \|f - \Pi_{k-1}^{\mathcal{F}} f\|_{0,\Omega} \right\}. \end{aligned} \quad (3.29)$$

We are now ready to establish the rates of convergence of our VEM/BEM scheme.

Theorem 3.2. *Under the assumptions that $u \in X \cap \prod_{i=1}^I \mathbf{H}^{k+1}(\Omega_i)$ and $f \in \prod_{i=1}^I \mathbf{H}^k(\Omega_i)$, there holds*

$$\|(u, \lambda) - (u_h, \lambda_h)\| := \|u - u_h\|_{1,\Omega} + \|\lambda - \lambda_h\|_{-1/2,\Gamma} \lesssim h^k \sum_{i=1}^I \left\{ \|u\|_{k+1,\Omega_i} + \|f\|_{k,\Omega_i} \right\}. \quad (3.30)$$

Proof. It reduces to bound each one of the terms in (3.29) by using our regularity assumptions on u and f , and the approximation properties of the projection and interpolation operators involved. Indeed, from (3.16) (cf. Lemma 3.3) we have that

$$|a^F(\Pi_k^F u, w_h) - a_h^F(\Pi_k^F u, w_h)| \lesssim h_F^k \|u\|_{k+1,F} \|w_h\|_{1,F} \quad \forall F \in \mathcal{F}_h, \quad (3.31)$$

which implies

$$\sup_{w_h \in X_h^k} \frac{\sum_{F \in \mathcal{F}_h} |a^F(\Pi_k^F u, w_h) - a_h^F(\Pi_k^F u, w_h)|}{\|w_h\|_{1,\Omega}} \lesssim h^k \sum_{i=1}^I \|u\|_{k+1,\Omega_i}. \quad (3.32)$$

Next, by applying (3.3) and (3.5), we readily deduce that

$$\begin{aligned} \|u - I_k^{\mathcal{F}} u\|_{1,\Omega} + \left(\sum_{F \in \mathcal{F}_h} \|u - \Pi_k^F u\|_{1,F}^2 \right)^{1/2} + \|f - \Pi_{k-1}^{\mathcal{F}} f\|_{0,\Omega} \\ \lesssim h^k \sum_{i=1}^I \left\{ \|u\|_{k+1,\Omega_i} + \|f\|_{k,\Omega_i} \right\}. \end{aligned} \quad (3.33)$$

On the other hand, by hypothesis $\lambda = \kappa \nabla u \cdot \mathbf{n}$ satisfies $\lambda|_{\Gamma_j} \in \mathbf{H}^{k-1/2}(\Gamma_j)$ on each straight segment Γ_j , $j \in \{1, \dots, J\}$, constituting Γ . Hence, Lemma 3.1 and the trace theorem yield

$$\|\lambda - \Pi_{k-1}^{\mathcal{E}} \lambda\|_{-1/2,\Gamma} \lesssim h^k \sum_{j=1}^J \|\lambda\|_{k-1/2,\Gamma_j} \lesssim h^k \sum_{i=1}^I \|u\|_{k+1,\Omega_i}. \quad (3.34)$$

Finally, replacing (3.32), (3.33), and (3.34) in (3.29) we obtain (3.30) and conclude the proof. \square

3.4 $L^2(\Omega)$ -error estimate

Our goal here is to derive rates of convergence for $\|u - u_h\|_{0,\Omega}$. To this end, we now recall the symmetry properties of the boundary integral operators V and W , which establish that (cf. [44], [52])

$$\langle \xi, V\mu \rangle = \langle \mu, V\xi \rangle \quad \forall \xi, \mu \in \mathbf{H}^{-1/2}(\Gamma) \quad \text{and} \quad \langle W\varphi, \psi \rangle = \langle W\psi, \varphi \rangle \quad \forall \varphi, \psi \in \mathbf{H}^{1/2}(\Gamma). \quad (3.35)$$

Next, we let $(z, \eta) \in \mathbf{X} := X \times \mathbf{H}_0^{-1/2}(\Gamma)$ be the unique solution of (2.10) with datum $u - u_h$ instead of f , that is

$$\mathbf{A}((z, \eta), (v, \mu)) = \int_{\Omega} (u - u_h) v \quad \forall (v, \mu) \in \mathbf{X}, \quad (3.36)$$

which implies, taking in particular $v \equiv 0$, that

$$V\eta + \left(\frac{\text{id}}{2} - K\right) \gamma z = 0 \quad \text{on } \Gamma. \quad (3.37)$$

Then, according to the definition of \mathbf{A} (cf. (2.11)), and using the symmetry of a as well as those of V and W (cf. (3.35)), we find that

$$\begin{aligned} \mathbf{A}((v, \mu), (z, -\eta)) &= a(v, z) + \langle W\gamma v, \gamma z \rangle - \langle \eta, V\mu \rangle - \langle \eta, \left(\frac{\text{id}}{2} - K\right) \gamma v \rangle - \langle \mu, \left(\frac{\text{id}}{2} - K\right) \gamma z \rangle \\ &= a(z, v) + \langle W\gamma z, \gamma v \rangle - \langle \mu, V\eta + \left(\frac{\text{id}}{2} - K\right) \gamma z \rangle - \langle \eta, \left(\frac{\text{id}}{2} - K\right) \gamma v \rangle, \end{aligned}$$

which, invoking (3.37) and using (3.36), yields

$$\mathbf{A}((v, \mu), (z, -\eta)) = \mathbf{A}((z, \eta), (v, \mu)) = \int_{\Omega} (u - u_h) v \quad \forall (v, \mu) \in \mathbf{X}. \quad (3.38)$$

In what follows we assume that $z \in X \cap \prod_{i=1}^I \mathbf{H}^2(\Omega_i)$ and that there exists $C > 0$ such that

$$\sum_{i=1}^I \|z\|_{2,\Omega_i} \leq C \|u - u_h\|_{0,\Omega}. \quad (3.39)$$

Then, we have the following result.

Theorem 3.3. *In addition to the above hypothesis on z , assume that $u \in X \cap \prod_{i=1}^I \mathbf{H}^{k+1}(\Omega_i)$ and that $f \in \prod_{i=1}^I \mathbf{H}^k(\Omega_i)$. Then, there holds*

$$\|u - u_h\|_{0,\Omega} \lesssim h^{k+1} \sum_{i=1}^I \left\{ \|u\|_{k+1,\Omega_i} + \|f\|_{k,\Omega_i} \right\}. \quad (3.40)$$

Proof. Choosing $(v, \mu) = (u - u_h, \lambda - \lambda_h)$ in (3.38), adding and subtracting $(I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)$ in the second component of \mathbf{A} , using (2.10), and then adding and subtracting the expressions

$$\mathbf{A}_h((u_h, \lambda_h), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)) = \int_{\Omega} (\Pi_{k-1}^{\mathcal{F}} f) I_k^{\mathcal{F}} z \quad \text{and} \quad \mathbf{A}((u_h, \lambda_h), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)),$$

we obtain

$$\begin{aligned} \|u - u_h\|_{0,\Omega}^2 &= \mathbf{A}((u - u_h, \lambda - \lambda_h), (z, -\eta)) \\ &= \mathbf{A}((u, \lambda), (z - I_k^{\mathcal{F}} z, \Pi_{k-1}^{\mathcal{E}} \eta - \eta)) + \mathbf{A}((u, \lambda), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)) - \mathbf{A}((u_h, \lambda_h), (z, -\eta)) \\ &= \mathbf{A}((u, \lambda), (z - I_k^{\mathcal{F}} z, \Pi_{k-1}^{\mathcal{E}} \eta - \eta)) + \int_{\Omega} (f - \Pi_{k-1}^{\mathcal{F}} f) I_k^{\mathcal{F}} z + \mathbf{A}_h((u_h, \lambda_h), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)) \\ &\quad - \mathbf{A}((u_h, \lambda_h), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)) + \mathbf{A}((u_h, \lambda_h), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)) - \mathbf{A}((u_h, \lambda_h), (z, -\eta)), \end{aligned}$$

which, using also the orthogonality condition satisfied by $\Pi_{k-1}^{\mathcal{F}}$, can be reordered as

$$\begin{aligned} \|u - u_h\|_{0,\Omega}^2 &= \mathbf{A}((u - u_h, \lambda - \lambda_h), (z - I_k^{\mathcal{F}} z, \Pi_{k-1}^{\mathcal{E}} \eta - \eta)) \\ &\quad + \int_{\Omega} (f - \Pi_{k-1}^{\mathcal{F}} f) (I_k^{\mathcal{F}} z - \Pi_{k-1}^{\mathcal{F}} (I_k^{\mathcal{F}} z)) \\ &\quad + \mathbf{A}_h((u_h, \lambda_h), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)) - \mathbf{A}((u_h, \lambda_h), (I_k^{\mathcal{F}} z, -\Pi_{k-1}^{\mathcal{E}} \eta)). \end{aligned} \quad (3.41)$$

We now proceed to bound the terms on the right hand side of (3.41). In fact, employing the boundedness of \mathbf{A} , the approximation properties of $I_k^{\mathcal{F}} z$ (cf. (3.5)) and $\Pi_{k-1}^{\mathcal{E}}$ (cf. Lemma 3.1), the fact that $\eta = \frac{\partial z}{\partial \mathbf{n}}$, the trace theorem, and the regularity estimate (3.39), we get

$$\begin{aligned} |\mathbf{A}((u - u_h, \lambda - \lambda_h), (z - I_k^{\mathcal{F}} z, \Pi_{k-1}^{\mathcal{E}} \eta - \eta))| &\lesssim \|(u - u_h, \lambda - \lambda_h)\| \|(z - I_k^{\mathcal{F}} z, \eta - \Pi_{k-1}^{\mathcal{E}} \eta)\| \\ &\lesssim h \|(u - u_h, \lambda - \lambda_h)\| \left\{ \sum_{i=1}^I \|z\|_{2,\Omega_i} + \sum_{j=1}^J \|\eta\|_{1/2,\Gamma_j} \right\} \\ &\lesssim h \|(u - u_h, \lambda - \lambda_h)\| \|u - u_h\|_{0,\Omega}. \end{aligned} \quad (3.42)$$

In turn, utilizing now the approximation property of $\Pi_{k-1}^{\mathcal{F}}$ (cf. (3.3)), the fact that $\|I_k^{\mathcal{F}} z\|_{1,\Omega} \lesssim |I_k^{\mathcal{F}} z|_{1,\Omega} \lesssim |z|_{1,\Omega}$, where the last inequality here follows from (3.5), and the a priori estimate for the solution of (3.36), we find that

$$\begin{aligned} \left| \int_{\Omega} (f - \Pi_{k-1}^{\mathcal{F}} f) (I_k^{\mathcal{F}} z - \Pi_{k-1}^{\mathcal{F}} (I_k^{\mathcal{F}} z)) \right| &\leq \|f - \Pi_{k-1}^{\mathcal{F}} f\|_{0,\Omega} \|I_k^{\mathcal{F}} z - \Pi_{k-1}^{\mathcal{F}} I_k^{\mathcal{F}} z\|_{0,\Omega} \\ &\lesssim h \|f - \Pi_{k-1}^{\mathcal{F}} f\|_{0,\Omega} \|I_k^{\mathcal{F}} z\|_{1,\Omega} \lesssim h \|f - \Pi_{k-1}^{\mathcal{F}} f\|_{0,\Omega} \|u - u_h\|_{0,\Omega} \\ &\lesssim h^{k+1} \|u - u_h\|_{0,\Omega} \sum_{i=1}^I \|f\|_{k,\Omega_i}. \end{aligned} \quad (3.43)$$

Next, according to the definitions of \mathbf{A} (cf. (2.11)) and \mathbf{A}_h (cf. (3.12)), we realize that the remaining expression in (3.41) becomes $a_h(u_h, I_k^{\mathcal{F}} z) - a(u_h, I_k^{\mathcal{F}} z)$, so that adding and subtracting $\Pi_k^{\mathcal{F}} u$ in the first component of each bilinear form, we obtain

$$\begin{aligned} |a_h(u_h, I_k^{\mathcal{F}} z) - a(u_h, I_k^{\mathcal{F}} z)| &\leq \sum_{F \in \mathcal{F}_h} |a_h^F(u_h - \Pi_k^F u, I_k^{\mathcal{F}} z) - a^F(u_h - \Pi_k^F u, I_k^{\mathcal{F}} z)| \\ &+ \sum_{F \in \mathcal{F}_h} |a_h^F(\Pi_k^F u, I_k^{\mathcal{F}} z) - a^F(\Pi_k^F u, I_k^{\mathcal{F}} z)|. \end{aligned} \quad (3.44)$$

Then, by virtue of the estimates (3.18) and (3.39), we have

$$\begin{aligned} \sum_{F \in \mathcal{F}_h} |a_h^F(\Pi_k^F u, I_k^{\mathcal{F}} z) - a^F(\Pi_k^F u, I_k^{\mathcal{F}} z)| \\ \lesssim h^{k+1} \sum_{F \in \mathcal{F}_h} \|u\|_{k+1, F} \|z\|_{2, F} \lesssim h^{k+1} \sum_{i=1}^I \|u\|_{k+1, \Omega_i} \|u - u_h\|_{0, \Omega}. \end{aligned} \quad (3.45)$$

Similarly, employing now (3.17) and (3.39), we deduce that

$$\begin{aligned} \sum_{F \in \mathcal{F}_h} |a_h^F(u_h - \Pi_k^F u, I_k^{\mathcal{F}} z) - a^F(u_h - \Pi_k^F u, I_k^{\mathcal{F}} z)| &\lesssim h \sum_{F \in \mathcal{F}_h} \|u_h - \Pi_k^F u\|_{1, F} \|z\|_{2, F} \\ &\lesssim h \sum_{F \in \mathcal{F}_h} \left\{ \|u - u_h\|_{1, F} + \|u - \Pi_k^F u\|_{1, F} \right\} \|z\|_{2, F} \lesssim h^{k+1} \sum_{i=1}^I \|u\|_{k+1, \Omega_i} \|u - u_h\|_{0, \Omega}. \end{aligned} \quad (3.46)$$

Finally, replacing (3.45) and (3.46) back in (3.44), and then placing the resulting estimate together with (3.42) and (3.43) back in (3.41), we arrive at (3.40), thus concluding the proof. \square

3.5 Computable approximation of u

We now introduce the fully computable approximation of u given by $\hat{u} := \Pi_k^{\mathcal{F}} u_h$, and establish next the rates of convergence for $\|u - \hat{u}\|_{0, \Omega}$ and for the corresponding broken $\mathbf{H}^1(\Omega)$ -seminorm, that is

$$|u - \hat{u}|_{1, b, \Omega} := \left\{ \sum_{F \in \mathcal{F}_h} |u - \hat{u}_h|_{1, F}^2 \right\}^{1/2}.$$

Theorem 3.4. *Under the assumptions that $u \in X \cap \prod_{i=1}^I \mathbf{H}^{k+1}(\Omega_i)$ and $f \in \prod_{i=1}^I \mathbf{H}^k(\Omega_i)$, there holds*

$$\|u - \hat{u}_h\|_{0, \Omega} + h |u - \hat{u}|_{1, b, \Omega} \lesssim h^{k+1} \sum_{i=1}^I \left\{ \|u\|_{k+1, \Omega_i} + \|f\|_{k, \Omega_i} \right\}. \quad (3.47)$$

Proof. Let us first recall that $(\Pi_k^{\mathcal{F}} v)|_F := \Pi_k^F(v|_F)$ and that certainly $\|\Pi_k^F(v|_F)\|_{0, F} \leq \|v|_F\|_{0, F}$ for all $F \in \mathcal{F}_h$ and for all $v \in L^2(\Omega)$. Then, adding and subtracting $\Pi_k^{\mathcal{F}} u$, we readily obtain that

$$\|u - \hat{u}_h\|_{0, \Omega} \leq \|u - \Pi_k^{\mathcal{F}} u\|_{0, \Omega} + \|\Pi_k^{\mathcal{F}}(u - u_h)\|_{0, \Omega} \leq \|u - \Pi_k^{\mathcal{F}} u\|_{0, \Omega} + \|u - u_h\|_{0, \Omega}. \quad (3.48)$$

In turn, by choosing $\ell = 0$ in (3.3), we easily deduce that $|\Pi_k^F(v)|_{1, F} \lesssim |v|_{1, F}$ for all $F \in \mathcal{F}_h$ and for all $v \in \mathbf{H}^1(F)$. Hence, proceeding similarly to (3.48), we find that for each $F \in \mathcal{F}_h$ there holds

$$|u - \hat{u}_h|_{1, F} \leq |u - \Pi_k^F u|_{1, F} + |\Pi_k^F(u - u_h)|_{1, F} \lesssim |u - \Pi_k^F u|_{1, F} + |u - u_h|_{1, F},$$

which yields

$$|u - \hat{u}_h|_{1, b, \Omega} \lesssim |u - \Pi_k^{\mathcal{F}} u|_{1, b, \Omega} + |u - u_h|_{1, \Omega}. \quad (3.49)$$

In this way, applying (3.3) and the rates of convergence provided by (3.30) and (3.40) to the corresponding terms in (3.48) and (3.49), we arrive at (3.47) and finish the proof. \square

4 The VEM/BEM coupling in three dimensions

4.1 Preliminaries

For the sake of simplicity, we assume in what follows that $\kappa|_{\Omega_i}$ is a constant for $i = 1, \dots, I$. Then, we now let $\{\mathcal{T}_h\}_h$ be a family of decompositions of $\bar{\Omega}$ into polyhedral elements E of diameter $h_E \leq h$, and assume again that the meshes $\{\mathcal{T}_h\}_h$ are aligned with each Ω_i , $i = 1, \dots, I$. In turn, the boundary ∂E of each $E \in \mathcal{T}_h$ is subdivided into planar faces denoted by F , and we let \mathcal{F}_h be the set of faces of \mathcal{T}_h that are contained in Γ . In addition, we assume that the family $\{\mathcal{T}_h\}_h$ of meshes satisfy the following conditions: There exists $\rho \in (0, 1)$ such that

- (B1) each E of $\{\mathcal{T}_h\}_h$ is star-shaped with respect to a ball B_E of radius ρh_E ,
- (B2) for each E of $\{\mathcal{T}_h\}_h$, the diameters h_F of all its faces $F \subseteq \partial E$ satisfy $h_F \geq \rho h_E$,
- (B3) the faces of each $E \in \{\mathcal{T}_h\}_h$, viewed as 2-dimensional elements, satisfy the properties (A1) and (A2) (cf. Section 3.1) with the same ρ .

Next, given an integer $k \geq 1$ and $E \in \mathcal{T}_h$, and bearing in mind the definition (3.2), we set

$$X_h^k(\partial E) := \left\{ v \in C^0(\partial E) : v|_F \in X_h^k(F) \quad \forall F \subseteq \partial E \right\}, \quad (4.1)$$

and introduce the local virtual element space

$$W_h^k(E) := \left\{ v \in H^1(E) : v|_{\partial E} \in X_h^k(\partial E), \Delta v \in \mathcal{P}_k(E), \Pi_k^E v - \Pi_k^{\nabla, E} v \in \mathcal{P}_{k-2}(E) \right\}, \quad (4.2)$$

where, analogously to the 2D case (cf. Section 3.1), Π_k^E is now the $L^2(E)$ -orthogonal projection onto $\mathcal{P}_k(E)$, and the projection operator $\Pi_k^{\nabla, E} : H^1(E) \rightarrow \mathcal{P}_k(E)$ is defined as in (3.1) after replacing F with E . In addition, the degrees of freedom of $W_h^k(E)$ consist of:

- i) the values at the vertices of E ,
- ii) the moments of order $\leq k - 2$ on the edges of E ,
- iii) the moments of order $\leq k - 2$ on the faces of E , and
- iv) the moments of order $\leq k - 2$ on E .

We can then define the global virtual element space as

$$W_h^k := \left\{ v \in X : v|_E \in W_h^k(E) \quad \forall E \in \mathcal{T}_h \right\}. \quad (4.3)$$

Furthermore, and coherently with the notations of Section 3, given any integer $k \geq 0$, we let Π_k^E and $\Pi_k^{\mathcal{T}}$ be the L^2 -orthogonal projections onto $\mathcal{P}_k(E)$ and $\mathcal{P}_k(\mathcal{T}_h)$, respectively, and denote by $\mathbf{\Pi}_k^E$ and $\mathbf{\Pi}_k^{\mathcal{T}}$ their corresponding vectorial counterparts. Here again, we stress that $\mathcal{P}_k(E) \subseteq X_h^k(E)$ and that the projectors $\Pi_k^{\nabla, E} v$, $\Pi_k^E v$ and $\mathbf{\Pi}_{k-1}^E \nabla v$ are all computable for each $v \in X_h^k(E)$ (cf. [1]). In turn, we let $I_k^E : H^2(E) \rightarrow W_h^k(E)$ be the local interpolation operator, which is uniquely determined by the degrees of freedom of $W_h^k(E)$, and whose corresponding global operator is denoted $I_k^{\mathcal{T}} : H^2(\Omega) \rightarrow W_h^k$. The error estimates satisfied by the operators Π_k^E , $\Pi_k^{\nabla, E}$ and I_k^E are given by analogue versions of (3.3), (3.4) and (3.5), respectively, in which F is replaced with E .

On the other hand, we also introduce the simplicial submesh \mathfrak{F}_h of Γ obtained by subdividing each face $F \in \mathcal{F}_h$ into the set of triangles that arise after joining each vertex of F with the midpoint of the disc with respect to which F is star-shaped. Since we are assuming that the meshes satisfy conditions **(A1)** and **(A2)** (cf. Section 3.1), the triangles $T \in \mathfrak{F}_h$ have a shape ratio that is uniformly bounded with respect to h . According to the above, and in order to approximate the non-virtual boundary unknowns of our scheme (cf. Section 4.2 below), we now introduce the piecewise polynomial spaces

$$\Lambda_h^{k-1} := \left\{ \mu_h \in L^2(\Gamma) : \mu_h|_T \in P_{k-1}(T) \quad \forall T \in \mathfrak{F}_h \right\} \quad (4.4)$$

and

$$\Psi_h^k := \left\{ \varphi_h \in C^0(\Gamma) : \varphi_h|_T \in \mathcal{P}_k(T) \quad \forall T \in \mathfrak{F}_h \right\} \cap H_0^{1/2}(\Gamma). \quad (4.5)$$

Moreover, we let $\Pi_{k-1}^{\mathfrak{F}}$ be the $L^2(\Gamma)$ -orthogonal projection onto Λ_h^{k-1} , and let $\mathcal{L}_k^{\mathfrak{F}} : C^0(\Gamma) \rightarrow \Psi_h^k$ be the corresponding global Lagrange interpolation operator of order k . Then, denoting by $\{\Gamma_1, \dots, \Gamma_J\}$ the open polygons, contained in different hyperplanes of \mathbb{R}^3 , such that $\Gamma = \cup_{j=1}^J \bar{\Gamma}_j$, we now recall from [52] the following approximation properties of $\Pi_{k-1}^{\mathfrak{F}}$ and $\mathcal{L}_k^{\mathfrak{F}}$, which will be used later on.

Lemma 4.1. *Assume that $\mu \in H_0^{-1/2}(\Gamma) \cap H_b^r(\Gamma)$ for some $r \geq 0$. Then*

$$\left\| \mu - \Pi_{k-1}^{\mathfrak{F}} \mu \right\|_{-t, \Gamma} \lesssim h^{\min\{r, k\}+t} \|\mu\|_{r, b, \Gamma} \quad \forall t \in \{0, 1/2\}.$$

Proof. See [52, Theorem 4.3.20]. □

Lemma 4.2. *Assume that $\varphi \in H_b^{r+1/2}(\Gamma) \cap H^1(\Gamma)$ for some $r > 1/2$. Then*

$$\left\| \varphi - \mathcal{L}_k^{\mathfrak{F}} \varphi \right\|_{t, \Gamma} \lesssim h^{\min\{r+1/2, k+1\}-t} \|\varphi\|_{r+1/2, b, \Gamma} \quad \forall t \in \{0, 1/2, 1\}.$$

Proof. See [52, Proposition 4.1.50]. □

4.2 A new variational formulation

We begin by stressing that the variational formulation (2.10) is not valid for a VEM/BEM coupling in three dimensions because, as noticed from definitions (4.1) and (4.2), the restriction of a VEM function to the boundary of a given element is not a polynomial function but a virtual function as well. As a consequence, the term $\langle \mu_h, (\frac{\text{id}}{2} - K)\gamma v_h \rangle$ of (3.11) is not computable for $v_h \in W_h^k$ and $\mu_h \in \Lambda_h^{k-1}$. Moreover, it can be easily shown that, replacing this term by $\langle \mu_h, (\frac{\text{id}}{2} - K)\Pi_k^{\mathcal{F}} \gamma v_h \rangle$ in the formulation of the discrete problem, results in a dramatic loss of accuracy because, as Γ is a polyhedral Lipschitz boundary, the integral operator K does not yield any further regularity.

Therefore, in order to devise a more suitable VEM/BEM coupling for the three dimensional version of our model, we need to avoid the interaction of a VEM variable with a BEM variable through a boundary integral operator. This can be achieved by introducing in what follows, not only the normal derivative $\lambda := \kappa \nabla u \cdot \mathbf{n} = \frac{\partial u_e}{\partial \mathbf{n}}$, but also the trace $\psi := \gamma u = \gamma u_e$, as boundary unknowns in the formulation. As a consequence, and instead of (2.2), the harmonic solution in the exterior region \mathcal{O}_e is computed now as

$$u_e(x) = \int_{\Gamma} \frac{\partial \mathbf{E}(|x-y|)}{\partial \mathbf{n}_y} \psi(y) \, ds_y - \int_{\Gamma} \mathbf{E}(|x-y|) \lambda(y) \, ds_y \quad \forall x \in \mathcal{O}_e, \quad (4.6)$$

and hence, the corresponding identities (2.5) and (2.6) become

$$0 = \left(\frac{\text{id}}{2} - K\right)\psi + V\lambda \quad \text{on } \Gamma, \quad (4.7)$$

and

$$\lambda = -W\psi + \left(\frac{\text{id}}{2} - K^\dagger\right)\lambda \quad \text{on } \Gamma. \quad (4.8)$$

Then, integrating by parts the first equation in (2.1), adding and subtracting the expression $\langle \lambda, \varphi \rangle$ with arbitrary $\varphi \in \mathbf{H}_0^{1/2}(\Gamma)$, and imposing weakly the relation $\psi = \gamma u$ in $\mathbf{H}^{1/2}(\Gamma)$, we are led at first instance to seek $(u, \psi, \lambda) \in \mathbb{X} := X \times \mathbf{H}_0^{1/2}(\Gamma) \times \mathbf{H}^{-1/2}(\Gamma)$ such that

$$\int_{\Omega} \kappa \nabla u \cdot \nabla v - \langle \lambda, \gamma v - \varphi \rangle - \langle \lambda, \varphi \rangle + \langle \mu, \gamma u - \psi \rangle = \int_{\Omega} f v \quad (4.9)$$

for all $(v, \varphi, \mu) \in \mathbb{X}$. Moreover, incorporating (4.8) and (4.7), respectively, into the third and fourth terms on the left hand side of (4.9), we arrive at our new variational formulation: Find $(u, \psi, \lambda) \in \mathbb{X}$ such that

$$\mathbb{A}((u, \psi, \lambda), (v, \varphi, \mu)) = \mathbb{F}(v, \varphi, \mu) := \int_{\Omega} f v \quad \forall (v, \varphi, \mu) \in \mathbb{X}, \quad (4.10)$$

where

$$\begin{aligned} \mathbb{A}((u, \psi, \lambda), (v, \varphi, \mu)) &= \mathbf{A}((u, \psi, \lambda), (v, \varphi, \mu)) + \langle W\psi, \varphi \rangle \\ &+ \langle \mu, V\lambda \rangle - \langle \lambda, \left(\frac{\text{id}}{2} - K\right)\varphi \rangle + \langle \mu, \left(\frac{\text{id}}{2} - K\right)\psi \rangle \end{aligned} \quad (4.11)$$

and

$$\mathbf{A}((u, \psi, \lambda), (v, \varphi, \mu)) = a(u, v) - \langle \lambda, \gamma v - \varphi \rangle + \langle \mu, \gamma u - \psi \rangle, \quad (4.12)$$

with a and its local version a^E being defined as in the 2D case (cf. (3.8) with E instead of F). Analogously as observed in Section 2, it is easy to see here, thanks again to Lemma 2.1, that \mathbb{A} is bounded and elliptic in \mathbb{X} with respect to the usual norm of this product space, and therefore the well-posedness of (4.10) follows also from a straightforward application of the Lax-Milgram lemma.

Analogously to Section 2, we now stress that the transmission conditions employed in the derivation of the present continuous formulation are recovered from (4.10) and (4.6). Indeed, taking separately $(v, \varphi) = (0, 0)$ and $(v, \mu) = (0, 0)$ in (4.10), we obtain $\gamma u = -V\lambda + \left(\frac{\text{id}}{2} + K\right)\psi = \gamma u_e$ on Γ , and $\lambda = -W\psi + \left(\frac{\text{id}}{2} - K^\dagger\right)\lambda = \frac{\partial u_e}{\partial \mathbf{n}}$ on Γ , respectively. In addition, choosing $(\varphi, \mu) = (0, 0)$ in (4.10), it follows that $\text{div}(\kappa \nabla u) = -f$ in Ω and $\lambda = \kappa \nabla u \cdot \mathbf{n}$ on Γ , and hence $\lambda = \kappa \nabla u \cdot \mathbf{n} = \frac{\partial u_e}{\partial \mathbf{n}}$ on Γ . Finally, knowing that u_e can also be represented with γu_e instead of ψ in (4.6), we arrive at $W\psi = W\gamma u_e$, and thus the ellipticity of W (cf. (2.8)) yields $\psi = \gamma u_e = \gamma u$.

4.3 A first VEM/BEM scheme

Having in mind the finite dimensional subspaces defined in (4.3), (4.4), and (4.5), here we propose the following discrete formulation for (4.10): Find $(u_h, \psi_h, \lambda_h) \in \mathbb{X}_h := W_h^k \times \Psi_h^k \times \Lambda_h^{k-1}$ such that

$$\mathbb{A}_h((u_h, \psi_h, \lambda_h), (v_h, \varphi_h, \mu_h)) = \mathbb{F}_h(v_h, \varphi_h, \mu_h) := \int_{\Omega} \Pi_{k-1}^{\mathcal{T}} f v_h \quad (4.13)$$

for all $(v_h, \varphi_h, \mu_h) \in \mathbb{X}_h$, where

$$\begin{aligned} \mathbb{A}_h((u_h, \psi_h, \lambda_h), (v_h, \varphi_h, \mu_h)) &= \mathbf{A}_h((u_h, \psi_h, \lambda_h), (v_h, \varphi_h, \mu_h)) + \langle W\psi_h, \varphi_h \rangle \\ &+ \langle \mu_h, V\lambda_h \rangle - \langle \lambda_h, \left(\frac{\text{id}}{2} - K\right)\varphi_h \rangle + \langle \mu_h, \left(\frac{\text{id}}{2} - K\right)\psi_h \rangle, \end{aligned} \quad (4.14)$$

and

$$\begin{aligned} \mathbf{A}_h((u_h, \psi_h, \lambda_h), (v_h, \varphi_h, \mu_h)) &= a_h(u_h, v_h) - \sum_{F \in \mathcal{F}_h} \int_F \lambda_h \Pi_{k-1}^F(\gamma v_h - \varphi_h) \\ &+ \sum_{F \in \mathcal{F}_h} \int_F \mu_h \Pi_{k-1}^F(\gamma u_h - \psi_h), \end{aligned} \quad (4.15)$$

with the bilinear form a_h being constructed as in Section 3. Namely, denoting by $\mathcal{E}(E)$ and $\mathcal{F}(E)$ the sets of edges and faces, respectively, of a given $E \in \mathcal{T}_h$, we introduce

$$S_h^E(v, z) := \sum_{e \in \mathcal{E}(E)} \int_e \Pi_k^e v \Pi_k^e z + h_E^{-1} \sum_{F \in \mathcal{F}(E)} \int_F \Pi_{k-2}^F v \Pi_{k-2}^F z \quad \forall v, z \in W_h^k(E), \quad (4.16)$$

set

$$a_h^E(v, z) := \int_E \kappa \Pi_{k-1}^E \nabla v \cdot \Pi_{k-1}^E \nabla z + S_h^E(v - \Pi_k^{\nabla, E} v, z - \Pi_k^{\nabla, E} z) \quad \forall v, z \in H^1(E), \quad (4.17)$$

and define

$$a_h(v, z) := \sum_{E \in \mathcal{T}_h} a_h^E(v, z) \quad \forall v, z \in W_h^k. \quad (4.18)$$

The discrete problem (4.13) is meaningful since $S_h^E(\cdot, \cdot)$ is computable on $W_h^k(E) \times W_h^k(E)$. Moreover, it can be shown that $S_h^E(v, z)$ scales like $a^E(v, z) := \int_E \kappa \nabla v \cdot \nabla z$ on the kernel of $\Pi_k^{\nabla, E}$ in $W_h^k(E)$. In other words, the three-dimensional counterpart of (3.7) holds true (cf. [14, Section 5.5]), which implies, in particular, that we have the corresponding 3D versions of (3.15) and (3.21) as well.

4.4 Solvability and error estimates

We begin this section by introducing further notations to be employed later on. In fact, for any $s \geq 0$ we define the broken Sobolev spaces

$$\mathbf{H}^s(\mathcal{T}_h) := \prod_{E \in \mathcal{T}_h} \mathbf{H}^s(K), \quad \mathbf{H}^s(\mathcal{F}_h) := \prod_{F \in \mathcal{F}_h} \mathbf{H}^s(F),$$

which are endowed with the Hilbertian norms and corresponding seminorms, given respectively, by

$$\|v\|_{s, \mathcal{T}_h}^2 := \sum_{E \in \mathcal{T}_h} \|v\|_{s, E}^2, \quad \|\varphi\|_{s, \mathcal{F}_h}^2 := \sum_{F \in \mathcal{F}_h} \|\varphi\|_{s, F}^2.$$

and

$$|v|_{s, \mathcal{T}_h}^2 := \sum_{E \in \mathcal{T}_h} |v|_{s, E}^2, \quad |\varphi|_{s, \mathcal{F}_h}^2 := \sum_{F \in \mathcal{F}_h} |\varphi|_{s, F}^2,$$

for all $v \in \mathbf{H}^s(\mathcal{T}_h)$ and for all $\varphi \in \mathbf{H}^s(\mathcal{F}_h)$. In addition, we set as usual $\mathbf{H}^0(\mathcal{T}_h) = \mathbf{L}^2(\mathcal{T}_h)$ and $\mathbf{H}^0(\mathcal{F}_h) = \mathbf{L}^2(\mathcal{F}_h)$.

Now, concerning the solvability of (4.13), we first notice, in virtue of the comments at the end of the previous section, that the boundedness of \mathbf{A}_h follows exactly as proved for the 2D case (cf. Section 3.3). Then, we continue the analysis with the \mathbb{X}_h -ellipticity of \mathbf{A}_h with respect to the usual product norm of \mathbb{X} .

Lemma 4.3. *There holds*

$$\mathbf{A}_h((v_h, \varphi_h, \mu_h), (v_h, \varphi_h, \mu_h)) \gtrsim \|(v_h, \varphi_h, \mu_h)\|^2 \quad (4.19)$$

for all $(v_h, \varphi_h, \mu_h) \in \mathbb{X}_h$.

Proof. Given $(v_h, \varphi_h, \mu_h) \in \mathbb{X}_h$, it follows from (4.14) and (4.15) that

$$\mathbb{A}_h((v_h, \varphi_h, \mu_h), (v_h, \varphi_h, \mu_h)) = a_h(v_h, v_h) + \langle W\varphi_h, \varphi_h \rangle + \langle \mu_h, V\mu_h \rangle,$$

and hence the 3D version of (3.21) and Lemma 2.1 finish the proof. \square

Consequently, applying once again the Lax-Milgram lemma, we deduce that (4.13) has a unique solution $(u_h, \psi_h, \lambda_h) \in \mathbb{X}_h$. We now aim to establish the corresponding a priori error estimate. To this end, and following the same notations from Section 3.1, for each planar face $F \in \mathcal{F}_h$ we let Π_k^F be the $L^2(F)$ -orthogonal projection onto $\mathcal{P}_k(F)$ with vectorial counterpart $\mathbf{\Pi}_k^F$. In addition, $\Pi_k^{\mathcal{F}}$ and $\mathbf{\Pi}_k^{\mathcal{F}}$ stand for their global extensions to $L^2(\Gamma)$ and $L^2(\Gamma)^2$, respectively, which are assembled cellwise. Moreover, the approximation properties of Π_k^F (and hence of $\mathbf{\Pi}_k^F$, $\Pi_k^{\mathcal{F}}$ and $\mathbf{\Pi}_k^{\mathcal{F}}$) are exactly those given by (or derived from) (3.3).

The following result corresponds to the 3D analogue of Theorem 3.1.

Theorem 4.1. *Under the assumption that $u \in X \cap \prod_{i=1}^I \mathbf{H}^2(\Omega_i)$, there holds*

$$\begin{aligned} \|(u, \psi, \lambda) - (u_h, \psi_h, \lambda_h)\| &\lesssim \|f - \Pi_{k-1}^{\mathcal{T}} f\|_{0,\Omega} + \|(u, \psi, \lambda) - (I_k^{\mathcal{T}} u, \mathcal{L}_k^{\mathcal{F}} \psi, \Pi_{k-1}^{\mathcal{F}} \lambda)\| \\ &+ \sup_{\substack{(w_h, \phi_h, \xi_h) \in \mathbb{X}_h \\ (w_h, \phi_h, \xi_h) \neq \mathbf{0}}} \frac{|\mathbf{A}((u, \psi, \lambda), (w_h, \phi_h, \xi_h)) - \mathbf{A}_h((I_k^{\mathcal{T}} u, \mathcal{L}_k^{\mathcal{F}} \psi, \Pi_{k-1}^{\mathcal{F}} \lambda), (w_h, \phi_h, \xi_h))|}{\|(w_h, \phi_h, \xi_h)\|}. \end{aligned} \quad (4.20)$$

Proof. We follow basically the same sequence of arguments provided in the proof of Theorem 3.1. Indeed, according to the definitions of \mathbb{F} (cf. (4.10)), \mathbb{F}_h (cf. (4.13)), \mathbb{A} (cf. (4.11) - (4.12)) and \mathbb{A}_h (cf. (4.14) - (4.15)), which yields, in particular

$$(\mathbb{A} - \mathbb{A}_h)((v_h, \varphi_h, \mu_h), (w_h, \phi_h, \xi_h)) = (\mathbf{A} - \mathbf{A}_h)((v_h, \varphi_h, \mu_h), (w_h, \phi_h, \xi_h))$$

for all $(v_h, \varphi_h, \mu_h), (w_h, \phi_h, \xi_h) \in \mathbb{X}_h$, and using the boundedness of \mathbf{A} , we find that a direct application of the first Strang Lemma (cf. [27, Theorem 4.1.1]) to the context given now by (4.10) and (4.13), gives

$$\begin{aligned} \|(u, \psi, \lambda) - (u_h, \psi_h, \lambda_h)\| &\lesssim \|f - \Pi_{k-1}^{\mathcal{T}} f\|_{0,\Omega} + \inf_{(v_h, \varphi_h, \mu_h) \in \mathbb{X}_h} \left\{ \|(u, \psi, \lambda) - (v_h, \varphi_h, \mu_h)\| \right. \\ &+ \left. \sup_{\substack{(w_h, \phi_h, \xi_h) \in \mathbb{X}_h \\ (w_h, \phi_h, \xi_h) \neq \mathbf{0}}} \frac{|\mathbf{A}((u, \psi, \lambda), (w_h, \phi_h, \xi_h)) - \mathbf{A}_h((v_h, \varphi_h, \mu_h), (w_h, \phi_h, \xi_h))|}{\|(w_h, \phi_h, \xi_h)\|} \right\}. \end{aligned} \quad (4.21)$$

Next, the hypothesis guarantees that both u and $\psi = \gamma u$ are continuous, and hence $I_k^{\mathcal{T}} u$ and $\mathcal{L}_k^{\mathcal{F}} \psi$ are meaningful. In addition, the fact that $u \in \prod_{i=1}^I \mathbf{H}^2(\Omega_i)$ implies that $\lambda = \kappa \nabla u \cdot \mathbf{n} \in \mathbf{H}_b^{1/2}(\Gamma) \subseteq L^2(\Gamma)$, and hence $\Pi_{k-1}^{\mathcal{F}} \lambda$ is meaningful as well. In this way, taking in particular $(v_h, \varphi_h, \mu_h) = (I_k^{\mathcal{T}} u, \mathcal{L}_k^{\mathcal{F}} \psi, \Pi_{k-1}^{\mathcal{F}} \lambda) \in \mathbb{X}_h$ in (4.21) we arrive at (4.20) and conclude the proof. \square

Similarly to our analysis for the 2D case, we now aim to estimate the supremum in (4.20). For this purpose, we first observe from the definitions of \mathbf{A} (cf. (4.12)) and \mathbf{A}_h (cf. (4.15)), and using that $\psi = \gamma u$, that

$$\begin{aligned} \mathbf{A}((u, \psi, \lambda), (w_h, \phi_h, \xi_h)) - \mathbf{A}_h((I_k^{\mathcal{T}} u, \mathcal{L}_k^{\mathcal{F}} \psi, \Pi_{k-1}^{\mathcal{F}} \lambda), (w_h, \phi_h, \xi_h)) &= a(u, w_h) - a_h(I_k^{\mathcal{T}} u, w_h) \\ &- \langle \lambda, \gamma w_h - \phi_h \rangle + \int_{\Gamma} \Pi_{k-1}^{\mathcal{F}} \lambda \Pi_{k-1}^{\mathcal{F}} (\gamma w_h - \phi_h) - \int_{\Gamma} \xi_h \Pi_{k-1}^{\mathcal{F}} (\gamma I_k^{\mathcal{T}} u - \mathcal{L}_k^{\mathcal{F}} \psi) \end{aligned} \quad (4.22)$$

for all $(w_h, \phi_h, \xi_h) \in \mathbb{X}_h$. Then, recalling that κ has been assumed to be piecewise constant, and noting that certainly $\nabla \Pi_k^E u \in \mathcal{P}_{k-1}(E)^3$, we deduce, according to the definition of a_h^E (cf. (4.17)), that

$$a_h^E(\Pi_k^E u, w_h) = a^E(\Pi_k^E u, w_h) \quad \forall E \in \mathcal{T}_h, \quad \forall w_h \in W_h^k(E),$$

and therefore, adding and subtracting $\Pi_k^E u$ in the first components of a^E and a_h^E , we readily find that

$$a(u, w_h) - a_h(I_k^T u, w_h) = \sum_{E \in \mathcal{T}_h} \left\{ a^E(u - \Pi_k^E u, w_h) + a_h^E(\Pi_k^E u - I_k^E u, w_h) \right\} \quad \forall w_h \in W_h^k.$$

In this way, thanks to the foregoing identity and the boundedness of a^E and a_h^E , the latter being proved similarly to the proof of Lemma 3.2, and then adding and subtracting u in the expression resulting from bounding a_h^E , we arrive at

$$|a(u, w_h) - a_h(I_k^T u, w_h)| \lesssim \left\{ |u - I_k^T u|_{1,\Omega} + |u - \Pi_k^T u|_{1,\mathcal{T}_h} \right\} |w_h|_{1,\Omega}. \quad (4.23)$$

On the other hand, noting that $\Pi_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \in \Lambda_h^{k-1}$ (cf. (4.4)), and employing the orthogonality condition satisfied by $\Pi_{k-1}^{\tilde{\mathcal{F}}}$, as well as the symmetry of $\Pi_{k-1}^{\mathcal{F}}$, we obtain

$$\begin{aligned} -\langle \lambda, \gamma w_h - \phi_h \rangle + \int_{\Gamma} \Pi_{k-1}^{\tilde{\mathcal{F}}} \lambda \Pi_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) &= -\langle \lambda, \gamma w_h - \phi_h \rangle + \int_{\Gamma} \lambda \Pi_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \\ &= -\langle \lambda, \gamma w_h - \phi_h \rangle + \int_{\Gamma} \Pi_{k-1}^{\mathcal{F}} \lambda (\gamma w_h - \phi_h) = \langle \Pi_{k-1}^{\mathcal{F}} \lambda - \lambda, \gamma w_h - \phi_h \rangle, \end{aligned}$$

from which, according to the duality pairing between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$, and using the trace theorem, we obtain

$$\left| \int_{\Gamma} \Pi_{k-1}^{\tilde{\mathcal{F}}} \lambda \Pi_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) - \langle \lambda, \gamma w_h - \phi_h \rangle \right| \lesssim \|\lambda - \Pi_{k-1}^{\mathcal{F}} \lambda\|_{-1/2,\Gamma} \left\{ \|w_h\|_{1,\Omega} + \|\phi_h\|_{1/2,\Gamma} \right\}. \quad (4.24)$$

In turn, adding and subtracting $\gamma u = \psi$, we readily get

$$-\int_{\Gamma} \xi_h \Pi_{k-1}^{\mathcal{F}}(\gamma I_k^T u - \mathcal{L}_k^{\tilde{\mathcal{F}}} \psi) = \int_{\Gamma} \xi_h \Pi_{k-1}^{\mathcal{F}}(\gamma(u - I_k^T u) - (\psi - \mathcal{L}_k^{\tilde{\mathcal{F}}} \psi)),$$

from which, applying the Cauchy-Schwarz inequality in $L^2(\Gamma)$ and the inverse inequality satisfied by Λ_h^{k-1} (cf. (4.4)), we find that

$$\left| \int_{\Gamma} \xi_h \Pi_{k-1}^{\mathcal{F}}(\gamma I_k^T u - \mathcal{L}_k^{\tilde{\mathcal{F}}} \psi) \right| \lesssim h^{-1/2} \left\{ \|\gamma(u - I_k^T u)\|_{0,\Gamma} + \|\psi - \mathcal{L}_k^{\tilde{\mathcal{F}}} \psi\|_{0,\Gamma} \right\} \|\xi_h\|_{-1/2,\Gamma}. \quad (4.25)$$

Consequently, using (4.23), (4.24), and (4.25) to bound (4.22), and then replacing the resulting estimate into (4.20), we arrive at the following a priori error estimate

$$\begin{aligned} \|(u, \psi, \lambda) - (u_h, \psi_h, \lambda_h)\| &\lesssim \|f - \Pi_{k-1}^T f\|_{0,\Omega} + |u - I_k^T u|_{1,\Omega} + \|\psi - \mathcal{L}_k^{\tilde{\mathcal{F}}} \psi\|_{1/2,\Gamma} \\ &\quad + \|\lambda - \Pi_{k-1}^{\tilde{\mathcal{F}}} \lambda\|_{-1/2,\Gamma} + |u - \Pi_k^T u|_{1,\mathcal{T}_h} + \|\lambda - \Pi_{k-1}^{\mathcal{F}} \lambda\|_{-1/2,\Gamma} \\ &\quad + h^{-1/2} \left\{ \|\gamma(u - I_k^T u)\|_{0,\Gamma} + \|\psi - \mathcal{L}_k^{\tilde{\mathcal{F}}} \psi\|_{0,\Gamma} \right\}. \end{aligned} \quad (4.26)$$

Analogously to the 2D case, the foregoing equation constitutes the key estimate to derive the rates of convergence of the present 3D VEM/BEM scheme. Additionally, and in order to bound one of the terms involved, we also need the scaled trace inequality, which is stated as follows.

Lemma 4.4. For each $E \in \mathcal{T}_h$ there holds

$$\|v\|_{0,\partial E}^2 \lesssim \left\{ h_E^{-1} \|v\|_{0,E}^2 + h_E |v|_{1,E}^2 \right\} \quad \forall v \in \mathbf{H}^1(E). \quad (4.27)$$

Proof. See [31, Lemma 1.49]. \square

Then, we have the following main result.

Theorem 4.2. Under the assumptions that $u \in X \cap \prod_{i=1}^I \mathbf{H}^{k+1}(\Omega_i)$ and $f \in \prod_{i=1}^I \mathbf{H}^k(\Omega_i)$, there holds

$$\begin{aligned} \|(u, \psi, \lambda) - (u_h, \psi_h, \lambda_h)\| &:= \|u - u_h\|_{1,\Omega} + \|\psi - \psi_h\|_{1/2,\Gamma} + \|\lambda - \lambda_h\|_{-1/2,\Gamma} \\ &\lesssim h^k \sum_{i=1}^I \left\{ \|u\|_{k+1,\Omega_i} + \|f\|_{k,\Omega_i} \right\}. \end{aligned} \quad (4.28)$$

Proof. We begin by noticing, thanks to the regularity assumption on u , that $\psi = \gamma u \in \mathbf{H}_b^{k+1/2}(\Gamma)$ and $\lambda = \kappa \nabla u \cdot \mathbf{n} \in \mathbf{H}_b^{k-1/2}(\Gamma)$. In what follows we identify the terms on the right hand side of (4.26) according to the order they have been written there, from left to right and from up to down. Then, applying the 3D versions of (3.3) (to the first and fifth terms), (3.5) (to the second term), and Lemma 3.1 (to the sixth term), and using by the trace theorem that $\|\lambda\|_{k-1/2,b,\Gamma} \leq c \sum_{i=1}^I \|u\|_{k+1,\Omega_i}$, we obtain

$$\begin{aligned} \|f - \Pi_{k-1}^{\mathcal{T}} f\|_{0,\Omega} + |u - I_k^{\mathcal{T}} u|_{1,\Omega} + |u - \Pi_k^{\mathcal{T}} u|_{1,\mathcal{T}_h} + \|\lambda - \Pi_{k-1}^{\mathcal{F}} \lambda\|_{-1/2,\Gamma} \\ \lesssim h^k \sum_{i=1}^I \left\{ \|f\|_{k,\Omega_i} + \|u\|_{k+1,\Omega_i} \right\}. \end{aligned} \quad (4.29)$$

In turn, invoking Lemmas 4.2 and 4.1 to bound the third and fourth terms, respectively, and employing also by trace theorem that $\|\psi\|_{k+1/2,b,\Gamma} \leq c \sum_{i=1}^I \|u\|_{k+1,\Omega_i}$, we find that

$$\begin{aligned} \|\psi - \mathcal{L}_k^{\mathfrak{F}} \psi\|_{1/2,\Gamma} + \|\lambda - \Pi_{k-1}^{\mathfrak{F}} \lambda\|_{-1/2,\Gamma} \\ \lesssim h^k \left\{ \|\psi\|_{k+1/2,b,\Gamma} + \|\lambda\|_{k-1/2,b,\Gamma} \right\} \lesssim h^k \sum_{i=1}^I \|u\|_{k+1,\Omega_i}. \end{aligned} \quad (4.30)$$

On the other hand, another straightforward application of Lemma 4.2, but now to the eighth term, gives

$$\|\psi - \mathcal{L}_k^{\mathfrak{F}} \psi\|_{0,\Gamma} \lesssim h^{k+1/2} \|\psi\|_{k+1/2,b,\Gamma},$$

which yields

$$h^{-1/2} \|\psi - \mathcal{L}_k^{\mathfrak{F}} \psi\|_{0,\Gamma} \lesssim h^k \sum_{i=1}^I \|u\|_{k+1,\Omega_i}. \quad (4.31)$$

Finally, taking advantage of the scaled trace inequality (4.27), and making use once again of the 3D version of (3.5), we obtain that for each face F of an element $E \in \mathcal{T}_h$ there holds

$$\begin{aligned} h_F^{-1} \|\gamma(u - I_k^E u)\|_{0,F}^2 &\leq h_F^{-1} \|\gamma(u - I_k^E u)\|_{0,\partial E}^2 \\ &\lesssim h_E^{-2} \|u - I_k^E u\|_{0,E}^2 + |u - I_k^E u|_{1,E} \lesssim h_E^{2k} \|u\|_{k+1,E}^2, \end{aligned}$$

from which we deduce that

$$h^{-1/2} \|\gamma(u - I_k^{\mathcal{T}} u)\|_{0,\Gamma} \lesssim h^k \sum_{i=1}^I \|u\|_{k+1,\Omega_i}. \quad (4.32)$$

In this way, utilizing (4.29), (4.30), (4.31), and (4.32) in (4.26), we arrive at (4.28), thus ending the proof. \square

4.5 A second VEM/BEM scheme

Having in mind again the subspaces defined in (4.3), (4.4), and (4.5), we now propose the following alternative VEM/BEM scheme for (4.10): Find $(u_h, \psi_h, \lambda_h) \in \mathbb{X}_h := W_h^k \times \Psi_h^k \times \Lambda_h^{k-1}$ such that

$$\mathbb{B}_h((u_h, \psi_h, \lambda_h), (v_h, \varphi_h, \mu_h)) = \mathbb{F}_h(v_h, \varphi_h, \mu_h) := \int_{\Omega} \Pi_{k-1}^{\mathcal{T}} f v_h \quad (4.33)$$

for all $(v_h, \varphi_h, \mu_h) \in \mathbb{X}_h$, where

$$\begin{aligned} \mathbb{B}_h((u_h, \psi_h, \lambda_h), (v_h, \varphi_h, \mu_h)) &= \mathbf{B}_h((u_h, \psi_h), (v_h, \varphi_h)) + \langle W \psi_h, \varphi_h \rangle \\ &+ \langle \mu_h, V \lambda_h \rangle - \langle \lambda_h, (\frac{\text{id}}{2} - K) \varphi_h \rangle + \langle \mu_h, (\frac{\text{id}}{2} - K) \psi_h \rangle, \end{aligned} \quad (4.34)$$

and

$$\begin{aligned} \mathbf{B}_h((u_h, \psi_h), (v_h, \varphi_h)) &= a_h(u_h, v_h) - \sum_{F \in \mathcal{F}_h} \int_F \kappa \Pi_{k-1}^F \nabla u_h \cdot \mathbf{n} \Pi_{k-1}^F (\gamma v_h - \varphi_h) \\ &+ \sum_{F \in \mathcal{F}_h} \int_F \kappa \Pi_{k-1}^F \nabla v_h \cdot \mathbf{n} \Pi_{k-1}^F (\gamma u_h - \psi_h) + \sum_{F \in \mathcal{F}_h} \int_F h_F^{-1} \Pi_{k-1}^F (\gamma u_h - \psi_h) \Pi_{k-1}^F (\gamma v_h - \varphi_h), \end{aligned} \quad (4.35)$$

with a_h as defined in Section 4.3. Note that the last three expressions defining \mathbf{B}_h resembles those employed for the non-symmetric interior penalty discontinuous Galerkin method (cf. [31]).

Throughout this section we denote by $h_{\mathcal{T}} \in P_0(\mathcal{T}_h)$ the piecewise constant function defined by $h_{\mathcal{T}}|_E := h_E \forall E \in \mathcal{T}_h$. Similarly, $h_{\mathcal{F}} \in P_0(\mathcal{F}_h)$ is given by $h_{\mathcal{F}}|_F := h_F \forall F \in \mathcal{F}_h$. Then, it readily follows from (4.34), (4.35), the 3D version of (3.21), and Lemma 2.1, that \mathbb{B}_h is \mathbb{X}_h -elliptic with respect to the norm $||| \cdot |||$, whose square is defined as

$$|||(v_h, \varphi_h, \mu_h)|||^2 := |v_h|_{1,\Omega}^2 + \|\varphi_h\|_{1/2,\Gamma}^2 + \|\mu_h\|_{-1/2,\Gamma}^2 + \|h_{\mathcal{F}}^{-1/2} \Pi_{k-1}^{\mathcal{F}} (\gamma v_h - \varphi_h)\|_{0,\mathcal{F}_h}^2 \quad (4.36)$$

for all $(v_h, \varphi_h, \mu_h) \in \mathbb{X}_h$. As a consequence, the VEM/BEM scheme (4.33) admits a unique solution $(u_h, \psi_h, \lambda_h) \in \mathbb{X}_h$. Furthermore, the bilinear form \mathbf{A} (cf. (4.11)), being bounded with respect to the usual product norm of $\mathbb{X} := X \times H_0^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)$, is certainly bounded with respect to $||| \cdot |||$ as well. In this way, assuming from now on that $u \in X \cap \prod_{i=1}^I H^2(\Omega_i)$, and proceeding analogously to the proof of Theorem 4.1, in particular applying the first Strang Lemma (cf. [27, Theorem 4.1.1]) to the context given by (4.10) and (4.33), we deduce that

$$\begin{aligned} |||(u, \psi, \lambda) - (u_h, \psi_h, \lambda_h)||| &\lesssim \|f - \Pi_{k-1}^{\mathcal{T}} f\|_{0,\Omega} + |||(u, \psi, \lambda) - (I_k^{\mathcal{T}} u, \mathcal{L}_k^{\mathfrak{F}} \psi, \Pi_{k-1}^{\mathfrak{F}} \lambda)||| \\ &+ \sup_{\substack{(w_h, \phi_h, \xi_h) \in \mathbb{X}_h \\ (w_h, \phi_h, \xi_h) \neq \mathbf{0}}} \frac{|\mathbf{A}((u, \psi, \lambda), (w_h, \phi_h, \xi_h)) - \mathbf{B}_h((I_k^{\mathcal{T}} u, \mathcal{L}_k^{\mathfrak{F}} \psi), (w_h, \phi_h))|}{|||(w_h, \phi_h, \xi_h)|||}. \end{aligned} \quad (4.37)$$

Next, we observe from the definitions of \mathbf{A} (cf. (4.12)) and \mathbf{B}_h (cf. (4.35)), and using again that $\psi = \gamma u$, that

$$\begin{aligned} \mathbf{A}((u, \psi, \lambda), (w_h, \phi_h, \xi_h)) - \mathbf{B}_h((I_k^{\mathcal{T}} u, \mathcal{L}_k^{\mathfrak{F}} \psi), (w_h, \phi_h)) &= a(u, w_h) - a_h(I_k^{\mathcal{T}} u, w_h) \\ &- \langle \lambda, \gamma w_h - \phi_h \rangle + \int_{\Gamma} \kappa \Pi_{k-1}^{\mathcal{F}} \nabla I_k^{\mathcal{T}} u \cdot \mathbf{n} \Pi_{k-1}^{\mathcal{F}} (\gamma w_h - \phi_h) \\ &- \int_{\Gamma} \kappa \Pi_{k-1}^{\mathcal{F}} \nabla w_h \cdot \mathbf{n} \Pi_{k-1}^{\mathcal{F}} (\gamma I_k^{\mathcal{T}} u - \mathcal{L}_k^{\mathfrak{F}} \psi) \\ &- \int_{\Gamma} h_{\mathcal{F}}^{-1} \Pi_{k-1}^{\mathcal{F}} (\gamma I_k^{\mathcal{T}} u - \mathcal{L}_k^{\mathfrak{F}} \psi) \Pi_{k-1}^{\mathcal{F}} (\gamma w_h - \phi_h) \end{aligned} \quad (4.38)$$

for all $(w_h, \phi_h, \xi_h) \in \mathbb{X}_h$. Since the expression in the first row of (4.38) has already been estimated by (4.23), we now proceed to derive suitable upper bounds for the remaining three rows. Indeed, we begin by recalling that κ is piecewise constant and that $\lambda = \kappa \nabla u \cdot \mathbf{n}$. Hence, adding and subtracting u to $I_k^T u$, and using that $\kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla u \cdot \mathbf{n} \in \mathcal{P}_{k-1}(\mathcal{F}_h)$ and $\mathbf{n} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \in \mathcal{P}_{k-1}(\mathcal{F}_h)^3$, and bearing in mind the orthogonality conditions of $\mathbf{\Pi}_{k-1}^{\mathcal{F}}$ and $\mathbf{\Pi}_{k-1}^{\mathcal{F}}$, we can write

$$\begin{aligned}
& - \langle \lambda, \gamma w_h - \phi_h \rangle + \int_{\Gamma} \kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla I_k^T u \cdot \mathbf{n} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \\
& = \int_{\Gamma} \kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla (I_k^T u - u) \cdot \mathbf{n} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \\
& \quad - \int_{\Gamma} \kappa (\nabla u - \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla u) \cdot \mathbf{n} (\gamma w_h - \phi_h) \\
& = \int_{\Gamma} h_{\mathcal{F}}^{1/2} \kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla (I_k^T u - u) \cdot \mathbf{n} h_{\mathcal{F}}^{-1/2} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \\
& \quad - \int_{\Gamma} \kappa (\nabla u - \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla u) \cdot \mathbf{n} \{(\gamma w_h - \phi_h) - \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h)\},
\end{aligned}$$

from which applying Cauchy-Schwarz's inequality, the approximation property (3.3), and the trace theorem, we find that

$$\begin{aligned}
& \left| \langle \lambda, \gamma w_h - \phi_h \rangle - \int_{\Gamma} \kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla I_k^T u \cdot \mathbf{n} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \right| \\
& \lesssim \left\{ \|h_{\mathcal{F}}^{1/2} \nabla (u - I_k^T u)\|_{0, \mathcal{F}_h} + \|h_{\mathcal{F}}^{1/2} (\nabla u - \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla u)\|_{0, \mathcal{F}_h} \right\} \| (w_h, \phi_h, \xi_h) \|.
\end{aligned} \tag{4.39}$$

For the third row of (4.38) we need the following inverse inequality for the VEM, which has been proved in [26] and [56].

Lemma 4.5. *For each $F \in \mathcal{F}_h$ there holds*

$$|v|_{1, F} \lesssim h_F^{-1} \|v\|_{0, F} \quad \forall v \in X_h^k(F). \tag{4.40}$$

Proof. See [26, Theorem 3.6] and [56, Lemma 7.1]. \square

Then, employing Cauchy-Schwarz's inequality, adding and subtracting $\psi = \gamma u$, and applying (4.40) at the last step, we obtain

$$\begin{aligned}
& \int_{\Gamma} \kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla w_h \cdot \mathbf{n} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma I_k^T u - \mathcal{L}_k^{\mathfrak{F}} \psi) = \int_{\Gamma} \kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla (w_h - \mathbf{\Pi}_0^T w_h) \cdot \mathbf{n} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma I_k^T u - \mathcal{L}_k^{\mathfrak{F}} \psi) \\
& \lesssim \|h_{\mathcal{F}}^{-1/2} (\mathcal{L}_k^{\mathfrak{F}} \psi - \gamma I_k^T u)\|_{0, \mathcal{F}_h} \|h_{\mathcal{F}}^{1/2} \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla (w_h - \mathbf{\Pi}_0^T w_h)\|_{0, \mathcal{F}_h} \\
& \lesssim \left\{ \|h_{\mathcal{F}}^{-1/2} (\psi - \mathcal{L}_k^{\mathfrak{F}} \psi)\|_{0, \mathcal{F}_h} + \|h_{\mathcal{F}}^{-1/2} \gamma (u - I_k^T u)\|_{0, \mathcal{F}_h} \right\} \|h_{\mathcal{F}}^{1/2} \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla (w_h - \mathbf{\Pi}_0^T w_h)\|_{0, \mathcal{F}_h} \\
& \lesssim \left\{ \|h_{\mathcal{F}}^{-1/2} (\psi - \mathcal{L}_k^{\mathfrak{F}} \psi)\|_{0, \mathcal{F}_h} + \|h_{\mathcal{F}}^{-1/2} \gamma (u - I_k^T u)\|_{0, \mathcal{F}_h} \right\} \|h_{\mathcal{F}}^{-1/2} (w_h - \mathbf{\Pi}_0^T w_h)\|_{0, \mathcal{F}_h},
\end{aligned}$$

and hence, noting additionally by the scaled trace inequality (4.27) and the approximation property (3.3) that

$$h_F^{-1} \|w_h - \mathbf{\Pi}_0^T w_h\|_{0, F}^2 \lesssim \left\{ h_E^{-2} \|w_h - \mathbf{\Pi}_0^T w_h\|_{0, E}^2 + |w_h|_{1, E}^2 \right\} \lesssim |w_h|_{1, E}^2 \quad \forall F \subseteq \partial E, \quad \forall E \in \mathcal{T}_h,$$

we conclude that

$$\begin{aligned}
& \left| \int_{\Gamma} \kappa \mathbf{\Pi}_{k-1}^{\mathcal{F}} \nabla w_h \cdot \mathbf{n} \mathbf{\Pi}_{k-1}^{\mathcal{F}}(\gamma I_k^T u - \mathcal{L}_k^{\mathfrak{F}} \psi) \right| \\
& \lesssim \left\{ \|h_{\mathcal{F}}^{-1/2} (\psi - \mathcal{L}_k^{\mathfrak{F}} \psi)\|_{0, \mathcal{F}_h} + \|h_{\mathcal{F}}^{-1/2} \gamma (u - I_k^T u)\|_{0, \mathcal{F}_h} \right\} |w_h|_{1, \Omega}.
\end{aligned} \tag{4.41}$$

In turn, concerning the last row of (4.38), we apply again Cauchy-Schwarz's inequality and the fact that $\psi = \gamma u$, to readily get

$$\begin{aligned} & \left| \int_{\Gamma} h_{\mathcal{F}}^{-1} \Pi_{k-1}^{\mathcal{F}}(\gamma I_k^{\mathcal{T}} u - \mathcal{L}_k^{\mathfrak{F}} \psi) \Pi_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h) \right| \\ & \lesssim \|h_{\mathcal{F}}^{-1/2} \Pi_{k-1}^{\mathcal{T}}(\mathcal{L}_k^{\mathfrak{F}} \psi - \gamma I_k^{\mathcal{T}} u)\|_{0, \mathcal{F}_h} \|h_{\mathcal{F}}^{-1/2} \Pi_{k-1}^{\mathcal{F}}(\gamma w_h - \phi_h)\|_{0, \mathcal{F}_h} \\ & \lesssim \left\{ \|h_{\mathcal{F}}^{-1/2} (\psi - \mathcal{L}_k^{\mathfrak{F}} \psi)\|_{0, \mathcal{F}_h} + \|h_{\mathcal{F}}^{-1/2} \gamma(u - I_k^{\mathcal{T}} u)\|_{0, \mathcal{F}_h} \right\} \| (w_h, \phi_h, \xi_h) \|. \end{aligned} \quad (4.42)$$

In this way, we are able to establish now the following main result of this section.

Theorem 4.3. *Under the assumptions that $u \in X \cap \prod_{i=1}^I \mathbf{H}^2(\Omega_i)$, there holds*

$$\begin{aligned} & \| (u, \psi, \lambda) - (u_h, \psi_h, \lambda_h) \| \lesssim \left\{ |u - I_k^{\mathcal{T}} u|_{1, \Omega} + |u - \Pi_k^{\mathcal{T}} u|_{1, \mathcal{T}_h} + \|f - \Pi_{k-1}^{\mathcal{T}} f\|_{0, \Omega} \right. \\ & + \|\psi - \mathcal{L}_k^{\mathfrak{F}} \psi\|_{1/2, \Gamma} + \|\lambda - \Pi_{k-1}^{\mathfrak{F}} \lambda\|_{-1/2, \Gamma} + \|h_{\mathcal{F}}^{-1/2} (\psi - \mathcal{L}_k^{\mathfrak{F}} \psi)\|_{0, \mathcal{F}_h} \\ & \left. + \|h_{\mathcal{F}}^{-1/2} (u - I_k^{\mathcal{T}} u)\|_{0, \mathcal{F}_h} + \|h_{\mathcal{F}}^{1/2} \nabla(u - I_k^{\mathcal{T}} u)\|_{0, \mathcal{F}_h} + \|h_{\mathcal{F}}^{1/2} (\nabla u - \Pi_{k-1}^{\mathcal{F}} \nabla u)\|_{0, \mathcal{F}_h} \right\}. \end{aligned} \quad (4.43)$$

Proof. It follows from the Strang estimate (4.37), the definition of the norm $\| \cdot \|$ (cf. (4.36)), and the bound for the supremum in (4.37), which results after using (4.23), (4.39), (4.41), and (4.42) in (4.38). \square

The rates of convergence for our second VEM/BEM scheme, which are the same as those provided by Theorem 4.2 for the first approach, are proved next.

Theorem 4.4. *Under the assumptions that $u \in X \cap \prod_{i=1}^I \mathbf{H}^{k+1}(\Omega_i)$ and $f \in \prod_{i=1}^I \mathbf{H}^k(\Omega_i)$, there holds*

$$\| (u, \psi, \lambda) - (u_h, \psi_h, \lambda_h) \| \lesssim h^k \sum_{i=1}^I \left\{ \|u\|_{k+1, \Omega_i} + \|f\|_{k, \Omega_i} \right\}. \quad (4.44)$$

Proof. The first seven terms on the right hand side of (4.43) were already bounded in the proof of Theorem 4.2, and thus we only need to bound the last two. Then, given $F \in \mathcal{F}_h$ and $E \in \mathcal{T}_h$ such that $F \subseteq \partial E$, the trace inequality (4.27) and the approximation property (3.5) imply

$$h_F \|\nabla(u - I_k^E u)\|_{0, F}^2 \lesssim \|\nabla(u - I_k^E u)\|_{0, E}^2 + h_E^2 |\nabla(u - I_k^E u)|_{1, E}^2 \lesssim h_E^{2k} \|u\|_{k+1, E}^2,$$

from which we obtain that

$$\|h_{\mathcal{F}}^{1/2} \nabla(u - I_k^{\mathcal{T}} u)\|_{0, \mathcal{F}_h} \lesssim h^k \sum_{i=1}^I \|u\|_{k+1, \Omega_i}. \quad (4.45)$$

In turn, applying the approximation property (3.3) to $\nabla u \in \prod_{i=1}^I \mathbf{H}^{k-1/2}(\partial\Omega_i)^3$, we deduce that for each $F \in \mathcal{F}_h$ there holds

$$h_F \|\nabla u - \Pi_{k-1}^F \nabla u\|_{0, F}^2 \lesssim h_F^{2k} \|\nabla u\|_{k-1/2, F}^2,$$

which, using the trace theorem in each subdomain Ω_i containing faces of \mathcal{F}_h on its boundary, yields

$$\|h_{\mathcal{F}}^{1/2} (\nabla u - \Pi_{k-1}^F \nabla u)\|_{0, \mathcal{F}_h} \lesssim h^k \sum_{i=1}^I \|u\|_{k+1, \Omega_i}. \quad (4.46)$$

In this way, (4.43) together with (4.45), (4.46), and the aforementioned estimates from Theorem 4.2, lead to (4.44), which finishes the proof. \square

We end the paper by remarking that the analysis developed in Sections 3.4 and 3.5 can be easily extended to the VEM/BEM approaches from Sections 4.3 and the present one, thus providing rates of convergence for $\|u - u_h\|_{0,\Omega}$ and for $\left\{\|u - \hat{u}_h\|_{0,\Omega} + h|u - \hat{u}|_{1,b,\Omega}\right\}$ in this 3D case as well.

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