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Efficient construction of 2-chains representing a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$

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Abstract We present an efficient algorithm for the construction of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ via the Poincaré-Lefschetz duality theorem. Denoting by g the first Betti number of $\overline{\Omega}$ the idea is to find, first g different 1-boundaries of $\overline{\Omega}$ with supports contained in $\partial\Omega$ whose homology classes in $\mathbb{R}^3 \setminus \Omega$ form a basis of $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$, and then to construct a set of 2-chains in $\overline{\Omega}$ having these 1-boundaries as their boundaries. The Poincaré-Lefschetz duality theorem ensures that the relative homology classes of these 2-chains in $\overline{\Omega}$ modulo $\partial\Omega$ form a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$. We devise a simple procedure for the construction of the required set of 1-boundaries of $\overline{\Omega}$ that, combined with a fast algorithm for the construction of 2-chains with prescribed boundary, allows the efficient computation of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ via this very natural approach. Some numerical experiments show the efficiency of the method and its performance comparing with other algorithms.

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1 Introduction

Consider a bounded domain Ω of $\mathbb{R}^3$. Here by a domain of $\mathbb{R}^3$ we mean a non-empty connected open subset of $\mathbb{R}^3$. Suppose the closure $\overline{\Omega}$ of Ω in $\mathbb{R}^3$ is polyhedral and its boundary $\partial\Omega$ is locally flat, like that used for finite element approximation of differential problems. Our aim is to develop a set of fast and robust algorithms for the automatic identification and construction of those homological structures that influence the solvability of differential problems defined on Ω. Let us consider, as a significant example, the curl-div system

$$\begin{aligned} \operatorname{curl} \mathbf{u} &= \mathbf{F} && \text{in } \Omega \\ \operatorname{div} \mathbf{u} &= G && \text{in } \Omega \\ \mathbf{u}\cdot\mathbf{n} &= \varphi && \text{on } \partial\Omega\,, \end{aligned}$$

being $\mathbf{n}$ the outward unit normal vector field on $\partial\Omega$. It is well-known that the solution of this problem is not unique if g, the first Betti number of $\overline{\Omega}$, is greater than zero. Two different ways to fix a unique solution are: to prescribe the circulation around a set of 1-cycles of $\overline{\Omega}$ that are representatives of a basis of the first homology group $H_1(\overline{\Omega};\mathbb{Z})$ of $\overline{\Omega}$, or to prescribe the flux through a set of surfaces that are representatives of a basis of the second relative homology group $H_2(\overline{\Omega},\partial\Omega;\mathbb{Z})$ of $\overline{\Omega}$ modulo $\partial\Omega$.

Let us consider a triangulation of $\overline{\Omega}$; namely, a tetrahedral mesh of $\overline{\Omega}$ with n_T tetrahedra, n_F faces, n_E edges and n_V vertices. The incidence matrices of such a triangulation, tetrahedra-to-faces $D_3 \in \mathbb{Z}^{n_F\times n_T}$, faces-to-edges $D_2 \in \mathbb{Z}^{n_E\times n_F}$ and edges-to-vertices $D_1 \in \mathbb{Z}^{n_V\times n_E}$, are the integer matrix representations of the so-called boundary operators associated with the given triangulation of $\overline{\Omega}$. The standard procedure to compute the homology and cohomology groups of $\overline{\Omega}$ is based on the computation of the Smith normal form of these integer matrices D_i, a computationally demanding algorithm even in the case of sparse matrices (see e.g. [23] and [11, 16]). Thus, before the Smith normal form procedure is employed, the problem size is reduced using fast algorithms (usually algorithms that run in linear time) that remove homologically irrelevant parts of the triangulation (see e.g. [9, 22]). An implementation of these techniques has been integrated in the finite element mesh generator *Gmsh* by Pellikka et al. (see [24]). Other software that perform homology and cohomology computations, with less emphasis on finite element modeling, are *CHomP* [7], *jPlex* [28] and *GAP homology* [10]. A different approach, using chain contraction instead of the classical reduction algorithms, is described in [25], the computational cost is higher but it has more functionalities, since it provides more comprehensive homological information.

If the goal is to construct a basis of $H_2(\overline{\Omega},\partial\Omega;\mathbb{Z})$, specific algorithms could be more efficient that generic algorithms for the computation of homology and cohomology groups.

A specific approach for the construction of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ has been proposed by Kotiuga in [17–19] and [13]. There the aim is to construct the so-called *"cuts"* of Ω; namely, surfaces-with-boundary $\{S_i\}_{i=1}^g$ of $\overline{\Omega}$ with $\partial S_i \subset \partial\Omega$, which permit to construct a single-valued scalar potential in $\Omega \setminus \bigcup_{i=1}^g S_i$ of any given irrotational vector field in Ω. These cuts are nonsingular polyhedral representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$. The algorithm consists in two main steps. Starting with a basis of $H_1(\overline{\Omega}; \mathbb{Z})$, in the first step, one constructs a basis $\{f_i\}_{i=1}^g$ of the cohomology group $H^1(\overline{\Omega}; \mathbb{Z})$ approximating a differential problem with a finite element method. Then the second step is to construct the cuts of Ω as level sets of the maps $\{f_i\}_{i=1}^g$. The representatives of the basis are regular surfaces (nonsingular polyhedral surfaces indeed) and this justify the substantial complexity of the procedure. For an interesting interpretation of this approach in the framework of eddy current problems, see [20] that contains also the main ideas concerning the possibility of constructing a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ starting from $H_1(\partial\Omega; \mathbb{Z})$ and using the Poincaré-Lefschetz duality theorem. This duality is also exploited for the identification of self-adjoint realizations of the curl operator in [14].

In this paper we focus on the construction of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ using a geometric approach, based on the Poincaré-Lefschetz duality theorem again, which works on a given triangulation of $\overline{\Omega}$. Here we are not interested in questions concerning regularity. Indeed the representatives of the basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ we construct are formal linear combinations (with integer coefficients) of oriented faces of the triangulation of $\overline{\Omega}$; namely, they are 2-chains of $\overline{\Omega}$ without any further regularity. This allows to gain in efficiency from the computational point of view.

We recall that the boundary $\partial\Omega$ of the domain Ω is said to be *locally flat* if, for every point $x \in \partial\Omega$, there exist an open neighborhood U_x of x in $\mathbb{R}^3$ and a homeomorphism $\phi_x : U_x \longrightarrow \mathbb{R}^3$ such that $\phi_x(U_x \cap \partial\Omega) = P$, where P is the coordinate plane $\{(x, y, z) \in \mathbb{R}^3 \mid z = 0\}$ (see [4, 5]). This kind of domains includes all Lipschitz polyhedral domains, but also domains like the crossed bricks (see, e.g., Fig. 3.1 in [21]).

Fix a triangulation $\mathcal{T}$ of $\overline{\Omega}$. A *1-cycle* γ *of* $\mathcal{T}$ (or of $\overline{\Omega}$) is a formal linear combination (with integer coefficients) of oriented edges of $\mathcal{T}$ with null boundary. The 1-cycle γ is said to be a *1-boundary of* $\mathcal{T}$ (or of $\overline{\Omega}$) if it is equal to the boundary of a 2-chain S of $\mathcal{T}$. By a *2-chain of* $\mathcal{T}$ *(or of* $\overline{\Omega}$*) we mean a formal linear combination of oriented faces of* $\mathcal{T}$. *If such a 2-chain* S exists, we call it *homological Seifert surface of* γ *in* $\mathcal{T}$ (or in $\overline{\Omega}$). The support of the 1-cycle γ of $\mathcal{T}$ is the subset of $\overline{\Omega}$ defined as the union of all the edges of $\mathcal{T}$ which appear in the formal expression of γ with a nonzero coefficient (and with its fixed orientation). If the support of γ is contained in $\partial\Omega$ we say that γ is a *1-cycle of* $\partial\Omega$.

Given g different 1-boundaries $\{\sigma'_n\}_{n=1}^g$ of $\mathcal{T}$ with supports contained in $\partial\Omega$ and whose homology classes in $\mathbb{R}^3 \setminus \Omega$ form a basis of $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$, and given for each $n \in \{1, \ldots, g\}$ a homological Seifert surface S_n of σ'_n in $\mathcal{T}$, the Poincaré-Lefschetz duality theorem ensures that the relative homology classes of the 2-chains $\{S_n\}_{n=1}^g$ in $\overline{\Omega}$ modulo $\partial\Omega$ form a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$. In [1] we propose and analyze a very efficient algorithm that, given a 1-boundary γ of $\mathcal{T}$, computes a homological Seifert surface of γ in $\mathcal{T}$. Hence this algorithm allows the construction of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ once we know a set of 1-boundaries $\sigma'_1, \ldots, \sigma'_g$ of $\mathcal{T}$ with supports contained in $\partial\Omega$ and whose homology classes in $\mathbb{R}^3 \setminus \Omega$ form a basis of $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$.

If $\partial\Omega$ is connected, an algorithm for the construction of such a set of 1-boundaries have been analyzed in [15]. The first step is to construct a set of $2g$ 1-cycles $\{\gamma_l\}_{l=1}^{2g}$ of $\partial\Omega$ that are representatives of a basis of $H_1(\partial\Omega;\mathbb{Z})$. The second step is to compute g linear combinations $\{\widehat{\sigma}_n = \sum_{l=1}^{2g} B_{n,l}\gamma_l\}_{n=1}^{g}$ of these $2g$ 1-cycles γ_l in such a way that the homology classes of the $\widehat{\sigma}_n$'s in $\mathbb{R}^3 \setminus \Omega$ form a basis of the homology group $H_1(\mathbb{R}^3 \setminus \Omega;\mathbb{Z})$. If $\partial\Omega$ is connected, each 1-cycle $\widehat{\sigma}_n$ of $\partial\Omega$ turns out to be also 1-boundaries of $\overline{\Omega}$ so we can take $\sigma_n' = \widehat{\sigma}_n$ for every $n \in \{1, \dots, g\}$.

In [2] the construction of 1-cycles of $\partial\Omega$ representing a basis of $H_1(\mathbb{R}^3 \setminus \Omega;\mathbb{Z})$ is extended to the case in which $\partial\Omega$ is not connected. However, due to the lack of connectedness of $\partial\Omega$, these 1-cycles are not necessarily 1-boundaries of $\overline{\Omega}$.

To visualize this phenomenon consider the domain Ω of $\mathbb{R}^3$ defined as an open solid torus with a coaxial smaller closed solid torus removed (see Fig. 1). The 1-cycles $\widehat{\sigma}_1$ and σ_2 of $\partial\Omega$, represented by a continuous line in Fig. 1a and b respectively, are representatives of a basis of $H_1(\mathbb{R}^3 \setminus \Omega;\mathbb{Z})$, but they are not 1-boundaries of $\overline{\Omega}$. To obtain a 1-boundary σ_1' of $\overline{\Omega}$ homologous to $\widehat{\sigma}_1$ in $\mathbb{R}^3 \setminus \Omega$, we need to consider a 1-cycle σ_1^* of $\partial\Omega$, like the one represented by the dotted line in Fig. 1c. Then $\sigma_1' := \widehat{\sigma}_1 - \sigma_1^*$ is the boundary of a 2-chain S_1 of $\overline{\Omega}$ (see Fig. 1c again) and is homologous to $\widehat{\sigma}_1$ in $\mathbb{R}^3 \setminus \Omega$ because σ_1^* is a 1-boundary in $\mathbb{R}^3 \setminus \Omega$. Analogously, there exists a 1-cycle σ_2^* of $\partial\Omega$ such that σ_2^* is a 1-boundary of $\mathbb{R}^3 \setminus \Omega$ and the 1-cycle $\sigma_2' := \sigma_2 - \sigma_2^*$ of $\partial\Omega$ is the boundary of a 2-chain S_2 of $\overline{\Omega}$ (see Fig. 1d). It follows that σ_2 is homologous in $\mathbb{R}^3 \setminus \Omega$ to the 1-boundary σ_2' of $\overline{\Omega}$.

The main theoretical result of this paper is as follows: *starting from a set of $2g$ 1-cycles of $\partial\Omega$ representing a basis of $H_1(\partial\Omega;\mathbb{Z})$, we explicitly construct a set $\{\sigma_n'\}_{n=1}^{g}$ of 1-cycles of $\partial\Omega$ such that the σ_n''s are 1-boundaries of $\overline{\Omega}$ and their homology classes*

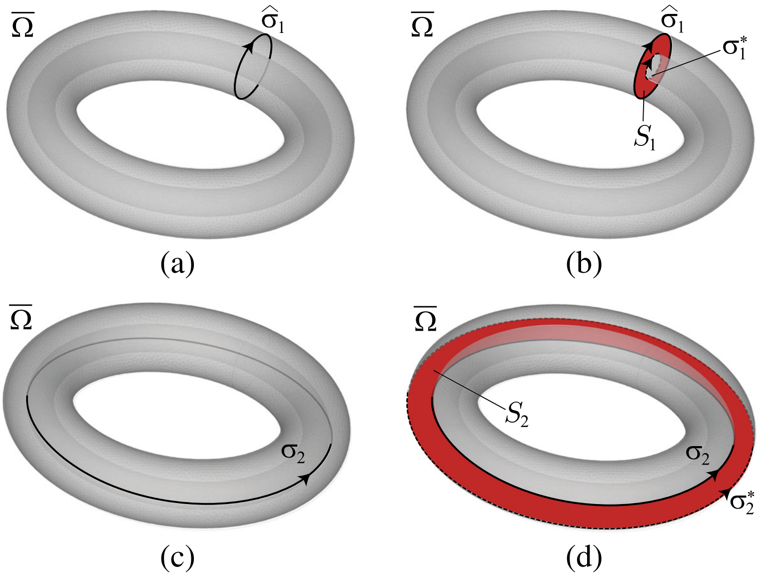


Fig. 1 The 1-boundaries

in $\mathbb{R}^3 \setminus \Omega$ *form a basis of* $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$. This is done in Section 2. In Section 3 we briefly describe the algorithm studied in [1] that allows us to construct a homological Seifert surface S_n of each σ'_n in $\overline{\Omega}$. The relative homology classes of the S_n's form a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$. Finally in Section 4 we present some numerical results illustrating the robustness and efficiency of this approach. We include also some comparisons with the results obtained using the cohomology solver integrated in *Gmsh*.

2 Construction of the 1-boundaries

2.1 The main result

Let $\mathcal{T} = (V, E, F, K)$ be a finite triangulation of $\overline{\Omega}$, where V is the set of vertices, E the set of edges, F the set of faces and K the set of tetrahedra of $\mathcal{T}$. Let $\mathcal{T}_\partial = (V_\partial, E_\partial, F_\partial)$ be the triangulation of $\partial\Omega$ induced by $\mathcal{T}$; namely, we have that $V_\partial = V \cap \partial\Omega$, E_∂ is the set of edges of $\mathcal{T}$ with support contained in $\partial\Omega$ and F_∂ is the set of faces with support contained in $\partial\Omega$. For a detailed description of all the homological notions related to $\mathcal{T}$ we will use below we refer the reader to Section 2 of [1].

For convenience, if c is a 1-cycle of $\mathbb{R}^3$ with support contained in a subset Z of $\mathbb{R}^3$, then we denote by $[c]_Z$ the homology class of c in $H_1(Z; \mathbb{Z})$.

The connected boundary case As indicated in the introduction, if $\partial\Omega$ *is connected*, then the desired 1-boundaries σ'_n are constructed in [15]. More precisely, under this connectedness condition the authors construct 1-cycles $\sigma_1, \dots, \sigma_g, \widehat{\sigma}_1, \dots, \widehat{\sigma}_g$ of $\mathcal{T}_\partial$ in such a way that their homology classes in $\mathcal{T}_\partial$ form a basis of $H_1(\mathcal{T}_\partial; \mathbb{Z})$ and it holds:

- $\sigma_1, \dots, \sigma_g$ are 1-boundaries of $\mathbb{R}^3 \setminus \Omega$ and their homology classes in $\overline{\Omega}$ form a basis of $H_1(\overline{\Omega}; \mathbb{Z})$; namely,

$$[\sigma_s]_{\mathbb{R}^3\setminus\Omega} = 0 \ \text{ for every } s \in \{1, \dots, g\}, \tag{1}$$

$$\left\{[\sigma_1]_{\overline{\Omega}}, \dots, [\sigma_g]_{\overline{\Omega}}\right\} \text{ is a basis of } H_1(\overline{\Omega}; \mathbb{Z}). \tag{2}$$

- $\widehat{\sigma}_1, \dots, \widehat{\sigma}_g$ are 1-boundaries of $\overline{\Omega}$ and their homology classes in $\mathbb{R}^3 \setminus \Omega$ form a basis of $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$; namely,

$$[\widehat{\sigma}_s]_{\overline{\Omega}} = 0 \ \text{ for every } s \in \{1, \dots, g\}, \tag{3}$$

$$\left\{[\widehat{\sigma}_1]_{\mathbb{R}^3\setminus\Omega}, \dots, [\widehat{\sigma}_g]_{\mathbb{R}^3\setminus\Omega}\right\} \text{ is a basis of } H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z}). \tag{4}$$

Defining $\sigma'_n := \widehat{\sigma}_n$ for every $n \in \{1, \dots, g\}$, we are done.

The not connected boundary case We now consider the more complicated case in which $\partial\Omega$ *is not connected*. Let us recall some results from Section 6 of [2]. Let $\Gamma_0, \Gamma_1, \dots, \Gamma_p$ denote the connected components of $\partial\Omega$ where $p \geq 1$. By the Jordan separation theorem, for every $r \in \{0, 1, \dots, p\}$, each open subset $\mathbb{R}^3 \setminus \Gamma_r$ of $\mathbb{R}^3$ has two connected components, both having Γ_r as boundary. Denote by D_r the bounded connected component of $\mathbb{R}^3 \setminus \Gamma_r$ and by g_r the first Betti number of its closure $\overline{D_r}$ in

$\mathbb{R}^3$. Rearranging the indices $r \in \{0, 1, \ldots, p\}$ if necessary, we can suppose that Γ_0 is the "external" component of $\partial\Omega$; namely, it holds: $\overline{\Omega} = \overline{D_0} \setminus \bigcup_{r=1}^{p} D_r$ and hence $\mathbb{R}^3 \setminus \Omega = (\mathbb{R}^3 \setminus D_0) \cup \bigcup_{r=1}^{p} \overline{D_r}$. Since $H_1(\partial\Omega; \mathbb{Z})$ is isomorphic to $\bigoplus_{r=0}^{p} H_1(\Gamma_r; \mathbb{Z})$, we have that $2g = \sum_{r=0}^{p} 2g_r$ or, equivalently, $g = \sum_{r=0}^{p} g_r$.

For every $r \in \{0, 1, \ldots, p\}$, $\partial D_r = \Gamma_r$ is connected so, as we said above, we can construct 1-cycles $\{\sigma_{r,s}\}_{s=1}^{g_r} \cup \{\widehat{\sigma}_{r,s}\}_{s=1}^{g_r}$ of $\mathcal{T}_\partial$ with support contained in Γ_r such that:

$$[\sigma_{r,s}]_{\mathbb{R}^3 \setminus D_r} = 0 \ \text{ for every } s \in \{1, \ldots, g_r\}, \tag{5}$$

$$\left\{[\sigma_{r,1}]_{\overline{D_r}}, \ldots, [\sigma_{r,g_r}]_{\overline{D_r}}\right\} \text{ is a basis of } H_1(\overline{D_r}; \mathbb{Z}) \tag{6}$$

and

$$[\widehat{\sigma}_{r,s}]_{\overline{D_r}} = 0 \ \text{ for every } s \in \{1, \ldots, g_r\}, \tag{7}$$

$$\left\{[\widehat{\sigma}_{r,1}]_{\mathbb{R}^3 \setminus D_r}, \ldots, [\widehat{\sigma}_{r,g_r}]_{\mathbb{R}^3 \setminus D_r}\right\} \text{ is a basis of } H_1(\mathbb{R}^3 \setminus D_r; \mathbb{Z}). \tag{8}$$

Lemma 1 *The set of homology classes*

$$\left\{[\sigma_{0,s}]_{\overline{\Omega}}\right\}_{s=1}^{g_0} \cup \left\{[\widehat{\sigma}_{1,s}]_{\overline{\Omega}}\right\}_{s=1}^{g_1} \cup \ldots \cup \left\{[\widehat{\sigma}_{p,s}]_{\overline{\Omega}}\right\}_{s=1}^{g_p} \textit{ is a basis of } H_1(\overline{\Omega}; \mathbb{Z}) \tag{9}$$

and the set

$$\left\{[\widehat{\sigma}_{0,s}]_{\mathbb{R}^3\setminus\Omega}\right\}_{s=1}^{g_0} \cup \left\{[\sigma_{1,s}]_{\mathbb{R}^3\setminus\Omega}\right\}_{s=1}^{g_1} \cup \ldots \cup \left\{[\sigma_{p,s}]_{\mathbb{R}^3\setminus\Omega}\right\}_{s=1}^{g_p} \textit{ is a basis of } H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z}). \tag{10}$$

The homology classes of 1-cycles corresponding to Γ_r, $r \in \{0, 1, \ldots, p\}$, *are omitted if* $g_r = 0$.

Proof Since $\mathbb{R}^3 \setminus \Omega$ is equal to the disjoint union $(\mathbb{R}^3 \setminus D_0) \cup \bigcup_{r=1}^{p} \overline{D_r}$, (10) follows immediately from (8) with $r = 0$ and (6) with $r \geq 1$. For a proof of (9), we refer the reader to Theorem 3.2.2.1 of [8] or to Theorem 6 of [2]. □

The problem is now that we do not know if the 1-cycles in $S := \left\{\widehat{\sigma}_{0,s}\right\}_{s=1}^{g_0} \cup \left\{\sigma_{1,s}\right\}_{s=1}^{g_1} \cup \ldots \cup \left\{\sigma_{p,s}\right\}_{s=1}^{g_p}$ of $\mathcal{T}_\partial$ are 1-boundaries of $\mathcal{T}$. Our idea to overcome this difficulty consists in a sort of *projection/subtraction procedure* in which one replaces each 1-cycle in S with a 1-boundary of $\mathcal{T}$ without changing its homology class in $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$ by subtracting a 1-cycle of $\mathcal{T}_\partial$ that is a 1-boundary of $\mathbb{R}^3 \setminus \Omega$. To do that we introduce the auxiliary sets Ω_r, $r \in \{0, 1, \ldots, p\}$ by setting

$$\Omega_0 := \Omega \cup (\mathbb{R}^3 \setminus D_0) \ \text{ and } \ \Omega_r := \Omega \cup \overline{D_r} \ \text{ for every } \ r \in \{1, \ldots, p\}.$$

For convenience, we define $P := \{1, \ldots, p\}$ and $P_r := P \setminus \{r\}$ for every $r \in P$.

Notice that Ω_0 is an unbounded domain of $\mathbb{R}^3$ with $\partial\Omega_0 = \partial\overline{\Omega_0} = \partial\Omega \setminus \Gamma_0 = \bigcup_{i \in P} \Gamma_i$ and, for every $r \in P$, Ω_r is a bounded domain of $\mathbb{R}^3$ with $\partial\Omega_r = \partial\overline{\Omega_r} = \partial\Omega \setminus \Gamma_r = \Gamma_0 \cup \bigcup_{i \in P\setminus\{r\}} \Gamma_i$.

In Fig. 2 we represent the sets $\overline{\Omega_0}$ and $\overline{\Omega_1}$ when Ω is an open solid torus with a coaxial smaller closed solid torus removed.

Lemma 2 *It holds that*

$$\bigcup_{i \in P} \left\{[\widehat{\sigma}_{i,s}]_{\overline{\Omega_0}}\right\}_{s=1}^{g_i} \ \textit{ is a basis of } H_1(\overline{\Omega_0}; \mathbb{Z}) \tag{11}$$

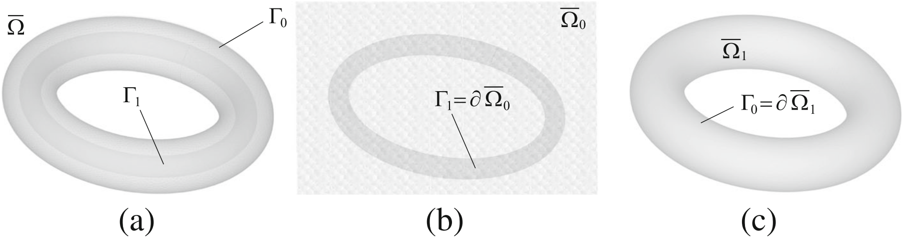


Fig. 2 The auxiliary sets $\overline{\Omega_0}$ and $\overline{\Omega_1}$

and

$$\big\{[\sigma_{0,s}]_{\overline{\Omega_r}}\big\}_{s=1}^{g_0} \cup \bigcup_{i\in P_r} \big\{[\widehat{\sigma}_{i,s}]_{\overline{\Omega_r}}\big\}_{s=1}^{g_i} \ \textit{ is a basis of } H_1(\overline{\Omega_r};\mathbb{Z}) \tag{12}$$

for every $r \in P$.

Proof Assertion (12) follows immediately by applying (9) with Ω equal to Ω_r. Let B be an open ball of $\mathbb{R}^3$ containing $\bigcup_{i\in P}\overline{D_i}$, then, by applying (9) with Ω equal to $B^* := B\setminus\bigcup_{i\in P}\overline{D_i}$, we infer that $\bigcup_{r\in P}\big\{[\widehat{\sigma}_{r,s}]_{\overline{B^*}}\big\}_{s=1}^{g_r}$ is a basis of $H_1(\overline{B^*};\mathbb{Z})$. Since $\overline{B^*}$ is a strong deformation retract of $\overline{\Omega_0}$, we obtain at once (11). $\square$

Remark 3 Since $\mathbb{R}^3\setminus\Omega_r$ is equal to the disjoint union $\bigcup_{i\in P}\overline{D_i}$ if $r=0$ and $(\mathbb{R}^3\setminus D_0)\cup\bigcup_{i\in P_r}\overline{D_i}$ if $r\in P$, we have also that

$$\bigcup_{i\in P}\big\{[\sigma_{i,s}]_{\mathbb{R}^3\setminus\Omega_0}\big\}_{s=1}^{g_i} \ \text{ is a basis of } H_1(\mathbb{R}^3\setminus\Omega_0;\mathbb{Z}) \tag{13}$$

and

$$\big\{[\widehat{\sigma}_{0,s}]_{\mathbb{R}^3\setminus\Omega_r}\big\}_{s=1}^{g_0} \cup \bigcup_{i\in P_r}\big\{[\sigma_{i,s}]_{\mathbb{R}^3\setminus\Omega_r}\big\}_{s=1}^{g_i} \ \text{ is a basis of } H_1(\mathbb{R}^3\setminus\Omega_r;\mathbb{Z}) \tag{14}$$

for every $r\in P$.

The key point of the above-mentioned projection/subtraction procedure is to write the homology classes $\{[\widehat{\sigma}_{0,s}]_{\overline{\Omega_0}}\}_{s=1}^{g_0}$ in terms of the basis of $H_1(\overline{\Omega_0};\mathbb{Z})$ given in (11) and, if $r\in P$, the homology classes $\{[\sigma_{r,s}]_{\overline{\Omega_r}}\}_{s=1}^{g_r}$ in terms of the basis of $H_1(\overline{\Omega_r};\mathbb{Z})$ given in (12).

For every $s\in\{1,\dots,g_0\}$, the support of $\widehat{\sigma}_{0,s}$ is contained in $\Gamma_0\subset\overline{\Omega_0}$. In this way, thanks to (11), there exist, and are unique, integers $\{\alpha_{i,j}^{0,s}\}_{i,j}$ such that

$$[\widehat{\sigma}_{0,s}]_{\overline{\Omega_0}} = \sum_{i\in P}\sum_{j=1}^{g_i}\alpha_{i,j}^{0,s}\,[\widehat{\sigma}_{i,j}]_{\overline{\Omega_0}}\,. \tag{15}$$

Similarly, for every $r\in P$ and for every $s\in\{1,\dots,g_r\}$, the support of $\sigma_{r,s}$ is contained in $\Gamma_r\subset\overline{\Omega_r}$. In this way, thanks to (12), there exist, and are unique, integers $\{\alpha_{i,j}^{r,s}\}_{i,j}$ such that

$$[\sigma_{r,s}]_{\overline{\Omega_r}} = \sum_{j=1}^{g_0}\alpha_{0,j}^{r,s}\,[\sigma_{0,j}]_{\overline{\Omega_r}} + \sum_{i\in P_r}\sum_{j=1}^{g_i}\alpha_{i,j}^{r,s}\,[\widehat{\sigma}_{i,j}]_{\overline{\Omega_r}}\,. \tag{16}$$

The 1-boundaries of $\mathcal{T}$ we are looking form are the 1-cycles of $\mathcal{T}_\partial$ constructed as follows:

$$\widehat{\sigma}'_{0,s} := \widehat{\sigma}_{0,s} - \sum_{i \in P} \sum_{j=1}^{g_i} \alpha_{i,j}^{0,s} \, \widehat{\sigma}_{i,j} \tag{17}$$

for every $s \in \{1, \dots, g_0\}$, and

$$\sigma'_{r,s} := \sigma_{r,s} - \sum_{j=1}^{g_0} \alpha_{0,j}^{r,s} \, \sigma_{0,j} - \sum_{i \in P_r} \sum_{j=1}^{g_i} \alpha_{i,j}^{r,s} \, \widehat{\sigma}_{i,j} \tag{18}$$

for every $r \in P$ and for every $s \in \{1, \dots, g_r\}$.

Figure 3 describes the projection/subtraction procedure ($\widehat{\sigma}_{0,1} \mapsto \widehat{\sigma}'_{0,1}$, $\sigma_{1,1} \mapsto \sigma'_{1,1}$) in the case Ω is an open solid torus with a coaxial smaller closed solid torus removed.

We are in position to proof the main theoretical result of this paper.

Proposition 4 *The 1-cycles of $\mathcal{T}_\partial$ constructed in (17) and in (18) have the following properties:*

(i) *They are 1-boundaries of $\mathcal{T}$; namely, their homology classes in $\overline{\Omega}$ are null.*
(ii) $[\widehat{\sigma}'_{0,s}]_{\mathbb{R}^3 \setminus \Omega} = [\widehat{\sigma}_{0,s}]_{\mathbb{R}^3 \setminus \Omega}$ *for every* $s \in \{1, \dots, g_0\}$ *and* $[\sigma'_{r,s}]_{\mathbb{R}^3 \setminus \Omega} = [\sigma_{r,s}]_{\mathbb{R}^3 \setminus \Omega}$ *for every* $r \in \{1, \dots, p\}$ *and for every* $s \in \{1, \dots, g_r\}$. *In particular, the set*

$$\left\{[\widehat{\sigma}'_{0,s}]_{\mathbb{R}^3 \setminus \Omega}\right\}_{s=1}^{g_0} \cup \left\{[\sigma'_{1,s}]_{\mathbb{R}^3 \setminus \Omega}\right\}_{s=1}^{g_1} \cup \ldots \cup \left\{[\sigma'_{p,s}]_{\mathbb{R}^3 \setminus \Omega}\right\}_{s=1}^{g_p}$$

is a basis of $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$.
(iii) *Let* $S_{0,s}$ *be a homological Seifert surface of* $\widehat{\sigma}'_{0,s}$ *in* $\mathcal{T}$ *for every* $s \in \{1, \dots, g_0\}$ *and let* $S_{r,s}$ *be a homological Seifert surface of* $\sigma'_{r,s}$ *in* $\mathcal{T}$ *for every* $r \in \{1, \dots, p\}$ *and for every* $s \in \{1, \dots, g_r\}$. *Then the relative homology classes*

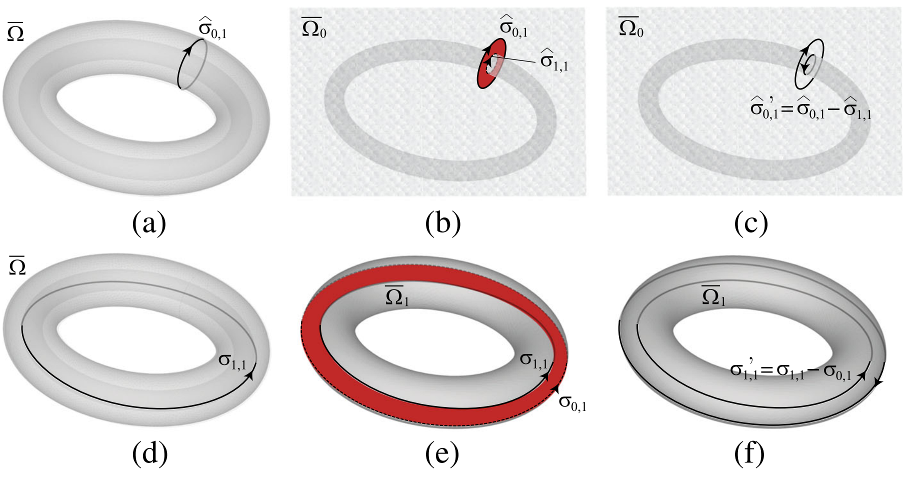


Fig. 3 The projection/subtraction procedure

of such 2-chains $\{S_{r,s}\}_{r\in\{0,1,\dots,p\},s\in\{1,\dots,g_r\}}$ *in* $\overline{\Omega}$ *modulo* $\partial\Omega$ *form a basis of* $H_2(\overline{\Omega},\partial\Omega;\mathbb{Z})$.

Proof (i) Let $s\in\{1,\dots,g_0\}$. We must prove that $[\widehat{\sigma}'_{0,s}]_{\overline{\Omega}}=0$. Observe that $\mathbb{R}^3=\overline{D_0}\cup\overline{\Omega_0}$ and $\overline{\Omega}=\overline{D_0}\cap\overline{\Omega_0}$. In this way, the Mayer-Vietoris exact sequence associated with the splitting $\mathbb{R}^3=\overline{D_0}\cup\overline{\Omega_0}$ implies that the following homomorphism is an isomorphism:

$$i_*\oplus j_*: H_1(\overline{\Omega};\mathbb{Z})\longrightarrow H_1(\overline{D_0};\mathbb{Z})\oplus H_1(\overline{\Omega_0};\mathbb{Z}),$$

where i_* and j_* are the homomorphisms induced by the inclusions $i:\overline{\Omega}\hookrightarrow\overline{D_0}$ and $j:\overline{\Omega}\hookrightarrow\overline{\Omega_0}$, respectively. It follows that $[\widehat{\sigma}'_{0,s}]_{\overline{\Omega}}=0$ if and only if $[\widehat{\sigma}'_{0,s}]_{\overline{D_0}}=i_*([\widehat{\sigma}'_{0,s}]_{\overline{\Omega}})=0$ and $[\widehat{\sigma}'_{0,s}]_{\overline{\Omega_0}}=j_*([\widehat{\sigma}'_{0,s}]_{\overline{\Omega}})=0$. By (15) and (17), we have that $[\widehat{\sigma}'_{0,s}]_{\overline{\Omega_0}}=0$. Since $\overline{D_r}\subset\overline{D_0}$ for every $r\in P$, equality (7) ensures that $[\widehat{\sigma}_{i,j}]_{\overline{D_0}}=0$ for every $i\in\{0,1,\dots,p\}$ and for every $j\in\{1,\dots,g_i\}$. In this way, by (17), we infer that $[\widehat{\sigma}'_{0s}]_{\overline{D_0}}=0$. This proves that $[\widehat{\sigma}'_{0,s}]_{\overline{\Omega}}=0$, as desired.

For any given $r\in P$ and $s\in\{1,\dots,g_r\}$, the proof of the fact that $[\sigma'_{r,s}]_{\overline{\Omega}}=0$ is similar. One must consider the Mayer-Vietoris sequence associated with splitting $\mathbb{R}^3=(\mathbb{R}^3\setminus D_r)\cup\overline{\Omega_r}$, points (16) and (18), and the inclusions $\mathbb{R}^3\setminus D_0\subset\mathbb{R}^3\setminus D_r$ and $\overline{D_i}\subset\mathbb{R}^3\setminus D_r$ for every $i\in P_r$, together with equalities (5) and (7).

(ii) Since $\mathbb{R}^3\setminus D_0\subset\mathbb{R}^3\setminus\Omega$ and $\overline{D_i}\subset\mathbb{R}^3\setminus\Omega$ for every $i\in P$, equalities (5) and (7) imply that $[\sigma_{0,j}]_{\mathbb{R}^3\setminus\Omega}=0$ for every $j\in\{1,\dots,g_0\}$ and $[\widehat{\sigma}_{i,j}]_{\mathbb{R}^3\setminus\Omega}=0$ for every $i\in P$ and for every $j\in\{1,\dots,g_i\}$. By (17) and (18), we have that $[\widehat{\sigma}'_{0,s}]_{\mathbb{R}^3\setminus\Omega}=[\widehat{\sigma}_{0,s}]_{\mathbb{R}^3\setminus\Omega}$ for every $s\in\{1,\dots,g_0\}$ and $[\sigma'_{r,s}]_{\mathbb{R}^3\setminus\Omega}=[\sigma_{r,s}]_{\mathbb{R}^3\setminus\Omega}$ for every $r\in P$ and for every $s\in\{1,\dots,g_r\}$. This proves the first part of (ii). The second part of (ii) now follows immediately from (10).

(iii) The existence of the homological Seifert surfaces $S_{r,s}$ is equivalent to (i). Point (iii) is a direct consequence of the second part of (ii) and of the Poincaré-Lefschetz duality theorem. $\square$

2.2 Computation of the 1-boundaries

The aim of this section is to describe an algorithm to compute explicitly the coefficients $\alpha^{r,s}_{i,j}$ that appear in equations (17) and (18).

2.2.1 A linking number matrix associated with $\overline{\Omega}$

We begin by recalling the notion of linking number and some of its properties, see, e.g., Rolfsen [26, pp. 132–136], and Seifert and Threlfall [27, Sects. 70, 73, 77].

Roughly speaking, given two 1-cycles γ and η of $\mathbb{R}^3$ with disjoint supports (namely, with $|\gamma|\cap|\eta|=\emptyset$), the linking number between them is the number of times that each 1-cycle winds around the other. A possible geometric way to give a rigorous definition is as follows. Choose a homological Seifert surface $S_\eta=\sum_{q=1}^k b_q f_q$ of η in $\mathbb{R}^3$; namely, $\partial_2 S_\eta=\eta$. It is well-known (and easy to see) that there exists a 1-cycle $\widehat{\gamma}=\sum_{p=1}^h\widehat{a}_p\widehat{e}_p$ homologous to γ in $\mathbb{R}^3\setminus|\eta|$ (and "arbitrarily close to γ" if necessary), which is transverse to S_η in the following sense: for every $p \in \{1, \dots, h\}$ and for every $q \in \{1, \dots, k\}$, the intersection $|\widehat{e}_p| \cap |f_q|$ is either empty or consists of a single point, which does not belong to $|\partial_1 \widehat{e}_p| \cup |\partial_2 f_q|$.

For every $p \in \{1, \dots, h\}$ and for every $q \in \{1, \dots, k\}$, we denote by $\boldsymbol{\tau}(\widehat{e}_p)$ the unit tangent vector of the oriented segment $\widehat{e}_p$ and by $\boldsymbol{\nu}(f_q)$ the unit normal vector of the oriented triangle f_q obtained by the right hand rule. Let us define $L_{pq} := 0$ if $|\widehat{e}_p| \cap |f_q| = \emptyset$ and $L_{pq} := \mathrm{sign}(\boldsymbol{\tau}(\widehat{e}_p) \cdot \boldsymbol{\nu}(f_q))$ otherwise. Here $\boldsymbol{\tau}(\widehat{e}_p) \cdot \boldsymbol{\nu}(f_q)$ is the scalar product of the vectors $\boldsymbol{\tau}(\widehat{e}_p)$ and $\boldsymbol{\nu}(f_q)$ and, given $r \in \mathbb{R}$, $\mathrm{sign}(r)$ is equal to -1 if $r < 0$, 0 if $r = 0$, and 1 if $r > 0$. The *linking number* $\ell_{\mathcal{K}}(\gamma, \eta)$ *between* γ *and* η is the integer defined as follows:

$$\ell_{\mathcal{K}}(\gamma, \eta) := \sum_{p=1}^{h} \sum_{q=1}^{k} \widehat{a}_p b_q L_{pq}. \tag{19}$$

This definition is well-posed: it depends only on γ and η, not on the choice of S_η and of $\widehat{\gamma}$.

The linking number is symmetric, $\ell_{\mathcal{K}}(\gamma, \eta) = \ell_{\mathcal{K}}(\eta, \gamma)$, and bilinear: $\ell_{\mathcal{K}}(a\gamma, \eta) = a\, \ell_{\mathcal{K}}(\gamma, \eta)$ for every $a \in \mathbb{Z}$ and, if γ^* is a 1-cycle of $\mathbb{R}^3$ with $|\gamma^*| \cap |\eta| = \emptyset$, $\ell_{\mathcal{K}}(\gamma + \gamma^*, \eta) = \ell_{\mathcal{K}}(\gamma, \eta) + \ell_{\mathcal{K}}(\gamma^*, \eta)$.

The linking number is a homological invariant in the following sense: if a 1-cycle γ^* of $\mathbb{R}^3$ is homologous to γ in $\mathbb{R}^3 \setminus |\eta|$, then

$$\ell_{\mathcal{K}}(\gamma, \eta) = \ell_{\mathcal{K}}(\gamma^*, \eta). \tag{20}$$

In particular, we have:

$$\ell_{\mathcal{K}}(\gamma, \eta) = 0 \text{ if } \gamma \text{ is a 1-boundary of } \mathbb{R}^3 \setminus |\eta|. \tag{21}$$

The linking number can be computed via the Gauss double integral:

$$\ell_{\mathcal{K}}(\gamma, \eta) = \frac{1}{4\pi} \oint_\gamma \left(\oint_\eta \frac{\mathbf{y} - \mathbf{x}}{|\mathbf{y} - \mathbf{x}|^3} \times \mathbf{ds}(\mathbf{y}) \right) \cdot \mathbf{ds}(\mathbf{x})\,. \tag{22}$$

For an efficient computation of the linking number see e.g. [3].

Another property of linking number, we will exploit to compute the coefficients $\alpha_{i,j}^{r,s}$ (see the proof of Lemma 5), is that it can be used to recognize 1-boundaries of $\overline{\Omega}$ among 1-cycles of $\overline{\Omega}$. This is possible by the Alexander duality theorem. Indeed, such a theorem ensures that $H_1(\mathbb{R}^3 \setminus \overline{\Omega}; \mathbb{Z})$ is isomorphic to $H_1(\overline{\Omega}; \mathbb{Z})$, and hence to $\mathbb{Z}^g$ if g is the first Betti number of $\overline{\Omega}$. Furthermore, if $\sigma_1^*, \dots, \sigma_g^*$ are 1-cycles of $\mathbb{R}^3$ with support in $\mathbb{R}^3 \setminus \overline{\Omega}$ whose homology classes in $\mathbb{R}^3 \setminus \overline{\Omega}$ form a basis of $H_1(\mathbb{R}^3 \setminus \overline{\Omega}; \mathbb{Z})$, then it holds:

A 1-cycle σ *of* $\overline{\Omega}$ *is a 1-boundary of* $\overline{\Omega}$ *if and only if* $\ell_{\mathcal{K}}(\sigma, \sigma_i^*) = 0$ *for every* $i \in \{1, \dots, g\}$.

For this topic, we refer the reader to [6] and to the references mentioned therein.

Let us define a block diagonal matrix $A \in \mathbb{Z}^{g \times g}$ whose entries are linking numbers.

Since $\partial\Omega$ has a collar in $\mathbb{R}^3 \setminus \Omega$, there exist 1-cycles $\{\widehat{\sigma}_{0,s}^-\}_{s=0}^{g_0} \cup \{\sigma_{1,s}^-\}_{s=1}^{g_1} \cup \ldots \cup \{\sigma_{p,s}^-\}_{s=1}^{g_p}$ of $\mathbb{R}^3$ with support contained in $\mathbb{R}^3 \setminus \overline{\Omega}$ (obtained by slightly moving the 1-cycles $\{\widehat{\sigma}_{0,s}\}_{s=0}^{g_0} \cup \{\sigma_{1,s}\}_{s=1}^{g_1} \cup \ldots \cup \{\sigma_{p,s}\}_{s=1}^{g_p}$ of $\mathcal{T}_\partial$ inside $\mathbb{R}^3 \setminus \overline{\Omega}$) such that $[\widehat{\sigma}_{0,s}^-]_{\mathbb{R}^3\setminus\Omega} = [\widehat{\sigma}_{0,s}]_{\mathbb{R}^3\setminus\Omega}$ for every $s \in \{1,\ldots,g_0\}$ and $[\sigma_{r,s}^-]_{\mathbb{R}^3\setminus\Omega} = [\sigma_{r,s}]_{\mathbb{R}^3\setminus\Omega}$ for every $r \in P$ and for every $s \in \{1,\ldots,g_r\}$. In particular, thanks to (13) and (14), we infer that

$$\bigcup_{i\in P} \{[\sigma_{i,s}^-]_{\mathbb{R}^3\setminus\overline{\Omega_0}}\}_{s=1}^{g_i} \text{ is a basis of } H_1(\mathbb{R}^3 \setminus \overline{\Omega_0}; \mathbb{Z}) \tag{23}$$

and

$$\{[\widehat{\sigma}_{0,s}^-]_{\mathbb{R}^3\setminus\overline{\Omega_r}}\}_{s=1}^{g_0} \cup \bigcup_{i\in P_r} \{[\sigma_{i,s}^-]_{\mathbb{R}^3\setminus\overline{\Omega_r}}\}_{s=1}^{g_i} \text{ is a basis of } H_1(\mathbb{R}^3 \setminus \overline{\Omega_r}; \mathbb{Z}) \tag{24}$$

for every $r \in P$.

For every $k, i \in \{0, 1, \ldots, p\}$, define the $(g_k \times g_i)$-matrix $A_{k,i}$ as follows:

$$\begin{aligned}
A_{0,0} &:= \left(\ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}^-, \sigma_{0,j})\right)_{l,j} \in \mathbb{Z}^{g_0\times g_0},\\
A_{0,i} &:= \left(\ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}^-, \widehat{\sigma}_{i,j})\right)_{l,j} \in \mathbb{Z}^{g_0\times g_i} \ \text{ if } i \in P,\\
A_{k,k} &:= \left(\ell_{\mathcal{K}}(\sigma_{k,l}^-, \widehat{\sigma}_{k,j})\right)_{l,j} \in \mathbb{Z}^{g_k\times g_k} \ \text{ if } k \in P,\\
A_{k,0} &:= \left(\ell_{\mathcal{K}}(\sigma_{k,l}^-, \sigma_{0,j})\right)_{l,j} \in \mathbb{Z}^{g_k\times g_0} \ \text{ if } k \in P,\\
A_{k,i} &:= \left(\ell_{\mathcal{K}}(\sigma_{k,l}^-, \widehat{\sigma}_{i,j})\right)_{l,j} \in \mathbb{Z}^{g_k\times g_i} \ \text{ if } k, i \in P \text{ and } k \neq i.
\end{aligned}$$

Denote by $A \in \mathbb{Z}^{g\times g}$ the matrix with blocks $(A_{k,i})_{k,i\in\{0,1,\ldots,p\}}$.

Lemma 5 *For every $k, i \in \{1,\ldots,p\}$ the matrices $A_{0,i}$ and $A_{k,0}$ are equal to zero, and if $k \neq i$ then also the matrix $A_{k,i}$ is equal to zero. In other words A is block diagonal.*

Proof First we recall that for every $r \in \{0, 1, \ldots, p\}$ and $s \in \{1,\ldots,g_r\}$ the supports of both the 1-cycles $\sigma_{r,s}$ and $\widehat{\sigma}_{r,s}$ are contained in Γ_r. Hence, if $k \neq i$ then the supports of the 1-cycles $\sigma_{k,l}$ and $\widehat{\sigma}_{i,j}$ are disjoint for $l \in \{1,\ldots,g_k\}$ and $j \in \{1,\ldots,g_i\}$, and $\ell_{\mathcal{K}}(\sigma_{k,l}, \widehat{\sigma}_{i,j}) = \ell_{\mathcal{K}}(\widehat{\sigma}_{i,j}, \sigma_{k,l})$ is well defined. Moreover $\ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}^-, \widehat{\sigma}_{i,j}) = \ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}, \widehat{\sigma}_{i,j})$ if $i \in P$, $\ell_{\mathcal{K}}(\sigma_{k,l}^-, \sigma_{0,j}) = \ell_{\mathcal{K}}(\sigma_{k,l}, \sigma_{0,j})$ if $k \in P$, and $\ell_{\mathcal{K}}(\sigma_{k,l}^-, \widehat{\sigma}_{i,j}) = \ell_{\mathcal{K}}(\sigma_{k,l}, \widehat{\sigma}_{i,j})$ if $k, i \in P$ and $k \neq i$.

Let us proof that $A_{0,i} = 0$ if $i \in P$. For every $j \in \{1,\ldots,g_i\}$ we have that $\widehat{\sigma}_{i,j} = \partial_2 S_{i,j}^*$ for some 2-chain $S_{i,j}^*$ in $\overline{D_i}$, while $|\widehat{\sigma}_{0,l}| \subset \Gamma_0$ for every $l \in \{1,\ldots,g_0\}$. Since $\Gamma_0 \cap \overline{D_i} = \emptyset$ if $i \in P$, then $A_{0,i} = (\ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}, \widehat{\sigma}_{i,j}))_{l,j} = 0$.

Analogously we can prove that $A_{k,0} = 0$ if $k \in P$. Indeed, for every $j \in \{1,\ldots,g_0\}$, $\sigma_{0,j} = \partial_2 S_{0,j}^*$ with $|S_{0,j}^*| \subset \mathbb{R}^3 \setminus D_0$ and $|\sigma_{k,l}| \subset \Gamma_k$ for every $l \in \{1,\ldots,g_l\}$. Again we have $\Gamma_k \cap (\mathbb{R}^3 \setminus D_0) = \emptyset$ if $k \in P$ and then $A_{k,0} = (\ell_{\mathcal{K}}(\sigma_{k,l}, \sigma_{0,j}))_{l,j} = 0$.

Finally $A_{k,i} = 0$ if $k, i \in P$ and $k \neq i$ because, for every $j \in \{1,\ldots,g_i\}$, $\widehat{\sigma}_{i,j} = \partial_2 S_{i,j}^*$ with $|S_{i,j}^*| \subset \overline{D_i}$, $|\sigma_{k,l}| \subset \Gamma_k$ for every $l \in \{1,\ldots,g_k\}$ and $\Gamma_k \cap \overline{D_i} = \emptyset$. Hence $A_{k,i} = (\ell_{\mathcal{K}}(\sigma_{k,l}, \widehat{\sigma}_{i,j}))_{l,j} = 0$. □

Remark 6 The computation of the entries $\ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}^{-}, \sigma_{0,j})$ and $\ell_{\mathcal{K}}(\sigma_{k,l}^{-}, \widehat{\sigma}_{k,j})$ of the matrices $A_{k,k}$ cannot be performed directly because $\{\widehat{\sigma}_{0,l}^{-}\}_l$ and $\{\sigma_{k,l}^{-}\}_{k,l}$ are 1-cycles of $\mathbb{R}^3 \setminus \Omega$, which is not triangulated (and is not convenient to triangulate). We overcome this difficulty by constructing 1-cycles $\{\sigma_{0,j}^{+}\}_{j=0}^{g_0} \cup \{\widehat{\sigma}_{1,j}^{+}\}_{j=1}^{g_1} \cup \ldots \cup \{\widehat{\sigma}_{p,j}^{+}\}_{j=1}^{g_p}$ of $\mathbb{R}^3$ with support contained in Ω such that $\sigma_{0,j}^{+}$ is homologous to $\sigma_{0,j}$ in $\overline{\Omega}$ and $\widehat{\sigma}_{k,j}^{+}$ is homologous to $\widehat{\sigma}_{k,j}$ in $\overline{\Omega}$. It turns out that $\ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}^{-}, \sigma_{0,j}) = \ell_{\mathcal{K}}(\widehat{\sigma}_{0,l}, \sigma_{0,j}^{+})$ for $l, j \in \{1, \ldots, g_0\}$ and, for every $k \in P$, $\ell_{\mathcal{K}}(\sigma_{k,l}^{-}, \widehat{\sigma}_{k,j}) = \ell_{\mathcal{K}}(\sigma_{k,l}, \widehat{\sigma}_{k,j}^{+})$ for $l, j \in \{1, \ldots, g_k\}$ (see [1, Lemma 2.1]). We will shown, in Section 2.2.4, how to construct $\sigma_{0,j}^{+}$ and $\widehat{\sigma}_{k,j}^{+}$.

2.2.2 Computation of the coefficients $(\alpha_{i,j}^{0,s})_{i,j}$ for $s \in \{1, \ldots, g_0\}$

Let $G_0 := \sum_{i \in P} g_i = g - g_0$ and let $A_{(0)}$ be the diagonal block matrix with blocks $(A_{k,k})_{k \in P} \in \mathbb{Z}^{G_0 \times G_0}$. It is important to observe that the entries of $A_{(0)}$ are the linking numbers between the representatives of a basis of $H_1(\mathbb{R}^3 \setminus \overline{\Omega_0}; \mathbb{Z})$ (see (23)) and the representatives of a basis of $H_1(\overline{\Omega_0}; \mathbb{Z})$ (see (11)). In this way, the Alexander duality theorem applied to $\overline{\Omega_0}$ ensures that

$$\left| \det \left(A_{(0)} \right) \right| = 1. \tag{25}$$

Consider the row vectors $\alpha_i^{0,s} := (\alpha_{i,1}^{0,s}, \ldots, \alpha_{i,g_i}^{0,s})$ and $\beta_i^{0,s} := \big(\ell_{\mathcal{K}}(\sigma_{i,1}, \widehat{\sigma}_{0,s}), \ldots, \ell_{\mathcal{K}}(\sigma_{i,g_i}, \widehat{\sigma}_{0,s})\big)$ for every $i \in P$, and the column vectors

$$\alpha^{0,s} := (\alpha_1^{0,s}, \ldots, \alpha_p^{0,s})^T \in \mathbb{Z}^{G_0} \quad \text{and} \quad \beta^{0,s} := (\beta_1^{0,s}, \ldots, \beta_p^{0,s})^T \in \mathbb{Z}^{G_0},$$

where the superscript "^{T}" denotes the transpose operation.

Bearing in mind the linearity of linking number and its homological invariance, equation (15) implies that

$$\ell_{\mathcal{K}}(\sigma_{k,h}, \widehat{\sigma}_{0,s}) = \sum_{i \in P} \sum_{j=1}^{g_i} \alpha_{i,j}^{0,s} \ell_{\mathcal{K}}(\sigma_{k,h}^{-}, \widehat{\sigma}_{i,j}) \ \text{ if } k \in P \text{ and } h \in \{1, \ldots, g_k\}. \tag{26}$$

Linear system (26) in the unknowns $(\alpha_{i,j}^{0,s})_{i,j}$ can be rewritten in the following compact form:

$$A_{(0)} \alpha^{0,s} = \beta^{0,s}, \tag{27}$$

where $\alpha^{0,s}$ is the unknown. Thanks to (25), equation (15) is equivalent to (27).

In this way, we conclude that the coefficients $(\alpha_{i,j}^{0,s})_{i,j}$ can be computed by solving linear system (27), namely solving p linear systems each one of dimension g_r, $r \in \{1, \ldots, p\}$.

2.2.3 Computation of the coefficients $(\alpha_{i,j}^{r,s})_{i,j}$ for $r \in P$ and $s \in \{1, \ldots, g_r\}$

Given $k, r \in P$, we define the integer $k_r \in \{0, 1, \ldots, p\} \setminus \{r\}$ by setting $k_r := k - 1$ if $k \leq r$ and $k_r := k$ if $k > r$. Let $G_r := g_0 + \sum_{i \in P_r} g_i = g - g_r$ and let $A_{(r)}$ be the diagonal block matrix $(A_{k_r, i_r})_{k,i \in P} \in \mathbb{Z}^{G_r \times G_r}$. By applying the Alexander duality theorem to $\overline{\Omega_r}$, we obtain:

$$\left|\det\left(A_{(r)}\right)\right| = 1. \tag{28}$$

Consider the row vectors $\alpha_0^{r,s} := (\alpha_{0,1}^{r,s}, \ldots, \alpha_{0,g_0}^{r,s})$, $\beta_0^{r,s} := \big(\ell_{\mathcal{K}}(\widehat{\sigma}_{0,1}, \sigma_{r,s}), \ldots, \ell_{\mathcal{K}}(\widehat{\sigma}_{0,g_0}, \sigma_{r,s})\big)$ and, for every $i \in P_r$, $\alpha_i^{r,s} := (\alpha_{i,1}^{r,s}, \ldots, \alpha_{i,g_i}^{r,s})$ and $\beta_i^{r,s} := \big(\ell_{\mathcal{K}}(\sigma_{i,1}, \sigma_{r,s}), \ldots, \ell_{\mathcal{K}}(\sigma_{i,g_i}, \sigma_{r,s})\big)$. Consider also the column vectors

$$\alpha^{r,s} := (\alpha_0^{r,s}, \alpha_1^{r,s}, \ldots, \alpha_{r-1}^{r,s}, \alpha_{r+1}^{r,s}, \ldots, \alpha_p^{r,s})^T \in \mathbb{Z}^{G_r}$$

and

$$\beta^{r,s} := (\beta_0^{r,s}, \beta_1^{r,s}, \ldots, \beta_{r-1}^{r,s}, \beta_{r+1}^{r,s}, \ldots, \beta_p^{r,s})^T \in \mathbb{Z}^{G_r}$$

By using equation (16) and the linking number, we infer that

$$\ell_{\mathcal{K}}(\widehat{\sigma}_{0,h}, \sigma_{r,s}) = \sum_{j=1}^{g_0} \alpha_{0,j}^{r,s} \ell_{\mathcal{K}}(\widehat{\sigma}_{0,h}^-, \sigma_{0,j}) + \sum_{i \in P_r} \sum_{j=1}^{g_i} \alpha_{i,j}^{r,s} \ell_{\mathcal{K}}(\widehat{\sigma}_{0,h}^-, \widehat{\sigma}_{i,j}) \tag{29}$$

if $h \in \{1, \ldots, g_0\}$ and

$$\ell_{\mathcal{K}}(\sigma_{k,h}, \sigma_{r,s}) = \sum_{j=1}^{g_0} \alpha_{0,j}^{r,s} \ell_{\mathcal{K}}(\sigma_{k,h}^-, \sigma_{0,j}) + \sum_{i \in P_r} \sum_{j=1}^{g_i} \alpha_{i,j}^{r,s} \ell_{\mathcal{K}}(\sigma_{k,h}^-, \widehat{\sigma}_{i,j}) \tag{30}$$

if $k \in P_r$ and $h \in \{1, \ldots, g_k\}$. Equations (29) and (30) can be rewritten as follows:

$$A_{(r)} \alpha^{r,s} = \beta^{r,s}. \tag{31}$$

Also in this case, for each $r \in P$, the matrix $A_{(r)}$ is block diagonal. Thanks to (28), equation (16) and linear system (31) are equivalent. Once again, we conclude that the coefficients $(\alpha_{i,j}^{r,s})_{i,j}$ can be computed by resolving linear system (31), namely solving p linear systems each one of dimension g_s, $s \in \{0, 1, \ldots, r-1, r+1, \ldots, p\}$.

2.2.4 Moving 1-cycles of $\partial\Omega$ inside Ω

In what follows, given any 1-cycle η of $\mathcal{T}_\partial$, we will construct a 1-cycle η^+ of Ω homologous to η in $\overline{\Omega}$. First we need to describe some geometric notions we will use in the mentioned construction. For a complete description of those notions, see [1, Section 2].

Given two different points $\mathbf{a}, \mathbf{b}$ in $\mathbb{R}^3$, we denote by $[\mathbf{a}, \mathbf{b}]$ the oriented segment of $\mathbb{R}^3$ from $\mathbf{a}$ to $\mathbf{b}$. The (not oriented) segment of $\mathbb{R}^3$ of vertices $\mathbf{a}, \mathbf{b}$ is the 2-set $\{\mathbf{a}, \mathbf{b}\}$. The unit tangent vector $\boldsymbol{\tau}([\mathbf{a}, \mathbf{b}])$ of the oriented segment $[\mathbf{a}, \mathbf{b}]$ is given by $\boldsymbol{\tau}([\mathbf{a}, \mathbf{b}]) := \frac{\mathbf{b}-\mathbf{a}}{|\mathbf{b}-\mathbf{a}|}$. Recall that a 1-chain (of $\mathbb{R}^3$) is a formal linear combination with integer coefficients of oriented segments, where we identify $-[\mathbf{a}, \mathbf{b}] = [\mathbf{b}, \mathbf{a}]$.

Analogously, if $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are three different not aligned points in $\mathbb{R}^3$, we denote by $[\mathbf{a}, \mathbf{b}, \mathbf{c}]$ the oriented triangle of $\mathbb{R}^3$. The (not oriented) triangle of $\mathbb{R}^3$ of vertices $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is the 3-set $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$. The unit normal vector $\boldsymbol{\nu}([\mathbf{a}, \mathbf{b}, \mathbf{c}])$ of the oriented triangle $[\mathbf{a}, \mathbf{b}, \mathbf{c}]$ is obtained by the right hand rule: $\boldsymbol{\nu}([\mathbf{a}, \mathbf{b}, \mathbf{c}]) := \frac{(\mathbf{b}-\mathbf{a})\times(\mathbf{c}-\mathbf{a})}{|(\mathbf{b}-\mathbf{a})\times(\mathbf{c}-\mathbf{a})|}$. Recall that a 2-chain (of $\mathbb{R}^3$) is a formal linear combination with integer coefficients of oriented triangles, where for every permutation $\rho : \{\mathbf{a}, \mathbf{b}, \mathbf{c}\} \longrightarrow \{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$ we identify $[\rho(\mathbf{a}), \rho(\mathbf{b}), \rho(\mathbf{c})] = [\mathbf{a}, \mathbf{b}, \mathbf{c}]$ if $\boldsymbol{\nu}([\rho(\mathbf{a}), \rho(\mathbf{b}), \rho(\mathbf{c})]) = \boldsymbol{\nu}([\mathbf{a}, \mathbf{b}, \mathbf{c}])$ and $[\rho(\mathbf{a}), \rho(\mathbf{b}), \rho(\mathbf{c})] = -[\mathbf{a}, \mathbf{b}, \mathbf{c}]$ if $\boldsymbol{\nu}([\rho(\mathbf{a}), \rho(\mathbf{b}), \rho(\mathbf{c})]) = -\boldsymbol{\nu}([\mathbf{a}, \mathbf{b}, \mathbf{c}])$.

We define the boundary of $[\mathbf{a}, \mathbf{b}, \mathbf{c}]$ in the following way: $\partial_2([\mathbf{a}, \mathbf{b}, \mathbf{c}]) = [\mathbf{b}, \mathbf{c}] - [\mathbf{a}, \mathbf{c}] + [\mathbf{a}, \mathbf{b}]$. By linearity this boundary operator can be extended to every 2-chains. It can be defined also for degenerate triangles $[\mathbf{a}, \mathbf{b}, \mathbf{c}]$ where $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are three different points in $\mathbb{R}^3$ not necessarily not aligned.

We will use also the barycenter of a segment $\{\mathbf{a}, \mathbf{b}\}$ and the barycenter of a triangle $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$: $B(\{\mathbf{a}, \mathbf{b}\}) = (\mathbf{a} + \mathbf{b})/2$, $B(\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}) = (\mathbf{a} + \mathbf{b} + \mathbf{c})/3$. Similarly, we set: $B([\mathbf{a}, \mathbf{b}]) = (\mathbf{a} + \mathbf{b})/2$, $B([\mathbf{a}, \mathbf{b}, \mathbf{c}]) = (\mathbf{a} + \mathbf{b} + \mathbf{c})/3$.

Let us fix an orientation of each edge and face of $\mathcal{T} = (V, E, F, K)$. This can be done as follows. Choose a total ordering $(\mathbf{v}_1, \ldots, \mathbf{v}_{n_V})$ of the elements of V. If the segment $e = \{\mathbf{v}_i, \mathbf{v}_j\}$ is an edge of $\mathcal{T}$ in E of vertices $\mathbf{v}_i, \mathbf{v}_j$ with $1 \leq i < j \leq n_V$, then e determines the oriented segment $[\mathbf{v}_i, \mathbf{v}_j]$, we denote again by e. Analogously, if the triangle $f = \{\mathbf{v}_i, \mathbf{v}_j, \mathbf{v}_k\}$ is a face of $\mathcal{T}$ in F of vertices $\mathbf{v}_i, \mathbf{v}_j, \mathbf{v}_k$ with $1 \leq i < j < k \leq n_V$, then f determines the oriented triangle $[\mathbf{v}_i, \mathbf{v}_j, \mathbf{v}_k]$, we denote again by f.

Let us recall some concepts concerning the block dual barycentric complex of $\mathcal{T}$ and the block dual barycentric complex of the triangulation $\mathcal{T}_\partial$ of $\partial\Omega$ induced by $\mathcal{T}$. More precisely we will use the oriented dual face $D(e)$ and the boundary oriented dual edge $D_\partial(e)$ of a boundary oriented edge e.

- For every oriented edge $e = [\mathbf{v}, \mathbf{w}]$ of $\mathcal{T}_\partial$, the oriented dual face $D(e)$ of $\mathcal{T}$ associated with e is a 2-chain defined as follows: if $F(e)$ denotes the set $\{f \in F \mid \{\mathbf{v}, \mathbf{w}\} \subset f\}$ of faces of $\mathcal{T}$ incident on e, then we set

$$D(e) := \sum_{f \in F(e)} \sum_{t \in K(f)} \operatorname{sign}\big(\boldsymbol{\tau}(e) \cdot \boldsymbol{\nu}([B(e), B(f), B(t)])\big)\, [B(e), B(f), B(t)],$$

where $K(f)$ is the set of tetrahedra of $\mathcal{T}$ incident on f (see Fig. 4). The reader observes that the support of $D(e)$ is the union of triangles of $\mathbb{R}^3$ with vertices $B(e)$, $B(f)$ and $B(t)$, where f varies in $F(e)$ and t in $K(f)$. Such triangles are oriented by e via the right hand rule.

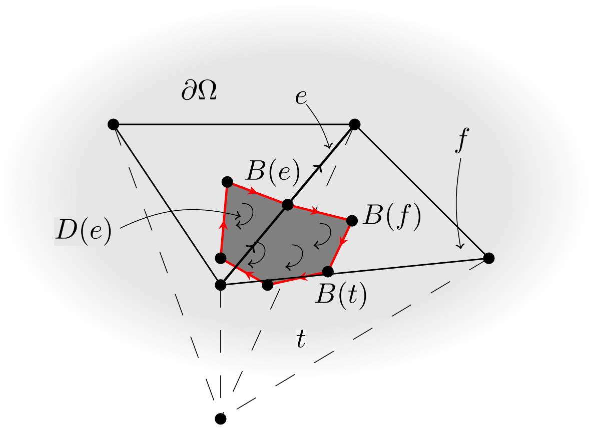


Fig. 4 The dual face $D(e)$ of a boundary edge e together with its boundary $\partial_2 D(e)$ in red

- For every oriented edge e of $\mathcal{T}_\partial$, the (boundary) oriented dual edge $D_\partial(e)$ of $\mathcal{T}_\partial$ associated with e is the 1-chain defined as follows. Let f_1 and f_2 be the boundary oriented faces incident on e, and let $\mathbf{n}(f_1)$ and $\mathbf{n}(f_2)$ be the outward unit normals of $\partial\Omega$ at $B(f_1)$ and at $B(f_2)$, respectively. Then we set

$$D_\partial(e) := \sum_{i=1}^{2} \operatorname{sign}\big(\boldsymbol{\tau}(e) \cdot (\mathbf{n}(f_i) \times \boldsymbol{\tau}([B(e), B(f_i)]))\big)[B(e), B(f_i)].$$

  $D_\partial(e)$ can be described as follows. By interchanging f_1 with f_2 if necessary, we can suppose that f_1 is on the left of e and f_2 on the right of e with respect to the orientation of $\partial\Omega$ induced by its outward unit vector field. Then we have:

$$D_\partial(e) = [B(f_1), B(e)] + [B(e), B(f_2)],$$

  see Fig. 5. A (non-oriented) dual edge of $\mathcal{T}_\partial$ is a 2-subset $\{\mathbf{a}, \mathbf{b}\}$ of $\partial\Omega$ such that $\{\mathbf{a}, \mathbf{b}\} = |\partial_1 D_\partial(e)|$ for some oriented edge e of $\mathcal{T}_\partial$. Denote by E'_∂ the set of all dual edges of $\mathcal{T}_\partial$.

Given a 1-cycle ℓ of $\mathcal{T}_\partial = (V_\partial, E_\partial, F_\partial)$, we say that ℓ is a *simple loop of* $\mathcal{T}_\partial$ if there exist distinct vertices $\mathbf{v}_{k(1)}, \ldots, \mathbf{v}_{k(R)}$ in V_∂ (for some indices $k(1), \ldots, k(R) \in \{1, \ldots, n_V\}$) such that each $\{\mathbf{v}_{k(r)}, \mathbf{v}_{k(r+1)}\}$ is an edge in E_∂ and $\ell = \sum_{r=1}^{R}[\mathbf{v}_{k(r)}, \mathbf{v}_{k(r+1)}]$, where $\mathbf{v}_{k(R+1)} = \mathbf{v}_{k(1)}$.

Denote by $\mathcal{E}_\partial$ the set of all boundary oriented edges in $\mathcal{T}_\partial$ (with the orientation fixed above). Consider an arbitrary 1-cycle $\eta = \sum_{e\in\mathcal{E}_\partial} \alpha_e e$ of $\mathcal{T}_\partial$. Let us show that η can be written as a finite linear combination (over the integers) of simple loops of $\mathcal{T}_\partial$. Let $\mathcal{S}$ be a spanning tree of the graph (V_∂, E_∂). We choose $\mathbf{v}_1$ as a root of $\mathcal{S}$. Given $\mathbf{v}_j \in V_\partial$, let $C_{\mathbf{v}_j}$ be the unique 1-chain in $\mathcal{S}$ from $\mathbf{v}_1$ to $\mathbf{v}_j$. For any oriented edge $e = [\mathbf{v}_k, \mathbf{v}_l] \in \mathcal{E}_\partial$ we denote by D_e the simple loop of $\mathcal{T}_\partial$ given by $C_{\mathbf{v}_k} + e - C_{\mathbf{v}_l}$. Then η can be written as $\eta = \sum_{e\in\mathcal{E}_\partial} \alpha_e e = \sum_{e\in\mathcal{E}_\partial} \alpha_e D_e$.

In this way, in order to construct $\eta^+ = \sum_{e\in\mathcal{E}_\partial} \alpha_e D_e^+$, we can assume that η is a simple loop of $\mathcal{T}_\partial$. Hence we can write η as follows: $\eta = \sum_{r=1}^{R_\eta}[\mathbf{v}_{k(r)}, \mathbf{v}_{k(r+1)}]$ with

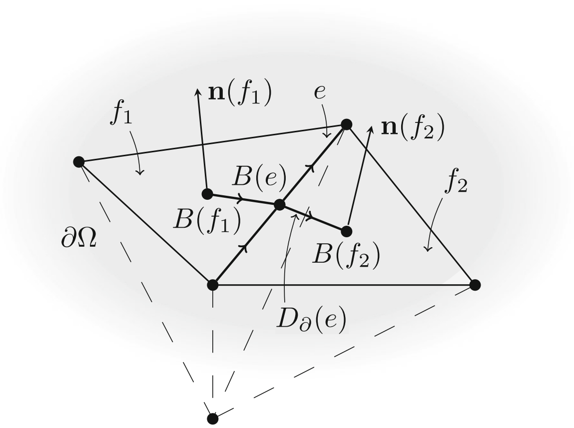


Fig. 5 The boundary dual edge $D_\partial(e)$

$\mathbf{v}_{k(1)} = \mathbf{v}_{k(R_\eta+1)}$, $\mathbf{v}_{k(r)} \in V_\partial$ for $1 \le r \le R_\eta$, $\mathbf{v}_{k(r)} \ne \mathbf{v}_{k(r')}$ if $1 \le r, r' \le R_\eta$ with $r \ne r'$ and $\{\mathbf{v}_{k(r)}, \mathbf{v}_{k(r+1)}\} \in E_\partial$ for $1 \le r \le R_\eta$.

For each $r \in \{1, \ldots, R_\eta\}$ we define the set $\mathcal{F}_r := \{\mathbf{w}_{r,0}, \mathbf{w}_{r,1}, \ldots, \mathbf{w}_{r,N_r}\}$ of vertices of V_∂ in the following way:

(i) $\mathbf{w}_{r,0} = \mathbf{v}_{k(r-1)}$ if $r > 1$ while $\mathbf{w}_{1,0} = \mathbf{v}_{k(R_\eta)}$,
(ii) $\mathbf{w}_{r,1}$ is the unique vertex in V_∂ such that $\nu([\mathbf{w}_{r,0}, \mathbf{v}_{k(r)}, \mathbf{w}_{r,1}])$ points outside Ω. If $\mathbf{w}_{r,1} = \mathbf{v}_{k(r+1)}$ then $N_r = 1$
(iii) If $N_r > 1$, for $s \ge 1$, $\mathbf{w}_{r,s+1}$ is the unique vertex in V_∂ such that $\mathbf{w}_{r,s+1} \ne \mathbf{w}_{r,s-1}$ and $\{\mathbf{w}_{r,s}, \mathbf{v}_{k(r)}, \mathbf{w}_{r,s+1}\} \in F_\partial$. If $\mathbf{w}_{r,s+1} = \mathbf{v}_{k(r+1)}$ then $N_r = s + 1$.

For $r \in \{1, \ldots, R_\eta\}$, for $s \in \{0, \ldots, N_r\}$ we denote by $B_{r,s}$ the barycenter of the edge $\{\mathbf{w}_{r,s}, \mathbf{v}_{k(r)}\}$ and for $s \in \{1, \ldots, N_r\}$ we denote by $B^*_{r,s}$ the barycenter of the triangle $\{\mathbf{w}_{r,s-1}, \mathbf{v}_{k(r)}, \mathbf{w}_{r,s}\}$ (see Fig. 6).

Consider the following 1-chain $\overline{\eta}$:

$$\overline{\eta} = \left(\sum_{r=1}^{R_\eta - 1} \left([\mathbf{v}_{k(r)}, B_{r+1,0}] + [B_{r+1,0}, \mathbf{v}_{k(r+1)}] \right) \right) + \left([\mathbf{v}_{k(R_\eta)}, B_{1,0}] + [B_{1,0}, \mathbf{v}_{k(1)}] \right)$$

$$= \sum_{r=1}^{R_\eta} \left([\mathbf{v}_{k(r)}, B_{r+1,0}] + [B_{r+1,0}, \mathbf{v}_{k(r+1)}] \right) ,$$

where we have denoted $B_{R_\eta+1,0} = B_{1,0}$. Clearly $\overline{\eta}$ is homologous to η in $\overline{\Omega}$ (in $\partial\Omega$ indeed). In fact

$$\partial_2 \left(\sum_{r=1}^{R_\eta} \left[\mathbf{v}_{k(r)}, B_{r+1,0}, \mathbf{v}_{k(r+1)} \right] \right) = \sum_{r=1}^{R_\eta} \Big(\left[B_{r+1,0}, \mathbf{v}_{k(r+1)} \right] - \left[\mathbf{v}_{k(r)}, \mathbf{v}_{k(r+1)} \right]$$
$$+ \left[\mathbf{v}_{k(r)}, B_{r+1,0} \right] \Big)$$
$$= \overline{\eta} - \eta \, .$$

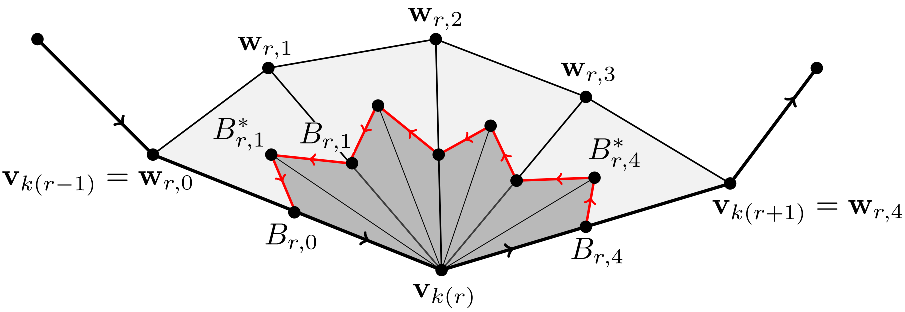


Fig. 6 The vertices $\mathbf{w}_{r,s}$, the barycenters $B_{r,s}$ and the barycenters $B^*_{r,s}$. In dark gray the 2-chain $\sum_{s=1}^{N_r} \left([B_{r,s-1}, \mathbf{v}_{k(r)}, B^*_{r,s}] + [B^*_{r,s}, \mathbf{v}_{k(r)}, B_{r,s}] \right)$. The red 1-chain together with $[B_{r,0}, \mathbf{v}_{k(r)}] + [\mathbf{v}_{k(r)}, B_{r,4}]$ is its boundary

Now we consider the 2-chain

$$S(\eta) = \sum_{r=1}^{R_\eta} \sum_{s=1}^{N_r} \left([B_{r,s-1}, \mathbf{v}_{k(r)}, B^*_{r,s}] + [B^*_{r,s}, \mathbf{v}_{k(r)}, B_{r,s}]\right)$$

and we define

$$\widehat{\eta} = \overline{\eta} - \partial_2 S(\eta)\,.$$

Notice that, since $B^*_{r,N_r} = B^*_{r+1,1}$, we can compute $\widehat{\eta}$ in this way:

$$\widehat{\eta} = \sum_{r=1}^{R_\eta} \sum_{s=1}^{N_r-1} D_\partial([\mathbf{v}_{k(r)}, \mathbf{w}_{r,s}])\,,$$

where the sum $\sum_{s=1}^{N_r-1} D_\partial([\mathbf{v}_{k(r)}, \mathbf{w}_{r,s}])$ is considered equal to 0 if $N_r = 1$ (see Fig. 7).

Finally we consider the following 2-chain $\widehat{S}(\eta)$ in the block dual barycentric complex of $\mathcal{T}$:

$$\widehat{S}(\eta) = \sum_{r=1}^{R_\eta} \sum_{s=1}^{N_r-1} D([\mathbf{v}_{k(r)}, \mathbf{w}_{r,s}])$$

(see Fig. 4 for the dual of a boundary edge), and we define η^+ of η by setting

$$\eta^+ = \widehat{\eta} - \partial_2 \widehat{S}(\eta)\,.$$

Summarizing, the algorithm for the construction of 1-cycle η^+ of Ω homologous to a simple loop η of $\mathcal{T}_\partial$ in $\overline{\Omega}$ first constructs the 1-chain $\hat{\eta}$ in Fig. 7 and then push inside Ω the barycenters $B_{r,s}$ subtracting $\partial_2 D([\mathbf{v}_{k(r)}, \mathbf{w}_{r,s}])$ to $D_\partial([\mathbf{v}_{k(r)}, \mathbf{w}_{r,s}])$.

2.3 The consequent algorithm

We are in position to write the complete algorithm for the computation of the 1-boundaries $\widehat{\sigma}'_{0,s}$ for $s \in \{1,\ldots,g_0\}$ and $\sigma'_{r,s}$ for $r \in \{1,\ldots,p\}$ and $s \in \{1,\ldots,g_r\}$. We introduce the following notation that allow us to descrive the algorithm in a more compact way, hiding the peculiarity of the external connected component Γ_0 of $\partial\Omega$:

$$\mathfrak{s}_{r,s} := \begin{cases} \widehat{\sigma}_{0,s} & \text{if } r = 0 \\ \sigma_{r,s} & \text{if } r \neq 0 \end{cases}, \quad \widehat{\mathfrak{s}}_{r,s} := \begin{cases} \sigma_{0,s} & \text{if } r = 0 \\ \widehat{\sigma}_{r,s} & \text{if } r \neq 0 \end{cases} \quad \text{and} \quad \mathfrak{s}'_{r,s} := \begin{cases} \widehat{\sigma}'_{0,s} & \text{if } r = 0 \\ \sigma'_{r,s} & \text{if } r \neq 0 \end{cases}$$

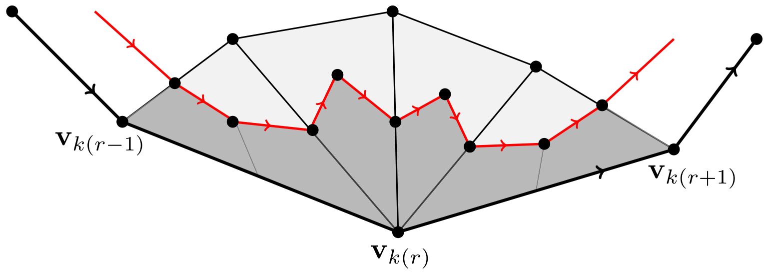


Fig. 7 The 1-chain $\widehat{\eta}$ in red

Algorithm 1

1. *For* $r \in \{0, 1, \ldots, p\}$
   (a) *compute a set of* $2g_r$ *1-cycles* $\{\gamma_{r,l}\}_{l=1}^{2g_r}$ *of* Γ_r *that are representatives of a basis of* $H_1(\Gamma_r; \mathbb{Z})$
   (via the Hiptmair-Ostrowski Algorithm [15]*).*
   (b) *compute*
   – g_r *1-cycles* $\{\sigma_{r,n}\}_{n=1}^{g_r}$ *whose homology classes in* $\overline{D_r}$ *form a basis of the homology group* $H_1(\overline{D}_r; \mathbb{Z})$
   – g_r *1-cycles* $\{\widehat{\sigma}_{r,n}\}_{n=1}^{g_r}$ *whose homology classes in* $\mathbb{R}^3 \setminus D_r$ *form a basis of the homology group* $H_1(\mathbb{R}^3 \setminus D_r; \mathbb{Z})$

   (via the Hiptmair-Ostrowski Algorithm [15]*).*
   (c) *for* $s \in \{1, \ldots, g_r\}$ *compute* $\mathfrak{s}_{r,s}$ *and* $\widehat{\mathfrak{s}}_{r,s}$.
   (d) *for* $s \in \{1, \ldots, g_r\}$ *compute the 1-cycles* $\widehat{\mathfrak{s}}_{r,s}^{+}$
   (via the algorithm in Section 2.2.4).
   (e) *compute the matrix* $A_{r,r} \in \mathbb{Z}^{g_r \times g_r}$ *with entries* $(A_{r,r})_{i,j} = \ell_{\mathcal{K}}(\mathfrak{s}_{r,i}, \widehat{\mathfrak{s}}_{r,j}^{+})$.
2. *For* $r \in \{0, 1, \ldots, p\}$
   (a) *for* $s \in \{1, \ldots, g_r\}$
   – *for* $l \in \{0, 1, \ldots, p\} \setminus \{r\}$
   (i) *compute the vector* $\beta_l^{r,s} \in \mathbb{Z}^{g_l}$ *with components* $(\beta_l^{r,s})_j = \ell_{\mathcal{K}}(\mathfrak{s}_{l,j}, \mathfrak{s}_{r,s})$
   (ii) *compute the vector* $\alpha_l^{r,s} \in \mathbb{Z}^{g_l}$ *solving the linear system* $A_{l,l}\alpha_l^{r,s} = \beta_l^{r,s}$.
   – *construct the 1-boundary*

$$\mathfrak{s}'_{r,s} = \mathfrak{s}_{r,s} - \sum_{\substack{l \in \{0,1,\ldots,p\},\\ l \neq r}} \sum_{j=1}^{g_l} \alpha_{l,j}^{r,s}\, \widehat{\mathfrak{s}}_{l,j} \,.$$

Summarizing the algorithm works in this way.

- For each connected component Γ_r of $\partial\Omega$ for $r \in \{0, 1, \ldots, p\}$, we construct $2g_r$ 1-cycles of Γ_r that are representatives of the first homology group of Γ_r and that can be divided in the following way: g_r whose homology class is not trivial in the connected component of $\mathbb{R}^3 \setminus \Gamma_r$ that contains Ω (and these are the 1- cycles $\widehat{\mathfrak{s}}_{r,s}$), and g_r whose homology class is not trivial in the other connected component $\mathfrak{D}_r$ of $\mathbb{R}^3 \setminus \Gamma_r$, the one not intersecting Ω (and these are the 1- cycles $\mathfrak{s}_{r,s}$).
- For $r \in \{0, 1, \ldots, p\}$ let Ω_r be the domain $\Omega \cup \Gamma_r \cup \mathfrak{D}_r$ of $\mathbb{R}^3$ as in Fig. 2. In Lemma 2 we proved that a basis of $H_1(\overline{\Omega_r}; \mathbb{Z})$ is given by

$$\bigcup_{\substack{l \in \{0,1,\ldots,p\},\\ l \neq r}} \{[\widehat{\mathfrak{s}}_{l,j}]_{\overline{\Omega_r}}\}_{j=1}^{g_l} \,.$$

- Now we write each homology class $[\mathfrak{s}_{r,s}]_{\overline{\Omega_r}}$ for $s \in \{1, \dots, g_r\}$ in terms of the above basis as in (15) and (16):

$$[\mathfrak{s}_{r,s}]_{\overline{\Omega_r}} = \sum_{\substack{l \in \{0,1,\dots,p\},\\ l \neq r}} \sum_{j=1}^{g_l} \alpha_{l,j}^{r,s} [\widehat{\mathfrak{s}}_{l,j}]_{\overline{\Omega_r}} .$$

- Finally

$$\mathfrak{s}'_{r,s} = \mathfrak{s}_{r,s} - \sum_{\substack{l \in \{0,1,\dots,p\},\\ l \neq r}} \sum_{j=1}^{g_l} \alpha_{l,j}^{r,s} \, \widehat{\mathfrak{s}}_{l,j} .$$

3 Construction of the homological Seifert surfaces

For the sake of completness we include in this section a brief description of the algorithm analyzed in [1] for the construction of homological Seifert surfaces of a given 1-boundary of $\mathcal{T} = (V, E, F, K)$.

Denote by $\mathcal{E}$ the set of all oriented edges of $\mathcal{T}$ and by $\mathcal{F}$ the set of all oriented faces of $\mathcal{T}$. The orientation was fixed in Section 2.2.4 above. Let $\gamma = \sum_{e\in\mathcal{E}} a_e e$ be a 1-boundary of $\mathcal{T}$. A 2-chain $S = \sum_{f\in\mathcal{F}} b_f f$ of $\mathcal{T}$ is a homological Seifert surface of γ in $\mathcal{T}$ if $\partial_2 S = \gamma$; namely,

$$\sum_{f\in\mathcal{F}} b_f \partial_2 f = \sum_{e\in\mathcal{E}} a_e e. \tag{32}$$

We can write this equation more explicitly as a linear system. Given $e \in \mathcal{E}$, let $\mathcal{F}(e)$ be the set $\left\{ f \in \mathcal{F} \,\middle|\, |e| \subset |f| \right\}$ of oriented faces in $\mathcal{F}$ incident on e and let $\mathrm{o}_e : \mathcal{F}(e) \longrightarrow \{-1, 1\}$ be the function sending $f \in \mathcal{F}(e)$ into the coefficient of e in the expression of $\partial_2 f$ as a formal linear combination of oriented edges in $\mathcal{E}$. Equation (32) is equivalent to the linear system

$$\sum_{f\in\mathcal{F}(e)} \mathrm{o}_e(f) b_f = a_e \quad \forall\, e \in \mathcal{E} ,$$

where the unknowns $\{b_f\}_{f\in\mathcal{F}}$ are integers. The matrix of this linear system is the incidence matrix between faces and edges of $\mathcal{T}$. Its entries take values in the set $\{-1, 0, 1\}$. This matrix is very sparse because it has just three nonzero entries per columns and the number of nonzero entries on each row is equal to the number of faces incident on the edge corresponding to the row. This kind of problems are usually solved using the Smith normal form, a computationally demanding algorithm even in the case of sparse matrices (see e.g. [11, 23]).

A first difficulty to devise a general and efficient algorithm to compute a homological Seifert surface S of a given 1-boundary γ of $\mathcal{T}$ is that the problem has not a unique solution. If $\mathfrak{t}$ is the number of tetrahedra of $\mathcal{T}$ and $\Gamma_0, \Gamma_1, \dots, \Gamma_p$ are the connected components of $\partial\Omega$, then the kernel of the incidence matrix is a free abelian group of rank $\mathfrak{t} + p$; namely, it is isomorphic to $\mathbb{Z}^{\mathfrak{t}+p}$. One of its basis is given by the boundaries of tetrahedra of $\mathcal{T}$ and by the 2-chains $\gamma_1, \dots, \gamma_p$ associated with the triangulations of $\Gamma_1, \dots, \Gamma_p$ induced by $\mathcal{T}$.

A natural strategy to obtain a unique solution S is to add $\mathtt{t}+p$ equations, by setting equal to zero the unknowns corresponding to suitable faces $f_1, \dots, f_{\mathtt{t}+p}$ of $\mathcal{T}$. From the geometric point of view, this is equivalent to impose that the homological Seifert surface S of γ does not contain the faces $f_1, \dots, f_{\mathtt{t}+p}$. From the computational point of view, it is equivalent to eliminate some unknowns of the problem to obtain a solvable linear system with a unique solution. We will use graph techniques to describe which unknowns set equal zero.

Let us recall the definition of complete dual graph of $\mathcal{T}$ introduced in [1, Subsection 2.2]. Besides the set E'_∂ of dual edges of $\mathcal{T}_\partial$ (whose definition was recalled in Section 2.2.4 above), we need the sets V' of dual vertices of $\mathcal{T}$, V'_∂ of dual vertices of $\mathcal{T}_\partial$ and E' of dual edges of $\mathcal{T}$. They are defined in the following way.

- For every tetrahedron t of $\mathcal{T}$, the dual vertex $D(t)$ of $\mathcal{T}$ associated with t is defined as the barycenter $B(t)$ of t: $D(t) := B(t)$. We denote by V' the set of all dual vertices of $\mathcal{T}$.

  For every face f of $\mathcal{T}_\partial$, the dual vertex $D_\partial(f)$ of $\mathcal{T}_\partial$ associated with f is defined as the barycenter of f: $D_\partial(f) := B(f)$. We denote by V'_∂ the set of all dual vertices of $\mathcal{T}_\partial$.
- For every oriented face $f = [\mathbf{v}, \mathbf{w}, \mathbf{y}] \in \mathcal{F}$, the oriented dual edge $D(f)$ of $\mathcal{T}$ associated with f is a 1-chain of $\mathbb{R}^3$ defined as follows: if $K(f)$ denotes the set $\{t \in K \,\big|\, \{\mathbf{v}, \mathbf{w}, \mathbf{y}\} \subset t\}$ of tetrahedra of $\mathcal{T}$ incident on f, we set

$$D(f) := \sum_{t \in K(f)} \operatorname{sign}\big(\boldsymbol{\nu}(f) \cdot \boldsymbol{\tau}([B(f), B(t)])\big)\, [B(f), B(t)].$$

  $D(f)$ can be described as follows. If the (oriented) face f is internal, then f is the common face of two tetrahedra t_1 and t_2 of $\mathcal{T}$, and the support of $D(f)$ is the union of the segment joining $B(f)$ with $B(t_1)$ and of the segment joining $B(f)$ and $B(t_2)$, see Fig. 8 (on the left). If f is a boundary face, then f is face of just one tetrahedron t, and the support of $D(f)$ is the segment joining $B(f)$

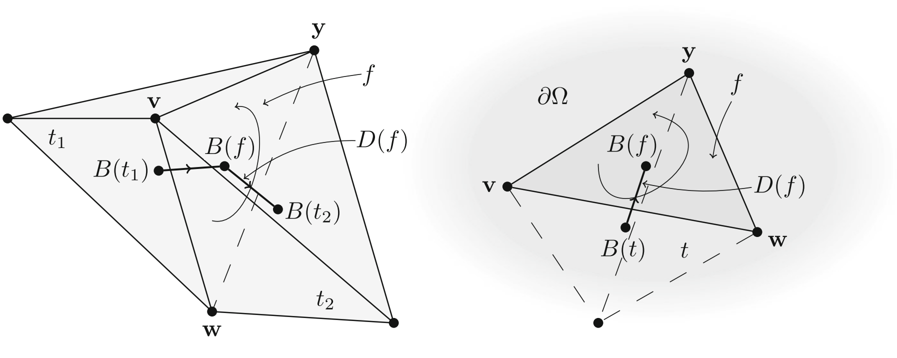


Fig. 8 The dual edge $D(f)$ in the case of an internal face (on the left) and in the case of a boundary face (on the right)

with $B(t)$, see Fig. 8 (on the right). In both cases, $D(f)$ is endowed with the orientation induced by f via the right hand rule.

A (non-oriented) dual edge of $\mathcal{T}$ is a 2-subset $\{v', w'\}$ of $\mathbb{R}^3$ such that $\{v', w'\} = |\partial_1 D(f)|$ for some $f \in \mathcal{F}$. We indicate by E' the set of all (non-oriented) dual edges of $\mathcal{T}$.

The *complete dual graph of* $\mathcal{T}$ is defined as the graph $\mathcal{A}' := (V' \cup V'_\partial, E' \cup E'_\partial)$.

Our idea is to consider a suitable spanning tree $\mathcal{B}'$ of $\mathcal{A}'$ and to set equal to zero the unknowns corresponding to faces of $\mathcal{T}$ whose dual edge belongs to $\mathcal{B}'$. The choice of $\mathcal{B}'$ is promising if and only if the number $N_{\mathcal{B}'}$ of faces of $\mathcal{T}$ whose dual edge belongs to $\mathcal{B}'$ (namely, the number of edges of $\mathcal{B}'$ not contained in $\partial\Omega$) is equal to $\mathfrak{t} + p$. Not all the spanning trees of $\mathcal{A}'$ satisfy this equality. It is not difficult to see that $N_{\mathcal{B}'} \geq \mathfrak{t} + p$ for all spanning tree $\mathcal{B}'$ of $\mathcal{A}'$. The equality holds true if and only if for each $i \in \{0, 1, \ldots, p\}$ the graph $\mathcal{B}'_i$ induced by $\mathcal{B}'$ on Γ_i is a spanning tree of $\mathcal{A}'_i$, the graph induced by $\mathcal{A}'$ on Γ_i. If the spanning tree $\mathcal{B}'$ of $\mathcal{A}'$ has the latter property, then we call it *Seifert dual spanning tree of* $\mathcal{T}$.

Let $\mathcal{B}' = (V' \cup V'_\partial, N')$ be a Seifert dual spanning tree of $\mathcal{T}$ and let $\mathcal{N}'$ be the corresponding set of oriented dual edges. In [1] we proved that the linear system

$$\begin{cases} \sum_{f \in \mathcal{F}(e)} \mathrm{o}_e(f) b_f = a_e & \text{if } e \in \mathcal{E} \\ b_f = 0 & \text{if } D(f) \in \mathcal{N}' \end{cases} \tag{33}$$

has a unique solution S and we give also an explicit formula for the solution. Roughly speaking the coefficient b_f of any face f of S with $D(f) \notin \mathcal{N}'$ is equal to the linking number between γ and the unique 1-cycle $\sigma_{\mathcal{B}'}(D(f))$ of $\mathcal{A}'$ with all the edges except $D(f)$ contained in $\mathcal{B}'$. These two 1-cycles could intersect on $\partial\Omega$. In this case, in order to define the correct linking number, it is necessary to perturb γ, moving it inside Ω. The definition of this perturbation is easier than the one used in the Section 2.2.4, because $\sigma_{\mathcal{B}'}(D(f))$ is a 1-cycle of $\mathcal{A}'$ and not of $\mathcal{T}$.

More precisely we proved that

$$b_f = \ell_{\mathcal{K}}\big(R_+(\gamma), \sigma_{\mathcal{B}'}(D(f))\big) \tag{34}$$

for every $f \in \mathcal{F}$, where the 1-cycle $R_+(\gamma)$ is defined in the following way. For every oriented edge $e = [\mathbf{v}, \mathbf{w}]$ in $\mathcal{E}_\partial$, choose a tetrahedron $t_e \in K$ incident on e (namely, $\{\mathbf{v}, \mathbf{w}\} \subset t_e$), denote by $\mathbf{d}_e$ the barycenter of the triangle of $\mathbb{R}^3$ of vertices $\mathbf{v}$, $\mathbf{w}$, $B(t_e)$, and define the 1-chain $r_+(e)$ of $\mathbb{R}^3$ by setting

$$r_+(e) := [\mathbf{v}, \mathbf{d}_e] + [\mathbf{d}_e, \mathbf{w}].$$

Given $\xi = \sum_{e \in \mathcal{E}} \alpha_e e$, we define:

$$R_+(\xi) := \sum_{e \in \mathcal{E} \setminus \mathcal{E}_\partial} \alpha_e e + \sum_{e \in \mathcal{E}_\partial} \alpha_e r_+(e).$$

However to solve (33), it is more convenient to adopt an elimination procedure and to use the explicit formula if the elimination procedure stops without having completed the solution. The resulting algorithm reads as follows.

Algorithm 2

1. $\mathcal{R} := \{f \in \mathcal{F} \mid D(f) \in \mathcal{N}'\}$, $\mathcal{D} := \mathcal{E}$.
2. *while* $\mathcal{R} \neq \mathcal{F}$
   (a) $n_{\mathcal{R}} := card(\mathcal{R})$
   (b) *for every* $e \in \mathcal{D}$
      (i) *if every oriented face of* $\mathcal{F}(e)$ *belong to* $\mathcal{R}$
         (A) $\mathcal{D} = \mathcal{D} \setminus \{e\}$
      (ii) *if exactly one oriented face* $f^* \in \mathcal{F}(e)$ *does not belong to* $\mathcal{R}$
         (A) *compute* b_f *via* (33)
         (B) $\mathcal{R} = \mathcal{R} \cup \{f\}$
         (C) $\mathcal{D} = \mathcal{D} \setminus \{e\}$
   (c) *if* $card(\mathcal{R}) = n_{\mathcal{R}}$
      (i) *pick* $f \notin \mathcal{R}$ *and compute* $b_f = \ell_{\mathcal{K}}(R_+(\gamma), \sigma_{\mathcal{B}'}(D(f)))$
      (ii) $\mathcal{R} = \mathcal{R} \cup \{f\}$

When using a bread first spanning tree $\mathcal{B}'$ of $\mathcal{A}'$, very often the elimination procedure computes the solution without using the explicit formula (34) (see [1]). In this case the computational cost is linear in the number of faces of the mesh $\mathcal{T}$.

If the 1-boundary γ is corner free (namely, no edge in the support of γ belongs to two distinct boundary faces contained in the same tetrahedron), then the homological Seifert surface S of γ constructed in this way is an internal homological Seifert surface; namely, all the faces in the support of S are internal faces of $\mathcal{T}$ (see [1]).

4 Numerical experiments

We have implemented the algorithm proposed in this paper in C++. All computations have been run on an Intel Core i7-3720QM @ 2.60GHz laptop with 16GB of RAM.

The more time consuming computation is the calculation of the linking number between two 1-cycles with disjoint supports.

The input is the tetrahedral mesh $\mathcal{T}$ of $\overline{\Omega}$ (that contains in particular the triangulation $\mathcal{T}_\partial$ of $\partial\Omega$). Then Algorithm 1 starts.

The first step is to construct, for each connected component of $\partial\Omega = \bigcup_{r=0}^{p} \Gamma_r$, a set of 1-cycles $\{\gamma_l^r\}_{l=1}^{2g_r}$ of Γ_r that are representatives of a basis of $H_1(\Gamma_r; \mathbb{Z})$. Then for each $r \in \{0, 1, \ldots, p\}$ we compute a set of g_r 1-cycles $\widehat{\sigma}_{r,s} = \sum_{l=1}^{2g_r} \hat{B}_{s,l}^r \gamma_l^r$ for $s \in \{1, \ldots, g_r\}$, whose homology classes in $\mathbb{R}^3 \setminus \Omega$ form a basis of the homology group $H_1(\mathbb{R}^3 \setminus D_r; \mathbb{Z})$, and another set of g_r 1-cycles $\sigma_{r,s} = \sum_{l=1}^{2g_r} B_{s,l}^r \gamma_l^r$ for $s \in \{1, \ldots, g_r\}$, whose homology classes in $\overline{\Omega}$ form a basis of the homology group $H_1(\overline{D}_r; \mathbb{Z})$. This step is done using the algorithm introduced in [15] and it requires the computation of $\sum_{r=0}^{p} (2g_r)^2$ linking numbers of the form $\ell_{\mathcal{K}}(\gamma_l^r, (\gamma_m^r)^+)$ with $1 \leq l, m \leq 2g_r$.

If $\partial\Omega$ is not connected the next step is to compute the 1-boundaries

$$\left\{\widehat{\sigma}'_{0,s}\right\}_{s=1}^{g_0} \cup \left\{\sigma'_{1,s}\right\}_{s=1}^{g_1} \cup \ldots \cup \left\{\sigma'_{p,s}\right\}_{s=1}^{g_p}$$

solving the linear systems (27) and (31) described in Section 2. For each connected component Γ_r of $\partial\Omega$, we have to solve g_r linear systems of dimension $g - g_r$. The main cost of this step is to compute the right-hand side vectors with coefficients $\beta^{r,s} \in \mathbb{Z}^{g-g_r}$ for $s \in \{1, \ldots, g_r\}$. So this step requires the computation of $\sum_{r=0}^{p} g_r(g - g_r) = g^2 - \sum_{r=0}^{p} g_r^2$ linking numbers.

The final step is to compute a homological Seifert surface for each 1-boundary via Algorithm 2. Usually this step does not require the computation of linking numbers because the explicit formula (34) is not used.

We will present 5 different test problems: a solid torus with a coaxial toric cavity, the complement of the (thickened) Borromean rings with respect to a box, the complement with respect to a solid two-torus of a (thickened) trefoil knot that embraces the holes of the solid two-torus, the complement with respect to a solid two-torus of the (thickened) Hopf link and a final example where the rank of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ is quite big (equal to 128) consisting in a solid 100-torus (namely, a solid torus with 100 holes) with eight cavities. The cavities are two solid 11-tori and six solid tori.

The first elementary example is a solid torus with a coaxial toric cavity. The boundary of the domain has two connected components and none of them is homologically trivial. The generators of $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$ are the two 1-cycles $\widehat{\sigma}_1$, σ_2 represented in Fig. 1a, c as continuous lines. Clearly none of them is the boundary of a 2-chain contained in $\overline{\Omega}$. Therefore the first step is to complete each one with a 1-cycle trivial in $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$ in order to obtain a 1-boundary in the same homology class.

In Fig. 9 we show the two representatives of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$: on the left the one corresponding to the 1-cycle $\widehat{\sigma}_1$, and on the right the one corresponding to the 1-cycle σ_2.

Table 1 contains the details on the number of edges and faces in the complex for four different meshes and the corresponding computational time divided into four contributions. *Mesh pre-processing* represents the time spent for loading the mesh from hard disk and computing all incidences between the elements of the complex. *Hiptmair–Ostrowski* is the time spent for computing the bases of $H_1(\overline{\Omega}; \mathbb{Z})$ and $H_1(\mathbb{R}^3 \setminus \Omega; \mathbb{Z})$ with the algorithm introduced in [15]. We remark that the support of

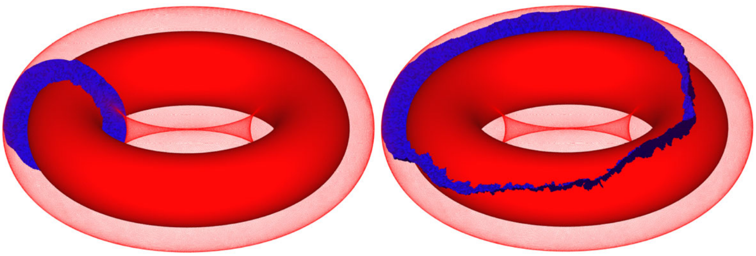


Fig. 9 The torus with a coaxial toric cavity. Representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ for the finest mesh are shown

Table 1 The torus with a coaxial toric cavity: the number of geometric elements of the triangulation and the computational time

Benchmark torus with toric cavity	Mesh 1	Mesh 2	Mesh 3	Mesh 4
Edges	51521	145963	1321902	10238231
Faces	76330	227314	2177158	17210016
Mesh pre-processing [s]	0.607	1.800	17.76	141.2
Hiptmair–Ostrowski [s]	0.084	0.216	0.863	3.909
Boundary retrieval [s]	0.012	0.034	0.122	0.513
Elimination algorithm [s]	0.061	0.193	2.720	24.52
Total Time (this paper) [s]	0.764	2.243	21.46	170.1
Total Time (GMSH [12]) [s]	1.544	5.538	86.28	> 2 hours
Speedup	2.0	2.5	4.0	–

each one of the g elements of the constructed bases is contained in a single connected component of the boundary $\partial\Omega$. *Boundary retrieval* is the time employed to find the 1-boundaries from the homology basis, which is the main contribution of this paper. Finally, *Elimination algorithm* represents the time needed for the construction of the homological Seifert surfaces using Algorithm 2.

In Table 1 (and in the next tables) we include also the time spent by a state-of-the-art implementation of the purely algebraic algorithm to compute the $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ generators contained in the popular mesh generator GMSH (see [12]). As one can see, the speed up of the technique proposed in this paper is about 2 in case of small

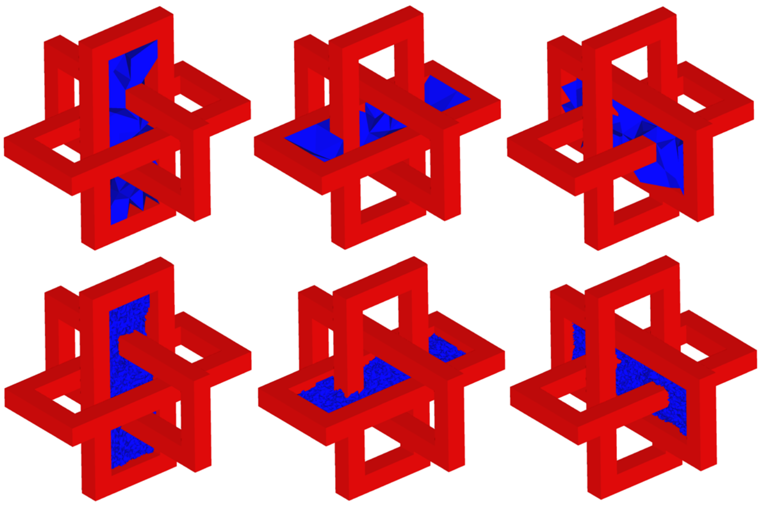


Fig. 10 The Borromean rings: on the top, three representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ for the coarsest mesh. On the bottom, three representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ for the finest mesh. The box is not shown for clarity

Table 2 The Borromean rings: the number of geometric elements of the triangulation and the computational time

Benchmark Borromean rings	Mesh 1	Mesh 2	Mesh 3	Mesh 4
Edges	29003	214807	1640732	11139998
Faces	46723	355752	2760283	18870406
Mesh pre-processing [s]	0.300	2.530	21.53	167.1
Hiptmair–Ostrowski [s]	0.020	0.080	0.410	2.165
Boundary retrieval [s]	0.010	0.010	0.030	0.183
Elimination algorithm [s]	0.030	0.320	3.460	30.98
Total Time (this paper) [s]	0.360	2.940	25.43	200.4
Total Time (GMSH [12]) [s]	1.076	11.19	121.1	$>$ 2 hours
Speedup	3.0	3.8	4.8	–

meshes but gets much bigger when considering real-life meshes with millions of tetrahedra.

The total number of linking numbers computed in this example is $g^2 + 3\sum_{r=0}^{p} g_r^2 = 2^2 + 3(1^2 + 1^2) = 10$

All observations related to this simple benchmark still hold true for other numerical experiments. In our second example the domain is the complement of the (thickened) Borromean rings with respect to a box. The number of connected components of the boundary is 4 and the first Betti number of the domain is equal to 3. The number of linking numbers to be computed is $3^2 + 3(1^2 + 1^2 + 1^2) = 18$. In Fig. 10 we show three representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ for two different meshes. Notice how the regularity of the representatives improves when refining the mesh.

Table 2 shows the dimension of the four different meshes considered, the computational time and the speed up with respect to GMSH. As can be seen, for the coarsest mesh the speed up is 3 and it increases when considering bigger meshes.

In the next two examples the domain is the complement with respect to a solid two-torus of a (thickened) trefoil knot (Example 3) and of the (thickened) Hopf link (Example 4).

In Example 3 the trefoil knot embraces the two holes of the solid two-torus. The boundary of the domain has 2 connected components and its first Betti number is

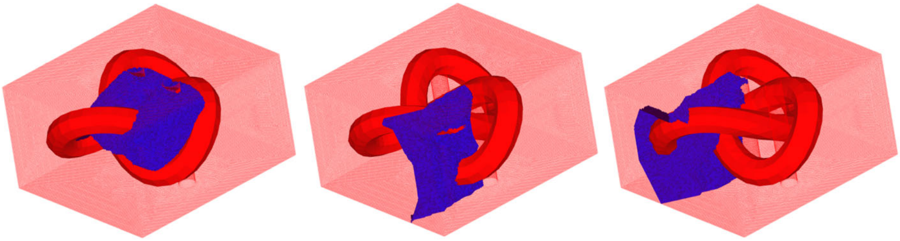


Fig. 11 The trefoil knot benchmark. Representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ for the finest mesh are shown. The exterior connected component of the boundary is a two-torus

Table 3 Benchmark trefoil knot: the number of geometric elements of the triangulation and the computational time

Benchmark trefoil knot	Mesh 1	Mesh 2	Mesh 3	Mesh 4
Edges	45018	176123	1260407	10264628
Faces	72305	283758	2086618	17305967
Pre-processing time [s]	0.554	2.103	16.72	153.6
Hiptmair–Ostrowski [s]	0.046	0.163	0.767	3.099
Boundary retrieval [s]	0.017	0.056	0.113	0.736
Elimination algorithm [s]	0.052	0.256	2.595	27.98
Total Time (this paper) [s]	0.669	2.578	20.20	185.4
Total Time (GMSH [12]) [s]	1.638	8.814	94287	> 2 hours
Speedup	2.5	3.4	4.7	–

3. The number of linking numbers to be computed is $3^2 + 3(2^2 + 1^2) = 24$. In Fig. 11 we show the three generators of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ for the trefoil benchmark and again, in Table 3, we give the dimension of the four different meshes considered, the computational time and the speed up with respect to GMSH with results similar to the previous examples.

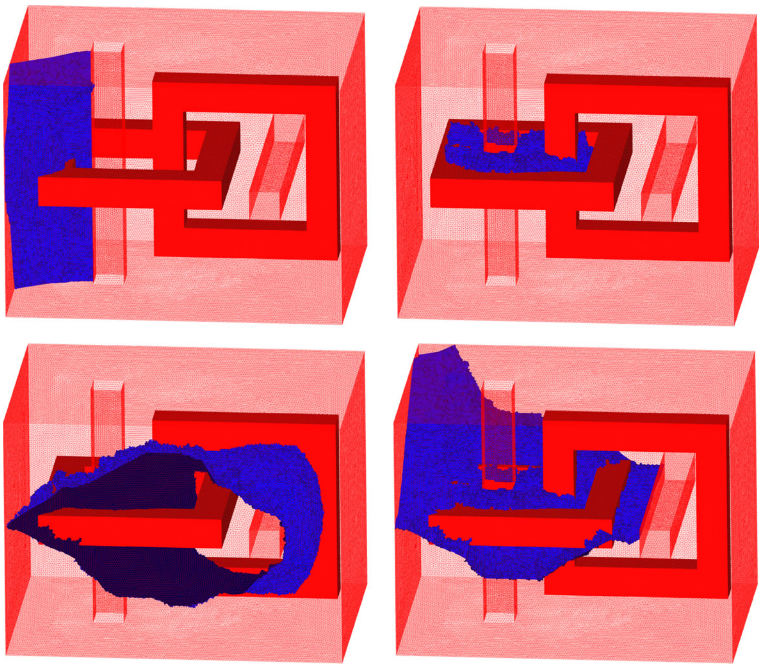
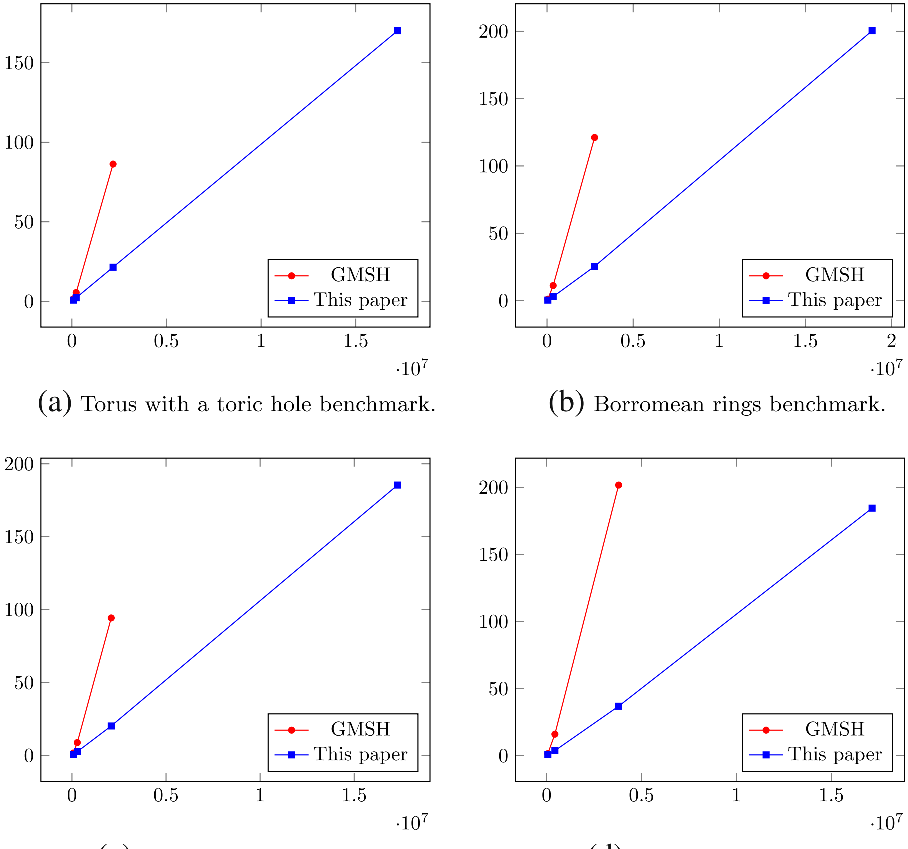


Fig. 12 The Hopf link benchmark. Representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ for the finest mesh are shown

Table 4 Benchmark Hopf link: the number of geometric elements of the triangulation and the computational time

Benchmark Hopf link	Mesh 1	Mesh 2	Mesh 3	Mesh 4
Edges	39692	263041	2255753	10152372
Faces	64007	434513	3794183	17148224
Mesh pre-processing [s]	0.857	3.183	30.98	153.1
Hiptmair–Ostrowski [s]	0.029	0.131	0.657	3.031
Boundary retrieval [s]	0.008	0.034	0.134	0.498
Elimination algorithm [s]	0.044	0.415	5.118	27.82
Total Time (this paper) [s]	0.938	3.763	36.89	184.5
Total Time (GMSH [12]) [s]	1.576	16.04	201.7	> 2 hours
Speedup	1.7	4.3	5.5	–



(a) Torus with a toric hole benchmark.

(b) Borromean rings benchmark.

(c) Trefoil knot benchmark.

(d) Hopf link benchmark.

Fig. 13 Time [s] vs mesh density [number of faces] for the GMSH code and the implementation of the algorithm proposed in this paper

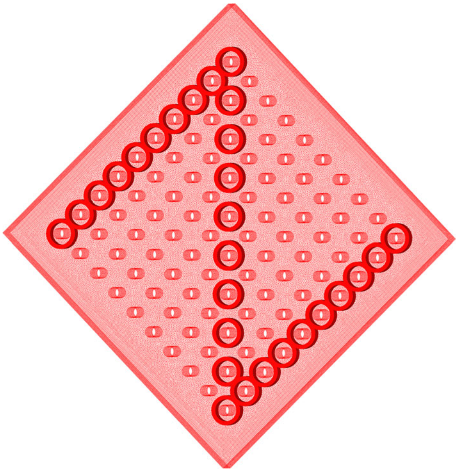


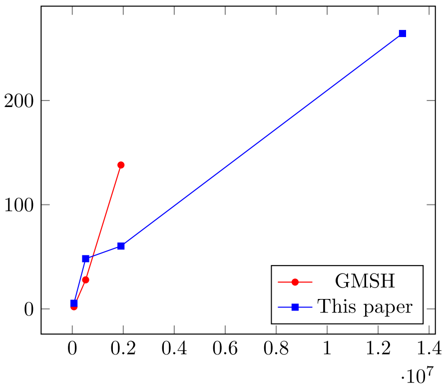
Fig. 14 The plate with holes benchmark

In Example 4 the the domain is the complement of the (thickened) Hopf link with respect to a solid two-torus. Each ring of the Hopf link turns around one of the holes of the solid two torus. In Fig. 12 we show the domain and four 2-chains that are representatives of a basis of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$. In this case the number of connected components of the boundary of the domain is 3, the first Betti number of the domain is 4, and the total number of linking numbers computed is $4^2 + 3(4 + 1 + 1) = 34$. In Table 4 we report the information about the meshes considered and the computational time. The speed up with respect to GMSH is similar to previous examples.

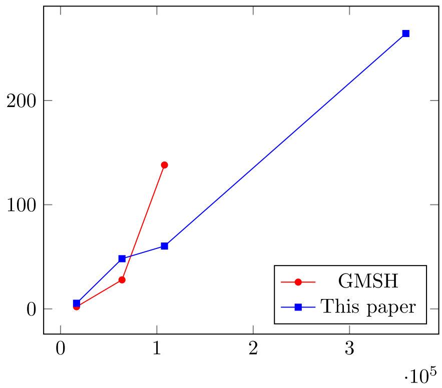
As expected, for these four benchmark problems the algorithm proposed in this paper has a linear complexity behavior as can be seen in Fig. 13 that illustrates also the speed up with respect to GMSH.

Table 5 Benchmark plate with holes: the number of geometric elements of the triangulation and the computational time

Benchmark plate with holes	Mesh 1	Mesh 2	Mesh 3	Mesh 4
Edges	45596	334526	1164992	7740566
Faces	65396	523825	1908897	12956479
Pre-processing time [s]	0.493	4.102	15.79	118.6
Hiptmair–Ostrowski [s]	3.251	23.14	17.60	50.66
Boundary retrival [s]	1.458	19.14	19.97	39.11
Elimination algorithm [s]	0.198	1.789	6.931	55.95
Total Time (this paper) [s]	5.400	48.17	60.30	264.3
Total Time (GMSH [12]) [s]	2.044	27.86	138.1	> 4 hours
Speedup	0.38	0.58	2.3	–



(a) Plate with holes benchmark.



(b) Plate with holes benchmark.

Fig. 15 Benchmark plate with holes: time [s] vs mesh density [on the left number of faces of $\mathcal{T}$, on the right number of faces of $\mathcal{T}_\partial$]

We finally consider an example where the rank of $H_2(\overline{\Omega}, \partial\Omega; \mathbb{Z})$ is much bigger (equal to 128) consisting in a solid 100-torus with eight cavities, see Fig. 14. The cavities are two solid 11-tori and six solid tori. So, the number of connected components of the boundary is 9 and the first Betti number of the domain is $100 + 22 + 6 = 128$.

In this case the number of linking numbers to compute is huge, equal to $128^2 + 3\,(100^2 + 2 \cdot 11^2 + 6) = 47128$. For this reason in the two smaller examples GMSH results faster than the approach proposed in this paper as one can be seen in Table 5. Yet, when the mesh cardinality gets into the range of real-life problems, we again get a sensible speed up. In particular, in the last mesh of more than 7 millions edges, GMSH wasn't able to produce a results after 4 hours of wall time, whereas our implementation took less than five minutes.

In Table 5 we can see that in this benchmark problem the time on small examples is dominated by the linking number computations so it is not linear (see Fig. 15).

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