

# CONSTRUCTION OF A FINITE ELEMENT BASIS OF THE FIRST DE RHAM COHOMOLOGY GROUP AND NUMERICAL SOLUTION OF 3D MAGNETOSTATIC PROBLEMS IN GENERAL TOPOLOGY

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**Abstract.** We devise an efficient algorithm for the finite element construction of discrete harmonic fields and the numerical solution of 3D magnetostatic problems. In particular, we construct a finite element basis of the first de Rham cohomology group of the computational domain. The proposed method works for general topological configurations and does not need the determination of “cutting” surfaces.

**1. Introduction.** The aim of this paper is two-fold. First, employing the edge finite elements introduced by Nédélec [48], we construct a discrete approximation of the space of harmonic fields

$$\mathbb{H}_\mu(\Omega) = \{ \mathbf{v} \in (L^2(\Omega))^3 \mid \operatorname{curl} \mathbf{v} = \mathbf{0}, \operatorname{div}(\mu \mathbf{v}) = 0, \mu \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \},$$

where  $\Omega$  is a bounded three-dimensional domain with a Lipschitz boundary,  $\mathbf{n}$  is the outward unit normal vector to  $\partial\Omega$ , and  $\mu$  is a symmetric matrix, uniformly positive definite in  $\Omega$  and with entries in  $L^\infty(\Omega)$  (in physical applications, the magnetic permeability).

In particular, we give a simple and efficient computational way for constructing the so-called *loop fields*, i.e., the irrotational vector fields  $\mathbf{T}_0$  that cannot be expressed in  $\Omega$  as the gradient of any single-valued scalar potential (therefore, there exists a loop in  $\Omega$  such that the line integral of  $\mathbf{T}_0$  on it is different from 0). These fields are of central importance for numerical electromagnetism in general topological domains (see, e.g., Kotiuga [39], Kettunen et al. [36]; see also Bossavit [13], Gross and Kotiuga [30]). To make precise one of their most important properties, let us first give a definition: if the only linear combination of a set of loop fields that equals a gradient is the trivial one, we say that those loop fields are linearly cohomologically independent. It is known that a maximal set of linearly cohomologically independent loop fields gives a basis of the first de Rham cohomology group of  $\Omega$ , namely, the quotient space between curl-free vector fields and gradients defined in  $\Omega$ .

Second, we furnish a finite element numerical solution to the magnetostatic problem, that reads as follows: given a divergence-free current density  $\mathbf{J}$ , with vanishing normal flux on all the connected components of  $\partial\Omega$ , find a magnetic field  $\mathbf{H}$  that satisfies

$$\begin{aligned} \operatorname{curl} \mathbf{H} &= \mathbf{J} && \text{in } \Omega \\ \operatorname{div}(\mu \mathbf{H}) &= 0 && \text{in } \Omega \\ \mu \mathbf{H} \cdot \mathbf{n} &= 0 && \text{on } \partial\Omega. \end{aligned} \tag{1.1}$$

In particular, the vector fields satisfying  $\operatorname{curl} \mathbf{H}_e = \mathbf{J}$  in  $\Omega$  are often called *source fields* in the electromagnetic literature, and are needed for formulating eddy current problems in terms of a magnetic scalar potential in the insulating region (see, e.g., Bossavit [13], Gross and Kotiuga [30], Alonso Rodríguez and Valli [3]).

Let us start by describing in more detail the first problem, namely, the approximation of  $\mathbb{H}_\mu(\Omega)$ . It is well-known that the dimension of this vector space is equal to the first Betti number of  $\Omega$ , that we will denote by  $g$  (see, e.g., Bossavit [13],

Hiptmair [34], Gross and Kotiuga [30]). The first Betti number is the rank of the first homology group of  $\Omega$ , that is, the number of a maximal set of independent non-bounding cycles in  $\Omega$ ; it is also the dimension of the first de Rham cohomology group of  $\Omega$ .

A theoretical way for determining a basis of  $\mathbb{H}_\mu(\Omega)$  is well-known (see, e.g., Foias and Temam [28], Bossavit [12], Amrouche et al. [5]), and is grounded on the fact that there exists  $g$  connected orientable Lipschitz surfaces  $\Sigma_n$ , with  $\partial\Sigma_n \subset \partial\Omega$ , each one “cutting” a non-bounding cycle in  $\bar{\Omega}$ . The construction procedure reads as follows. First, we can associate a loop field to any cutting surface  $\Sigma_n$ : having denoted by  $[\cdot]_{\Sigma_n}$  the jump across the surface  $\Sigma_n$ , and taking a function  $\varphi_n^*$  that is piecewise-smooth in  $\Omega \setminus \Sigma_n$  and satisfies  $[\varphi_n^*]_{\Sigma_n} = 1$ , we set  $\mathbf{T}_{0,n}^*$  the  $(L^2(\Omega))^3$ -extension of  $\text{grad } \varphi_n^*$ , where the (distributional) gradient has been computed in  $\Omega \setminus \Sigma_n$ . It is clear that  $\mathbf{T}_{0,n}^*$  has line integral equal to 1 on the non-bounding cycle that has been cut by the surface  $\Sigma_n$ ; therefore, it is a loop field. It is worth remarking that the function  $\varphi_n^*$  can be a discrete function (say, a finite element function); as a consequence,  $\mathbf{T}_{0,n}^*$  can be a finite element vector field. Second, we set  $\boldsymbol{\rho}_n = \mathbf{T}_{0,n}^* + \text{grad } \psi_n$ , where  $\psi_n \in H^1(\Omega)$  is the solution (uniquely determined up to an additive constant) to the classical Neumann problem

$$\int_{\Omega} \mu \text{grad } \psi_n \cdot \text{grad } \phi = - \int_{\Omega} \mu \mathbf{T}_{0,n}^* \cdot \text{grad } \phi \quad \forall \phi \in H^1(\Omega), \quad (1.2)$$

having introduced the Sobolev space  $H^1(\Omega) = \{\phi \in L^2(\Omega) \mid \text{grad } \phi \in (L^2(\Omega))^3\}$ . The vector functions  $\boldsymbol{\rho}_n$ ,  $n = 1, \dots, g$ , are a set of basis functions of  $\mathbb{H}_\mu(\Omega)$ . Moreover, if the loop field  $\mathbf{T}_{0,n}^*$  is a finite element, taking a finite element discretization of (1.2) we can construct a set of discrete fields  $\boldsymbol{\rho}_{n,h} = \mathbf{T}_{0,n}^* + \text{grad } \psi_{n,h}$ , finite element approximations of the basis functions  $\boldsymbol{\rho}_n$ .

It is now clear that the crucial point in the construction or in the approximation of the space of harmonic fields  $\mathbb{H}_\mu(\Omega)$  is the knowledge of a set of linearly cohomologically independent loop fields, and to this aim it is enough to determine the “cutting” surfaces  $\Sigma_n$ . There is an extensive literature concerning their construction (see Kotiuga [39], [40], [41], Harold and Simkin [31], Leonard et al. [43], Simkin et al. [58], Ren [53], Dular [26]). However, in general topological situations (for instance, in the case of domains that are the complement of “knotted” domains) and for real-sized finite element meshes this construction is not feasible, as it can be quite expensive from the computational point of view (see Bossavit [13], Dłotko et al. [25]).

Therefore, it is interesting to propose, as we do in this paper taking inspiration from Ghiloni [29], an alternative procedure for the determination of a set of linearly cohomologically independent discrete loop fields. Our method avoids the use of “cutting” surfaces and instead is based on the explicit knowledge of a maximal set of independent non-bounding cycles on  $\partial\Omega$ ; in other words, we only require the construction of a basis of the first homology group of  $\partial\Omega$ . We use a *spanning tree* (similar but different techniques, based on the so-called *belted tree*, have been proposed by several authors, but they do not work for all topological situations: see Ren and Razek [54], Kettunen et al. [37], Bossavit [13], Rapetti et al. [52], Henrotte and Hamayer [33], Dłotko et al. [25]). Another fundamental tool is the direct algorithm of Webb and Forghani [61]: however, since it is known to fail in certain topological situations (see Dłotko and Specogna [20]), we modify it in a suitable way, in order to be able to construct the finite element loop fields for every domain  $\Omega$ . A basic point here is the fact that we provide an explicit formula for expressing the discrete loop fields in terms of *linking numbers*.

Before concluding this survey, we want to recall that two other recent approaches have been proposed for computing cohomology generators, one based on algebraic techniques (Dłotko and Specogna [21]) and one more similar to our (Dłotko and Specogna [24]); the first one is proved to work for any topological situation, while the second one, though not completely general, is shown to be computationally more efficient than the former.

Going back to the second topic, namely, focusing on problem (1.1), it is readily seen that it is not well-posed, as uniqueness fails (just add a harmonic field to a solution  $\mathbf{H}$ ). The complete problem reads: given  $\mathbf{J} \in (L^2(\Omega))^3$  with  $\operatorname{div} \mathbf{J} = 0$  in  $\Omega$  and  $\int_{(\partial\Omega)_r} \mathbf{J} \cdot \mathbf{n} = 0$  for  $r = 0, 1, \dots, p$ , where  $(\partial\Omega)_r$  are the connected components of  $\partial\Omega$ , find the magnetic field  $\mathbf{H}$  such that

$$\begin{aligned} \operatorname{curl} \mathbf{H} &= \mathbf{J} && \text{in } \Omega \\ \operatorname{div}(\mu \mathbf{H}) &= 0 && \text{in } \Omega \\ \mu \mathbf{H} \cdot \mathbf{n} &= 0 && \text{on } \partial\Omega \\ \int_{\Omega} \mu \mathbf{H} \cdot \boldsymbol{\eta} &= 0 && \forall \boldsymbol{\eta} \in \mathbb{H}_{\mu}(\Omega). \end{aligned} \tag{1.3}$$

This problem has a solution (see, e.g., Saranen [56]), and uniqueness now is straightforward.

Let us also note that the complete curl-div problem

$$\begin{aligned} \operatorname{curl} \mathbf{u} &= \mathbf{J} && \text{in } \Omega \\ \operatorname{div}(\mu \mathbf{u}) &= f && \text{in } \Omega \\ \mu \mathbf{u} \cdot \mathbf{n} &= q && \text{on } \partial\Omega \\ \int_{\Omega} \mu \mathbf{u} \cdot \boldsymbol{\eta} &= 0 && \forall \boldsymbol{\eta} \in \mathbb{H}_{\mu}(\Omega), \end{aligned}$$

where  $f \in L^2(\Omega)$ ,  $q \in L^2(\Omega)$  and  $\int_{\Omega} f = \int_{\partial\Omega} q$ , can be solved by adding to the solution  $\mathbf{H}$  of problem (1.3) the gradient of the solution  $\omega$  (uniquely determined up to an additive constant) of the classical Neumann problem

$$\begin{aligned} \operatorname{div}(\mu \operatorname{grad} \omega) &= f && \text{in } \Omega \\ \mu \operatorname{grad} \omega \cdot \mathbf{n} &= q && \text{on } \partial\Omega. \end{aligned}$$

Therefore, when considering the complete curl-div system, the solution of problem (1.3) is anyhow the most important step.

Let us devise a suitable variational formulation of problem (1.3). Using the notation  $H^0(\operatorname{curl}; \Omega) = \{\mathbf{z} \in (L^2(\Omega))^3 \mid \operatorname{curl} \mathbf{z} = \mathbf{0}\}$ , it is well-known that any vector function  $\mathbf{z} \in H^0(\operatorname{curl}; \Omega)$  can be written as

$$\mathbf{z} = \operatorname{grad} \phi + \boldsymbol{\eta} \tag{1.4}$$

where  $\phi \in H^1(\Omega)$ ,  $\boldsymbol{\eta} \in \mathbb{H}_{\mu}(\Omega)$  and therefore  $\int_{\Omega} \mu \operatorname{grad} \phi \cdot \boldsymbol{\eta} = 0$  (see, e.g., Alonso Rodríguez and Valli [3]). It is readily verified that an equivalent formulation of problem (1.3) is: find  $\mathbf{H} \in (L^2(\Omega))^3$  such that

$$\begin{aligned} \operatorname{curl} \mathbf{H} &= \mathbf{J} && \text{in } \Omega \\ \int_{\Omega} \mu \mathbf{H} \cdot \mathbf{z} &= 0 && \forall \mathbf{z} \in H^0(\operatorname{curl}; \Omega). \end{aligned} \tag{1.5}$$

In fact, from (1.5) and integrating by parts we have

$$0 = \int_{\Omega} \mu \mathbf{H} \cdot \operatorname{grad} \phi = - \int_{\Omega} \operatorname{div}(\mu \mathbf{H}) \phi + \int_{\partial\Omega} \mu \mathbf{H} \cdot \mathbf{n} \phi.$$

Choosing  $\phi \in H^1(\Omega)$  with  $\phi|_{\partial\Omega} = 0$  it follows  $\operatorname{div}(\mu\mathbf{H}) = 0$  in  $\Omega$ ; hence we also have  $\int_{\partial\Omega} \mu\mathbf{H} \cdot \mathbf{n} \phi = 0$  for each  $\phi \in H^1(\Omega)$ , yielding  $\mu\mathbf{H} \cdot \mathbf{n} = 0$  on  $\partial\Omega$ .

Though formulation (1.5) looks quite simple, to our knowledge it has not been used as the starting point for devising an efficient numerical approximation algorithm for magnetostatics. This is what we propose in this paper.

With respect to this issue, let us start with a general overview. The finite element numerical approximation of the magnetostatic problem (1.3) has been considered since a long time, though very often in simple topological situation, as it is probably the “most frequently encountered field problem in electrical engineering design” (see Chari et al. [17]). We cannot present here an exhaustive description of the various methods employed; however, we want to mention some of the most important, in order to show the advantage of the finite element method based on (1.5).

A formulation in terms of a vector potential  $\mathbf{A}$  such that  $\operatorname{curl} \mathbf{A} = \mu\mathbf{H}$  is quite classical, and has been analyzed by Coulomb [18], Barton and Cendes [8], Preis et al. [51] (see also the new point of view involving mimetic finite differences presented in Brezzi and Buffa [14], Lipnikov et al. [44]): since the unknown is a vector field, the computational cost is higher than that needed to solve problem (1.5), that, as we will see in (2.1)–(2.3), is essentially a scalar problem. The same remark holds for the least squares approach of Chang and Gunzburger [16] and the even more expensive mixed methods of Kikuchi [38], Perugia [50], and Alotto and Perugia [4].

The co-volume method proposed by Nicolaides and Wu [49] is based on a system of two orthogonal grids like the classical Voronoi–Delaunay mesh pair, and for this reason this approach is not completely general, as some restrictions on the primal mesh and on the topological properties of the computational domain are needed.

Finally, the methods based on a magnetic scalar “potential” (the so-called reduced scalar potential) require the preliminary determination of a source field  $\mathbf{H}_e$ . Doing this by means of the Biot–Savart formula is not cheap from the computational point of view, and sometimes it induces cancellation errors (see Simkin and Trowbridge [59], Mayergoyz et al. [45], where it was proposed how to avoid this drawback by introducing an additional scalar potential; a complete analysis of this more complex formulation is in Bermudez et al. [10]). Let us also recall that a detailed presentation of the reasons behind these cancellation errors is given in Balac and Caloz [7].

We follow a different point of view. We start noting that a finite element approximation of (1.5) is standard provided that: (i) we know a discrete source field  $\mathbf{H}_{e,h}$  satisfying  $\operatorname{curl} \mathbf{H}_{e,h} = \mathbf{J}_h$ , where  $\mathbf{J}_h$  is a finite element approximation of the current density  $\mathbf{J}$ ; (ii) a suitable finite dimensional subspace of  $H^0(\operatorname{curl}; \Omega)$  is available.

With respect to the latter point (ii), we mimic the decomposition (1.4), and we consider the discrete functions  $\mathbf{z}_h = \operatorname{grad} \phi_h + \sum_{n=1}^g \xi_n \mathbf{T}_{0,n}$ , where  $\mathbf{T}_{0,n}$  are suitable finite element loop fields. Note that in this way we have lost the orthogonality relation  $\int_{\Omega} \mu \operatorname{grad} \phi \cdot \boldsymbol{\eta} = 0$ , that was true for the decomposition in (1.4), but this is not essential for our arguments. We prove that the error between the exact and the discrete solutions is bounded by the approximation error, uniformly with respect to the mesh size.

We are finally left with point (i), namely, the determination of the discrete source fields. This problem has been widely considered, mainly for simple topological domains (see, e.g., Webb and Forghani [61], Preis et al. [51], Dular et al. [27], Le Ménach et al. [42], Rapetti et al. [52], Dular [26], Badics and Cendes [6], Dłotko and Specogna [20]). We show that a discrete source field can be determined by adopting a similar procedure to that employed for the construction of the finite element

loop fields: again, the main point is the use of the Webb–Forghani algorithm, followed by the introduction of a dual graph for the edges whose degree of freedom has not been yet determined when the algorithm stops and by a simple algebraic direct solver (for a similar approach, see also Dłotko and Specogna [23]).

REMARK 1. *Let us note that we could also consider harmonic fields satisfying different boundary conditions, for instance  $\mu\mathbf{H} \cdot \mathbf{n} = 0$  on  $\Gamma_1$  and  $\mathbf{H} \times \mathbf{n} = \mathbf{0}$  on  $\Gamma_2$ , where  $\Gamma_1 \cup \Gamma_2 = \partial\Omega$  and  $\Gamma_1 \cap \Gamma_2 = \emptyset$ . Similarly, in the magnetostatic problem this set of boundary conditions could replace  $\mu\mathbf{H} \cdot \mathbf{n} = 0$  on  $\partial\Omega$ . The results we present here can be easily adapted to these situations.*

This paper is organized as follows. In Section 2 we introduce and analyze the finite element approximation of the magnetostatic problem (1.5). Section 3 is devoted to the description of some algebraic topology concepts and to the analysis of the fundamental discrete problem, that is the main tool for the construction of source fields and loop fields performed in Section 4. An explicit formula for describing the loop fields in terms of linking numbers is presented in Section 5. Section 6 contains the construction of the bases of the first homology groups of  $\bar{\Omega}$  and  $\mathbb{R}^3 \setminus \Omega$ , whose knowledge is needed for defining the fundamental discrete problem and for obtaining the explicit expression of the loop fields. Finally, in Section 7 we present some numerical results that illustrate the performances of the devised algorithms.

**2. Finite element approximation.** Let  $\Omega$  be a bounded Lipschitz polyhedral domain equipped with a tetrahedral triangulation  $\mathcal{T}_h = (V, E, F, T)$  of  $\bar{\Omega}$ .  $V$  is the set of vertices,  $E$  the set of edges,  $F$  the set of faces and  $T$  the set of tetrahedra in  $\mathcal{T}_h$ .

We consider the following spaces of finite elements:

- The space  $L_h$  of continuous piecewise linear finite elements. Its dimension is  $n_v$ , the number of vertices in  $\mathcal{T}_h$ .
- The space  $N_h$  of Nédélec edge elements of degree 1. Its dimension is  $n_e$ , the number of edges in  $\mathcal{T}_h$ .
- The space  $RT_h$  of Raviart–Thomas finite elements of degree 1. Its dimension is  $n_f$ , the number of faces in  $\mathcal{T}_h$ .

It is well-known that  $L_h \subset H^1(\Omega)$ ,  $N_h \subset H(\text{curl}; \Omega)$  and  $RT_h \subset H(\text{div}; \Omega)$ , where

$$\begin{aligned} H(\text{curl}; \Omega) &= \{\mathbf{v} \in (L^2(\Omega))^3 \mid \text{curl } \mathbf{v} \in (L^2(\Omega))^3\} \\ H(\text{div}; \Omega) &= \{\mathbf{v} \in (L^2(\Omega))^3 \mid \text{div } \mathbf{v} \in L^2(\Omega)\}. \end{aligned}$$

Moreover  $\text{grad } L_h \subset N_h$  and  $\text{curl } N_h \subset RT_h$  (see, e.g., Monk [46]).

Fix a total ordering  $v_1, \dots, v_{n_v}$  of the elements of  $V$ . This induces an orientation on the elements of  $E$  and  $F$ : if the end points of  $e_j$  are  $v_a$  and  $v_b$  for some  $a, b \in \{1, \dots, n_v\}$  with  $a < b$ , then the oriented edge  $e_j$  will be denoted by  $[v_a, v_b]$ , and therefore the unit tangent vector of  $e_j$  is given by  $\boldsymbol{\tau} = \frac{v_b - v_a}{|v_b - v_a|}$ ; on the other hand, if the face  $f$  has vertices  $v_a, v_b$  and  $v_c$  with  $a < b < c$ , the oriented face  $f$  will be denoted by  $[v_a, v_b, v_c]$  and its unit normal vector  $\boldsymbol{\nu}$  is obtained by the right hand rule.

Let us consider a basis of  $L_h$ ,  $\{\Phi_{h,1}, \dots, \Phi_{h,n_v}\}$ , such that

$$\Phi_{h,i}(v_j) = \delta_{i,j}$$

for  $1 \leq i, j \leq n_v$ , a basis of  $N_h$ ,  $\{\mathbf{w}_{h,1}, \dots, \mathbf{w}_{h,n_e}\}$ , such that

$$\int_{e_j} \mathbf{w}_{h,i} \cdot \boldsymbol{\tau} = \delta_{i,j}$$

for  $1 \leq i, j \leq n_e$ , and a basis of  $RT_h$ ,  $\{\mathbf{r}_{h,1}, \dots, \mathbf{r}_{h,n_f}\}$ , such that

$$\int_{f_j} \mathbf{r}_{h,i} \cdot \boldsymbol{\nu} = \delta_{i,j}$$

for  $1 \leq i, j \leq n_f$ . The finite element approximation of (1.5) reads as follows. Denoting as before the connected components of  $\partial\Omega$  by  $(\partial\Omega)_r$ ,  $r = 0, 1, \dots, p$ , and given  $\mathbf{J}_h \in RT_h$ , a suitable approximation of  $\mathbf{J}$ , with  $\operatorname{div} \mathbf{J}_h = 0$  and  $\int_{(\partial\Omega)_r} \mathbf{J}_h \cdot \mathbf{n} = 0$ , find  $\mathbf{H}_h \in N_h$  such that

$$\begin{aligned} \operatorname{curl} \mathbf{H}_h &= \mathbf{J}_h \\ \int_{\Omega} \mu \mathbf{H}_h \cdot \mathbf{z}_h &= 0 \quad \forall \mathbf{z}_h \in N_h \cap H^0(\operatorname{curl}; \Omega). \end{aligned} \quad (2.1)$$

Assuming that a function  $\mathbf{H}_{e,h} \in N_h$  such that  $\operatorname{curl} \mathbf{H}_{e,h} = \mathbf{J}_h$  is known, this problem can be easily rewritten as follows: find  $\mathbf{K}_h \in N_h \cap H^0(\operatorname{curl}; \Omega)$  such that

$$\int_{\Omega} \mu \mathbf{K}_h \cdot \mathbf{z}_h = - \int_{\Omega} \mu \mathbf{H}_{e,h} \cdot \mathbf{z}_h \quad \forall \mathbf{z}_h \in N_h \cap H^0(\operatorname{curl}; \Omega), \quad (2.2)$$

and define  $\mathbf{H}_h = \mathbf{K}_h + \mathbf{H}_{e,h}$ .

In the next section we present a general strategy for the computation of a suitable source field  $\mathbf{H}_{e,h}$  and a basis of  $N_h \cap H^0(\operatorname{curl}; \Omega)$ . The latter is based on the knowledge of a set of linearly cohomologically independent discrete loop fields: if they are denoted by  $\mathbf{T}_{0,j}$ ,  $j = 1, \dots, g$ , a basis of  $N_h \cap H^0(\operatorname{curl}; \Omega)$  is given by  $\{\operatorname{grad} \Phi_{h,1}, \dots, \operatorname{grad} \Phi_{h,n_v-1}\} \cup \{\mathbf{T}_{0,1}, \dots, \mathbf{T}_{0,g}\}$  (see Proposition 1). Therefore problem (2.2) can be rewritten as: find  $\beta_i \in \mathbb{R}$ ,  $i = 1, \dots, n_v - 1$ , and  $\eta_j \in \mathbb{R}$ ,  $j = 1, \dots, g$ , such that

$$\begin{aligned} \sum_{i=1}^{n_v-1} \beta_i \int_{\Omega} \mu \operatorname{grad} \Phi_{h,i} \cdot \operatorname{grad} \Phi_{h,l} + \sum_{j=1}^g \eta_j \int_{\Omega} \mu \mathbf{T}_{0,j} \cdot \operatorname{grad} \Phi_{h,l} \\ = - \int_{\Omega} \mu \mathbf{H}_{e,h} \cdot \operatorname{grad} \Phi_{h,l} \quad \forall l = 1, \dots, n_v - 1 \\ \sum_{i=1}^{n_v-1} \beta_i \int_{\Omega} \mu \operatorname{grad} \Phi_{h,i} \cdot \mathbf{T}_{0,n} + \sum_{j=1}^g \eta_j \int_{\Omega} \mu \mathbf{T}_{0,j} \cdot \mathbf{T}_{0,n} \\ = - \int_{\Omega} \mu \mathbf{H}_{e,h} \cdot \mathbf{T}_{0,n} \quad \forall n = 1, \dots, g; \end{aligned} \quad (2.3)$$

the solution of problem (2.1) is then determined by setting

$$\mathbf{H}_h = \sum_{i=1}^{n_v-1} \beta_i \operatorname{grad} \Phi_{h,i} + \sum_{j=1}^g \eta_j \mathbf{T}_{0,j} + \mathbf{H}_{e,h}. \quad (2.4)$$

The solution of problem (2.3) is quite standard and computationally cheap once the source field  $\mathbf{H}_{e,h}$  and the loop fields  $\mathbf{T}_{0,j}$  are available. Therefore in the following sections we will focus only on these two issues.

From the theoretical point of view, it is straightforward to furnish an error estimate. Let us denote by  $\Pi^{RT_h}$  and  $\Pi^{N_h}$  the interpolation operators defined for smooth functions and valued in  $RT_h$  and  $N_h$ , respectively.

**THEOREM 1.** *Assume that  $\mathbf{J}$  and the solution  $\mathbf{H}$  of problem (1.5) are smooth. Then the solution  $\mathbf{H}_h$  of problem (2.1) with  $\mathbf{J}_h = \Pi^{RT_h} \mathbf{J}$  satisfies the following error estimate*

$$\|\mathbf{H} - \mathbf{H}_h\|_0 + \|\operatorname{curl} \mathbf{H} - \operatorname{curl} \mathbf{H}_h\|_0 \leq C \|\mathbf{H} - \Pi^{N_h} \mathbf{H}\|_0 + \|\mathbf{J} - \Pi^{RT_h} \mathbf{J}\|_0. \quad (2.5)$$

*Proof.* We notice that

$$\int_{\Omega} \mu(\mathbf{H} - \mathbf{H}_h) \cdot \mathbf{z}_h = 0 \quad \forall \mathbf{z}_h \in N_h \cap H^0(\text{curl}; \Omega),$$

hence

$$\|\mathbf{H} - \mathbf{H}_h\|_0^2 \leq C_1 \int_{\Omega} \mu(\mathbf{H} - \mathbf{H}_h) \cdot (\mathbf{H} - \mathbf{H}_h) = C_1 \int_{\Omega} \mu(\mathbf{H} - \mathbf{H}_h) \cdot (\mathbf{H} - \mathbf{v}_h)$$

for each  $\mathbf{v}_h \in V_h(\mathbf{J}_h) := \{\mathbf{v}_h \in N_h \mid \text{curl } \mathbf{v}_h = \mathbf{J}_h\}$ . Thus we have the optimal error estimate

$$\|\mathbf{H} - \mathbf{H}_h\|_0 \leq C \inf_{\mathbf{v}_h \in V_h(\mathbf{J}_h)} \|\mathbf{H} - \mathbf{v}_h\|_0.$$

Since  $\mathbf{J}$  and  $\mathbf{H}$  are smooth, the interpolants  $\Pi^{RT_h} \mathbf{J}$  and  $\Pi^{N_h} \mathbf{H}$  are well defined; therefore from  $\mathbf{J}_h = \Pi^{RT_h} \mathbf{J}$  it clearly follows  $\Pi^{N_h} \mathbf{H} \in V_h(\mathbf{J}_h)$ , as  $\text{curl}(\Pi^{N_h} \mathbf{H}) = \Pi^{RT_h}(\text{curl } \mathbf{H})$ . In this case we conclude with (2.5), as  $\text{curl } \mathbf{H} = \mathbf{J}$  and  $\text{curl } \mathbf{H}_h = \mathbf{J}_h = \Pi^{RT_h} \mathbf{J}$ .  $\square$

We recall that the interpolants of  $\mathbf{J}$  and  $\mathbf{H}$  are well-defined if, for instance,  $\mathbf{J}$  and  $\mathbf{H}$  belong to  $(H^{1/2+\delta}(\Omega))^3$  with  $\delta > 0$ .

**3. The fundamental discrete problem.** In the recent years many works investigate the use of algebraic topology techniques in computational electromagnetism, exploiting the geometrical nature of Maxwell equations (see, e.g., Bossavit [13], Tarhasaari and Kettunen [60], Hiptmair [34], Gross and Kotiuga [30], Dłotko and Specogna [22]).

In the following we introduce some notions of homology theory and graph theory. We consider a mesh  $\mathcal{T}_h = (V, E, F, T)$  on  $\bar{\Omega}$ , having assigned the orientation to the edges and faces as explained before. The basic concept is that of chain: a 2-chain is a formal linear combination of oriented faces, a 1-chain a formal linear combination of oriented edges and a 0-chain a formal linear combination of vertices, in all cases taking the coefficients in  $\mathbb{Z}$ . We denote by  $C_k(\mathcal{T}_h, \mathbb{Z})$  the set of all the  $k$ -chains in  $\mathcal{T}_h$ ,  $k = 0, 1, 2$ .

Now we can define the boundary operator  $\partial_k : C_k(\mathcal{T}_h, \mathbb{Z}) \rightarrow C_{k-1}(\mathcal{T}_h, \mathbb{Z})$  for  $k = 1, 2$ . For the oriented face  $f = [v_{a_0}, v_{a_1}, v_{a_2}]$  we have

$$\partial_2 f := [v_{a_1}, v_{a_2}] - [v_{a_0}, v_{a_2}] + [v_{a_0}, v_{a_1}]$$

where  $[v_a, v_b]$  denotes the oriented edge from the vertex  $v_a$  to the vertex  $v_b$ . Analogously for the oriented edge  $e = [v_a, v_b]$  we have

$$\partial_1 e := v_b - v_a.$$

We extend the definition of the boundary operator to chains by linearity.

A 1-chain  $c$  of  $\mathcal{T}_h$  is a 1-cycle if  $\partial_1 c = 0$ , and is a 1-boundary if there exists a 2-chain  $C$  such that  $\partial_2 C = c$ . Notice that all 1-boundaries are 1-cycles but, in general, not all 1-cycles are 1-boundaries.

Let us denote by  $Z_1(\mathcal{T}_h, \mathbb{Z})$  the set of 1-cycles,  $Z_1(\mathcal{T}_h, \mathbb{Z}) := \ker(\partial_1)$ , and  $B_1(\mathcal{T}_h, \mathbb{Z})$  the set of 1-boundaries,  $B_1(\mathcal{T}_h, \mathbb{Z}) := \text{im}(\partial_2)$ . Two 1-cycles  $c$  and  $c'$  are called homologous in  $\mathcal{T}_h$  if  $c - c'$  is a 1-boundary in  $\mathcal{T}_h$ . If  $c$  is homologous to the zero 1-cycle (namely, it is a 1-boundary), then we say that  $c$  bounds in  $\mathcal{T}_h$ .

The first homology group of  $\mathcal{T}_h$  consists of all homology classes of 1-cycles of  $\mathcal{T}_h$ , that is, it is the quotient group

$$\mathcal{H}_1(\mathcal{T}_h, \mathbb{Z}) = Z_1(\mathcal{T}_h, \mathbb{Z})/B_1(\mathcal{T}_h, \mathbb{Z}).$$

It is well-known that, up to isomorphisms,  $\mathcal{H}_1(\mathcal{T}_h, \mathbb{Z})$  depends only on  $\bar{\Omega}$  and not on  $\mathcal{T}_h$ . For this reason, we can refer to  $\mathcal{H}_1(\mathcal{T}_h, \mathbb{Z})$  as the first homology group of  $\bar{\Omega}$ , and we can write  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$  instead of  $\mathcal{H}_1(\mathcal{T}_h, \mathbb{Z})$ . This group is an abelian group of rank  $g$ , the first Betti number of  $\bar{\Omega}$  (see Munkres [47, p. 24]). More precisely, it is a free abelian group, namely,  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$  is isomorphic to  $\mathbb{Z}^g$  (see Gross and Kotiuga [30, Sect. 3D], and Benedetti et al. [9, Lemma 5.4]). It is worth remarking that  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$  is also isomorphic to the (singular) homology group  $\mathcal{H}_1(\Omega, \mathbb{Z})$  of  $\Omega$  (see Munkres [47, Chap. 4] for the definition of the latter group).

The vertices and edges of the mesh  $\mathcal{T}_h = (V, E, F, T)$  form a graph. A spanning tree  $\mathcal{S}_h = (V, L)$  is a maximal subgraph of  $(V, E)$  (maximal because it visits all vertices) without loops (this means that it is a tree).

Given the tetrahedral triangulation  $\mathcal{T}_h = (V, E, F, T)$  of  $\bar{\Omega}$ , let  $\{\sigma_n\}_{n=1}^g$  be a set of 1-cycles that are representative of a basis of the homology group  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$  (their construction is performed in Section 6). Let us also consider a spanning tree  $\mathcal{S}_h = (V, L)$  of the graph  $(V, E)$ . We focus now on the *main problem* of our approach, namely: find  $\mathbf{Z}_h \in N_h$  such that

$$\begin{aligned} \operatorname{curl} \mathbf{Z}_h &= \mathbf{J}_h \\ \oint_{\sigma_n} \mathbf{Z}_h \cdot ds &= \kappa_n \quad \forall n = 1, \dots, g \\ \int_e \mathbf{Z}_h \cdot \boldsymbol{\tau} &= 0 \quad \forall e \in L, \end{aligned} \quad (3.1)$$

where  $\kappa_1, \dots, \kappa_g$  are real numbers.

The formulation of this problem uses a tree-cotree decomposition, similar to what has been previously done by many authors (see, for instance, Albanese and Rubinacci [1], Kettunen et al. [37], Bossavit [13], Henrotte and Hamayer [33], Henneron et al. [32]).

**THEOREM 2.** *Assume that  $\mathbf{J}_h \in RT_h$ ,  $\operatorname{div} \mathbf{J}_h = 0$  and  $\int_{(\partial\Omega)_r} \mathbf{J}_h \cdot \mathbf{n} = 0$  for any connected component  $(\partial\Omega)_r$  of  $\partial\Omega$ ,  $r = 0, 1, \dots, p$ . Then problem (3.1) has a solution and this solution is unique.*

*Proof.* If  $\mathbf{Z}_h$  and  $\tilde{\mathbf{Z}}_h$  are two different solutions of (3.1), then  $\mathbf{Z}_h - \tilde{\mathbf{Z}}_h \in N_h$ ,  $\operatorname{curl}(\mathbf{Z}_h - \tilde{\mathbf{Z}}_h) = \mathbf{0}$  and  $\oint_{\sigma_n} (\mathbf{Z}_h - \tilde{\mathbf{Z}}_h) \cdot ds = 0$  for all  $n = 1, \dots, g$ . From the de Rham theorem for Whitney forms (see Hiptmair [34]) there exists  $\psi_h \in L_h$  such that  $\mathbf{Z}_h - \tilde{\mathbf{Z}}_h = \operatorname{grad} \psi_h$ . Since the degrees of freedom of  $\operatorname{grad} \psi_h$  are equal to 0 for each edge of the spanning tree  $\mathcal{S}_h$ , we can conclude that  $\psi_h$  is constant: in fact if the edge  $e$  from  $v_a$  to  $v_b$  belongs to  $\mathcal{S}_h$  we have  $0 = \int_e \operatorname{grad} \psi_h \cdot ds = \psi_h(v_b) - \psi_h(v_a)$ , then  $\psi_h(v_a) = \psi_h(v_b)$ , and  $\psi_h$  is constant because  $\mathcal{S}_h$  is a spanning tree.

Concerning the existence of a solution, the assumptions on  $\mathbf{J}_h$  assure that there exists  $\mathbf{H}^* \in (L^2(\Omega))^3$  such that  $\operatorname{curl} \mathbf{H}^* = \mathbf{J}_h$ ,  $\operatorname{div} \mathbf{H}^* = 0$  and  $\mathbf{H}^* \cdot \mathbf{n} = 0$  in  $\partial\Omega$  (see, e.g., Saranen [56]). Since  $\Omega$  is a Lipschitz bounded polyhedral domain there exists  $s_\Omega \in (1/2, 1)$  such that  $H(\operatorname{curl}; \Omega) \cap H_0(\operatorname{div}; \Omega) \subset (H^{s_\Omega}(\Omega))^3$  (see, e.g., Alonso and Valli [2]). Hence  $\mathbf{H}^* \in (H^{s_\Omega}(\Omega))^3$  and  $\operatorname{curl} \mathbf{H}^* = \mathbf{J}_h \in (L^p(\Omega))^3$  for some  $p > 2$ , thus the Nédélec interpolant of  $\mathbf{H}^*$ ,  $\Pi^{N_h} \mathbf{H}^*$ , is well defined (see Amrouche et al. [5], Monk [46, Lemma 5.38]).

Now we want to prove the existence of  $\mathbf{W}_h \in N_h \cap H^0(\operatorname{curl}; \Omega)$  such that

$$\begin{aligned} \oint_{\sigma_n} \mathbf{W}_h \cdot ds &= \kappa_n - \oint_{\sigma_n} \Pi^{N_h} \mathbf{H}^* \cdot ds \quad \forall n = 1, \dots, g \\ \int_e \mathbf{W}_h \cdot \boldsymbol{\tau} &= - \int_e \Pi^{N_h} \mathbf{H}^* \cdot \boldsymbol{\tau} \quad \forall e \in L. \end{aligned}$$



This is a linear system of  $g + n_v - 1$  equations. It is well-known that the dimension of  $N_h \cap H^0(\text{curl}; \Omega)$  is  $g + n_v - 1$  (see, e.g., Hiptmair [34]), hence existence follows from uniqueness, that has been already proved. Finally, setting  $\mathbf{Z}_h = \mathbf{W}_h + \Pi^{N_h} \mathbf{H}^*$  we have found a solution to (3.1).  $\square$

Clearly, a field  $\mathbf{H}_{e,h}$  such that  $\text{curl } \mathbf{H}_{e,h} = \mathbf{J}_h$ , namely, a discrete source field, can be computed solving (3.1), having chosen the constants  $\kappa_n$  in any arbitrary way.

On the other hand, as shown in the following proposition, a set of linearly cohomologically independent finite element loop fields  $\mathbf{T}_{0,j}$ ,  $j = 1, \dots, g$ , can be determined by solving (3.1) with  $\mathbf{J}_h = \mathbf{0}$  and  $\kappa_n = m_{n,j}$ , for any choice of a non-singular matrix  $M$  with entries  $m_{n,j}$ . In particular, a basis of  $N_h \cap H^0(\text{curl}; \Omega)$  can be computed starting from  $\{\Phi_{h,1}, \dots, \Phi_{h,n_v}\}$ , a basis of  $L_h$ .

**PROPOSITION 1.** *Let  $\mathbf{T}_{0,j}$ ,  $j = 1, \dots, g$ , be the solutions to problem (3.1) with  $\mathbf{J}_h = \mathbf{0}$  and  $\kappa_n = m_{n,j}$ , where the matrix  $M = (m_{n,j})$  is non-singular. Then they are linearly cohomologically independent and the set*

$$\{\text{grad } \Phi_{h,1}, \dots, \text{grad } \Phi_{h,n_v-1}\} \cup \{\mathbf{T}_{0,1}, \dots, \mathbf{T}_{0,g}\}$$

*is a basis of  $N_h \cap H^0(\text{curl}; \Omega)$ .*

*Proof.* Since the dimension of  $N_h \cap H^0(\text{curl}; \Omega)$  is equal to  $g + n_v - 1$ , it is enough to prove linear independence. If we have  $\sum_{i=1}^{n_v-1} p_i \text{grad } \Phi_{h,i} + \sum_{j=1}^g q_j \mathbf{T}_{0,j} = \mathbf{0}$ , it follows for all  $n = 1, \dots, g$

$$0 = \sum_{i=1}^{n_v-1} p_i \oint_{\sigma_n} \text{grad } \Phi_{h,i} \cdot ds + \sum_{j=1}^g q_j \oint_{\sigma_n} \mathbf{T}_{0,j} \cdot ds = \sum_{j=1}^g q_j m_{n,j},$$

hence  $q_j = 0$  for each  $j = 1, \dots, g$ . We thus have  $\sum_{i=1}^{n_v-1} p_i \text{grad } \Phi_{h,i} = \mathbf{0}$ , hence  $\sum_{i=1}^{n_v-1} p_i \Phi_{h,i} = \text{const}$ ; the conclusion follows from the fact that  $\Phi_{h,i}(v_{n_v}) = 0$  for each  $i = 1, \dots, n_v - 1$ .

The proof that the loop fields  $\mathbf{T}_{0,j}$  are linearly cohomologically independent follows the same argument.  $\square$

**4. The construction of source fields and loop fields.** In this section we introduce an algorithm for solving problem (3.1). Since we are looking for a solution  $\mathbf{Z}_h$  of (3.1), we need to compute its degrees of freedom  $\int_{e_k} \mathbf{Z}_h \cdot \boldsymbol{\tau}$ , for  $k = 1, \dots, n_e$ .

The first step is very simple: we just assigne value 0 to the degrees of freedom associated to any edge  $e \in L$  (namely, belonging to the spanning tree), solving in this way (3.1)<sub>3</sub>.

After that, the standard technique for taking into account (3.1)<sub>2</sub>, namely, the homological equations, is based on the use of a *belted tree* instead of a spanning tree. Before continuing, we warn the reader that we do not follow this approach in this paper, since we prefer to follow a cheaper procedure that avoids the construction of a belted tree; however, for the sake of completeness, we present here the main features of this technique. The notion of belted tree has been proposed by Ren and Razek [54] (see also Kettunen et al. [37], Bossavit [13], Rapetti et al. [52], Dłotko et al. [25]), and it consists in a spanning tree with  $g$  additional edges  $e_1^*, \dots, e_g^*$ . Note that, since any graph obtained from a spanning tree adding an edge contains a 1-cycle, the belted tree is no longer a tree. The additional edges  $e_n^*$ ,  $n = 1, \dots, g$ , are chosen such that each one closes a non-bounding 1-cycle  $\sigma_n^*$ , and the set of these 1-cycles  $\{\sigma_n^*\}_{n=1}^g$  represents a basis of  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$ . Clearly, the degree of freedom corresponding to the edge  $e_n^*$  is equal to  $\kappa_n$ .

The final step is as follows. Since the degrees of freedom of a function  $\mathbf{v}_h \in RT_h$  are the fluxes  $\int_f \mathbf{v}_h \cdot \boldsymbol{\nu}$  for  $f \in F$ , relations (3.1)<sub>1</sub> are in fact a linear system with  $n_f$  (number of faces in  $\mathcal{T}_h$ ) equations and  $n_e$  (number of edges in  $\mathcal{T}_h$ ) unknowns. For each face  $f \in F$  we have

$$\int_f \mathbf{J}_h \cdot \boldsymbol{\nu} = \int_f \operatorname{curl} \mathbf{Z}_h \cdot \boldsymbol{\nu} = \oint_{\partial_2 f} \mathbf{Z}_h \cdot d\mathbf{s}. \quad (4.1)$$

so each row has exactly three non-zero entries.

Having assigned, as described in the first two steps, the degrees of freedom on the belted tree, other unknowns can be easily eliminated by the following algorithm:

ALGORITHM 1.

1.  $D := L \cup \{e_1^*, \dots, e_g^*\}$ ,  $N := F$
2. *while*  $D \neq E$ 
  - (a)  $n_D := \operatorname{card}(D)$
  - (b) *for every*  $f \in N$ 
    - i. *if every edge of the boundary of*  $f$  *belongs to*  $D$ , *then*
      - A.  $N = N \setminus \{f\}$
    - ii. *if exactly one edge*  $e$  *of the boundary of*  $f$  *does not belong to*  $D$ 
      - A. *compute*  $\int_e \mathbf{Z}_h \cdot \boldsymbol{\tau}$  *from* (4.1)
      - B.  $D = D \cup \{e\}$
  - (c) *if*  $\operatorname{card}(D) = n_D$  *then* *STOP*.

This algorithm has been proposed in a simpler form by Webb and Forghani [61], setting as initial step  $D = L$ . It is quite natural: at any step,  $D$  is the set of edges whose degree of freedom is known. If there are faces with two edges in this set, one computes from (4.1) the degree of freedom corresponding to the third edge of such a face.

Two questions are in order: does the algorithm start? Does the algorithm terminate with  $D = E$ ?

If the spanning tree  $\mathcal{S}_h$  is constructed in a suitable way, for instance a breadth-first spanning tree, there exist faces in  $F$  with exactly two sides in  $L$ , the set of edges of  $\mathcal{S}_h$ : therefore, in these cases the algorithm does start.

A careful analysis of the termination properties of this algorithm can be found in Dłotko and Specogna [20], where it is referred to as GSTT (generalized spanning tree technique). The authors also analyze its properties when the starting set  $D$  coincides with  $L$ , calling it STT (spanning tree technique). Clearly, if the domain  $\Omega$  has a simple topological shape (namely,  $g = 0$ ) the two algorithms coincide.

In [20] it is shown that the termination properties of GSTT and STT are strongly dependent on the choice of the spanning tree; for instance, with a depth-first spanning tree these algorithms can fail even if the domain  $\Omega$  has a simple topological shape, and no choice of the spanning tree is known that allows the termination of the algorithms if the domain  $\Omega$  is the complement of a trefoil knot.

Therefore, in a general topological situation it is not possible to say that these algorithms are able to determine all the degrees of freedom, and it is necessary to provide a strategy for the computation of the remaining unknowns.

To this aim, in the case of a domain of simple topological shape Dłotko and Specogna [23] proposed ESTT (extended spanning tree technique), based on symbolic computations that can be implemented in any object oriented programming language.

The algorithm that we propose is valid for any topological situation and reads as follows: first, we assign the value 0 on all the edges of the spanning tree; then, without introducing a belted tree, we apply Algorithm 1 with the initial set  $D = L$  (namely, STT). This procedure can stop without having determined all the degrees of freedom: in this case, we check if the homological equations  $(3.1)_2$  permit to compute one or more unknowns, and we restart STT. When the homological equations are no longer able to give additional information, we adopt a *dual graph* approach, that has some similarities with ESTT and indeed shows to be very efficient.

Let us describe the procedure: we are left with some faces where only one degree of freedom has been determined (say, 1-faces), and some faces where no degree of freedom has been determined (say, 0-faces). We construct a graph based on the fact that a 1-face naturally connects its two non-assigned edges: in other words, in this graph the nodes are the non-assigned edges and the arcs are the 1-faces.

In general, this graph is not connected; on each connected component  $\mathcal{G}_p$ ,  $p = 1, \dots, P$ , we choose a spanning tree and a root of the spanning tree. Each unknown associated to an edge of a fixed connected component can be expressed in an affine way with respect to the value of the corresponding root. In particular, the equations associated to the 0-faces are affine equations in terms of no more than three roots, and also the remaining homological equations can be expressed in terms of the unknowns corresponding to the roots.

We have thus reduced the problem to the solution of a small and sparse linear system with as many unknowns as the number of connected components of the dual graph (and as many equations as the number of 0-faces plus  $g_*$ ,  $0 \leq g_* \leq g$ ). This problem has a unique solution, hence it can be solved by using an algebraic direct method.

Let us summarize the algorithm we have proposed:

ALGORITHM 2.

1.  $D := L$ ,  $N := F$
2. *while*  $D \neq E$ 
  - (a)  $n_D := \text{card}(D)$
  - (b) *for every*  $f \in N$ 
    - i. *if every edge of the boundary of*  $f$  *belongs to*  $D$ , *then*
      - A.  $N = N \setminus \{f\}$
    - ii. *if exactly one edge*  $e$  *of the boundary of*  $f$  *does not belong to*  $D$ 
      - A. *compute*  $\int_e \mathbf{Z}_h \cdot \boldsymbol{\tau}$  *from* (4.1)
      - B.  $D = D \cup \{e\}$
  - (c) *for every cycle*  $\sigma_n$ 
    - i. *if*  $\sigma_n$  *has exactly one edge*  $e$  *that does not belong to*  $D$ 
      - A. *compute*  $\int_e \mathbf{Z}_h \cdot \boldsymbol{\tau}$  *from the homological equation* (3.1)<sub>2</sub>
      - B.  $D = D \cup \{e\}$
  - (d) *if*  $\text{card}(D) = n_D$  *then*
    - i. *construct the dual graph and compute*  $\int_e \mathbf{Z}_h \cdot \boldsymbol{\tau}$  *for all*  $e \notin D$  *solving the reduced linear system by a direct method*
    - ii.  $D = E$ .

Moreover, if the right hand side  $\mathbf{J}_h$  is vanishing we furnish in the next section an explicit formula for the solution to (3.1) in terms of linking numbers. The computation of a linking number can be done efficiently by means of a sum of simple double integrals (see Bertolazzi and Ghiloni [11]); however, for a fine mesh the number of edges can be quite large, hence this formula turns out to be too expensive if used for all the

edges in  $E \setminus L$ . The recipe we adopt is the following: in Algorithm 2 replace (d) by the computation of the value of one single unknown using this explicit formula (see Algorithm 3). In the numerical experiments presented in Section 7 we show that the use of the explicit formula is necessary very few times.

**5. An explicit formula for the loop fields.** The use of linking numbers is a crucial point of the procedure aiming at furnishing an explicit formula for the determination of the loop fields. We recall that the linking number is an integer that, given two closed and disjoint curves in the three-dimensional space, represents the number of times that each curve winds around the other (see, e.g., Rolfsen [55, pp. 132–136]). We use this concept in a slightly different case, that is natural in the homological framework (see Seifert and Threlfall [57, Sects. 70, 73, 77]). We consider a 1-cycle  $\gamma$  in  $\mathbb{R}^3$  of the form  $\gamma = \sum_{i=1}^K \alpha_i [v_{a_i}, v_{b_i}]$ , where  $\alpha_i \in \mathbb{Z}$ ,  $[v_{a_i}, v_{b_i}]$  is the oriented segment from  $v_{a_i}$  to  $v_{b_i}$ , and the boundary  $\partial_1 \gamma = \sum_{i=1}^K \alpha_i (v_{b_i} - v_{a_i})$  is null. The support of  $\gamma$  is the union of the segments joining  $v_{a_i}$  and  $v_{b_i}$  for which  $\alpha_i \neq 0$ . For a continuous vector field  $\mathbf{U}$  we set

$$\int_{\gamma} \mathbf{U} \cdot d\mathbf{s} = \sum_{i=1}^K \alpha_i \int_{[v_{a_i}, v_{b_i}]} \mathbf{U} \cdot \tau, \quad \int_{\gamma} \mathbf{U} \times d\mathbf{s} = \sum_{i=1}^K \alpha_i \int_{[v_{a_i}, v_{b_i}]} \mathbf{U} \times \tau,$$

where  $\tau$  is the unit tangent vector of  $[v_{a_i}, v_{b_i}]$ .

The linking number is a double line integral.

DEFINITION 1. Given  $\gamma = \sum_{i=1}^K \alpha_i [v_{a_i}, v_{b_i}]$  and  $\gamma' = \sum_{j=1}^M \beta_j [v_{c_j}, v_{d_j}]$ , two 1-cycles in  $\mathbb{R}^3$  with disjoint supports, we define their linking number by

$$\begin{aligned} lk(\gamma, \gamma') &:= \frac{1}{4\pi} \int_{\gamma} \int_{\gamma'} \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|^3} \cdot d\mathbf{s}(\mathbf{x}) \times d\mathbf{s}(\mathbf{y}) \\ &= \frac{1}{4\pi} \int_{\gamma} \left( \int_{\gamma'} \frac{\mathbf{y} - \mathbf{x}}{|\mathbf{y} - \mathbf{x}|^3} \times d\mathbf{s}(\mathbf{y}) \right) \cdot d\mathbf{s}(\mathbf{x}). \end{aligned}$$

Let us observe that  $lk(\gamma, \gamma') = \frac{1}{4\pi} \sum_{i=1}^K \sum_{j=1}^M \alpha_i \beta_j L_{ij}$ , where

$$L_{ij} = \int_{[v_{a_i}, v_{b_i}]} \int_{[v_{c_j}, v_{d_j}]} \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|^3} \cdot d\mathbf{s}(\mathbf{x}) \times d\mathbf{s}(\mathbf{y}).$$

Therefore, in order to compute the integer  $lk(\gamma, \gamma')$ , it suffices to have an efficient way for evaluating the double integrals  $L_{ij}$ . We recall again that this can be done via an exact explicit formula (see Bertolazzi and Ghiloni [11]).

We also need the following definitions. For each 1-cycle  $\sigma$  of  $\partial\Omega$ , we denote by  $\sigma^+$  the homology class of  $\sigma$  in  $\overline{\Omega}$ . Similarly, we indicate by  $\sigma^-$  the homology class of  $\sigma$  in  $\mathbb{R}^3 \setminus \Omega$ .

Now we describe how a basis of loop fields can be explicitly computed by choosing in (3.1) the constants  $\kappa_n$  equal to suitable linking numbers. Recall that  $\mathcal{S}_h = (V, L)$  is a spanning tree of the graph  $(V, E)$ , with  $\mathcal{T}_h = (V, E, F, T)$ . Given  $v_j \in V$ , let  $C_{v_j}$  be the unique 1-chain in  $\mathcal{S}_h$  from  $v_1$  to  $v_j$ . If  $e_k \in E$  is the edge with end points  $v_a$  and  $v_b$  with  $a < b$ , we denote by  $D_{e_k}$  the 1-cycle of  $\mathcal{T}_h$  given by  $D_{e_k} := C_{v_a} + e_k - C_{v_b}$  (note that, if  $e_k \in L$ ,  $C_{v_b} = C_{v_a} + e_k$ , hence  $D_{e_k} = 0$ ).

THEOREM 3. Given a 1-cycle  $\hat{\gamma}$  of  $\mathbb{R}^3 \setminus \overline{\Omega}$ , let us consider the function  $q : E \rightarrow \mathbb{R}$  given by

$$q(e_k) := \begin{cases} 0 & \text{if } e_k \in L \\ lk(D_{e_k}, \hat{\gamma}) & \text{if } e_k \notin L, \end{cases} \quad (5.1)$$

namely,  $q(e_k) = lk(D_{e_k}, \hat{\gamma})$ . Let us denote by  $\boldsymbol{\eta}_{h, \hat{\gamma}} \in N_h$  the function defined as  $\boldsymbol{\eta}_{h, \hat{\gamma}} = \sum_{k=1}^{n_e} q(e_k) \mathbf{w}_{h,k}$ , where  $\mathbf{w}_{h,k}$  are the basis function of  $N_h$ . The following assertions hold:

- i)  $\oint_{\gamma} \boldsymbol{\eta}_{h, \hat{\gamma}} \cdot d\mathbf{s} = lk(\gamma, \hat{\gamma})$  for each 1-cycle  $\gamma$  of  $\mathcal{T}_h$ .
- ii)  $\text{curl } \boldsymbol{\eta}_{h, \hat{\gamma}} = \mathbf{0}$ .

*Proof.* Let  $\gamma$  be a 1-cycle of  $\mathcal{T}_h$  and let  $\alpha_r \in \mathbb{Z}$ ,  $r = 1, \dots, n_e$ , such that  $\gamma = \sum_{r=1}^{n_e} \alpha_r e_r$ , where  $e_r \in E$  is the oriented edge  $[v_{r,1}, v_{r,2}]$ . Hence we have

$$\oint_{\gamma} \boldsymbol{\eta}_{h, \hat{\gamma}} \cdot d\mathbf{s} = \sum_{r=1}^{n_e} \alpha_r \int_{e_r} \left( \sum_{k=1}^{n_e} q(e_k) \mathbf{w}_{h,k} \right) \cdot \boldsymbol{\tau} = \sum_{r=1}^{n_e} \alpha_r \left( \sum_{k=1}^{n_e} q(e_k) \int_{e_r} \mathbf{w}_{h,k} \cdot \boldsymbol{\tau} \right).$$

Since  $\int_{e_r} \mathbf{w}_{h,k} \cdot \boldsymbol{\tau} = \delta_{k,r}$  one has

$$\oint_{\gamma} \boldsymbol{\eta}_{h, \hat{\gamma}} \cdot d\mathbf{s} = \sum_{r=1}^{n_e} \alpha_r q(e_r) = \sum_{r=1}^{n_e} \alpha_r lk(D_{e_r}, \hat{\gamma}).$$

Notice that

$$\begin{aligned} \sum_{r=1}^{n_e} \alpha_r D_{e_r} &= \sum_{r=1}^{n_e} \alpha_r (C_{v_{r,1}} + e_r - C_{v_{r,2}}) \\ &= \gamma - \sum_{r=1}^{n_e} \alpha_r (C_{v_{r,2}} - C_{v_{r,1}}) = \gamma. \end{aligned}$$

In fact, being  $\gamma$  a 1-cycle, we have that its boundary satisfies

$$0 = \partial_1 \gamma = \sum_{r=1}^{n_e} \alpha_r (v_{r,2} - v_{r,1});$$

since  $C_{v_{r,1}}$  and  $C_{v_{r,2}}$  depend only on  $v_{r,1}$  and  $v_{r,2}$ , respectively, we obtain

$$\sum_{r=1}^{n_e} \alpha_r (C_{v_{r,2}} - C_{v_{r,1}}) = 0$$

as well. In conclusion,

$$\oint_{\gamma} \boldsymbol{\eta}_{h, \hat{\gamma}} \cdot d\mathbf{s} = \sum_{r=1}^{n_e} \alpha_r lk(D_{e_r}, \hat{\gamma}) = lk(\gamma, \hat{\gamma}),$$

and we have proved i).

Concerning ii), for each  $f \in F$  we have

$$\int_f \text{curl } \boldsymbol{\eta}_{h, \hat{\gamma}} \cdot \mathbf{n} = \oint_{\partial_2 f} \boldsymbol{\eta}_{h, \hat{\gamma}} \cdot d\mathbf{s} = lk(\partial_2 f, \hat{\gamma}) = 0.$$

Since  $\text{curl } \boldsymbol{\eta}_{h, \hat{\gamma}}$  belongs to the space of Raviart–Thomas finite elements of degree 1, this means that all its degrees of freedom are vanishing, so it is equal to  $\mathbf{0}$ .  $\square$

Let us now assume that we know a set of 1-cycles  $\{\sigma_n\}_{n=1}^g \cup \{\hat{\sigma}_n\}_{n=1}^g$  of  $\partial\Omega$  such that: they are representatives of a basis of the homology group of  $\partial\Omega$ ;  $\{\sigma_n\}_{n=1}^g$  (respectively,  $\{\hat{\sigma}_n\}_{n=1}^g$ ) represent a basis of the homology group  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$  (respectively,

of the homology group of  $\mathbb{R}^3 \setminus \Omega$ ). The construction of these two sets of 1-cycles is faced in the next section.

We recall that we have denoted by  $\sigma_j^+$  the homology class of  $\sigma_j$  in  $\overline{\Omega}$  and by  $\widehat{\sigma}_j^-$  the homology class of  $\widehat{\sigma}_j$  in  $\mathbb{R}^3 \setminus \Omega$ . Here below we also introduce the 1-cycle  $R^+\sigma_j$ , a representative of  $\sigma_j^+$  whose support is completely contained in  $\Omega$ , and the 1-cycle  $R^-\widehat{\sigma}_j$ , a representative of  $\widehat{\sigma}_j^-$  whose support is completely contained in  $\mathbb{R}^3 \setminus \overline{\Omega}$ .  $R^+\sigma_j$  can be obtained by slightly “retracting”  $\sigma_j$  inside  $\Omega$ , and similarly  $R^-\widehat{\sigma}_j$  by slightly “retracting”  $\widehat{\sigma}_j$  inside  $\mathbb{R}^3 \setminus \overline{\Omega}$ .

PROPOSITION 2. *The vector fields*

$$\mathbf{T}_{0,j} := \boldsymbol{\eta}_{h,R^-\widehat{\sigma}_j}, \quad j = 1, \dots, g,$$

are a set of linearly cohomologically independent set of finite element loop fields, hence they represent a finite element basis of the first de Rham cohomology group of  $\Omega$ .

*Proof.* The vector fields  $\mathbf{T}_{0,j}$  are the solutions of

$$\begin{aligned} \operatorname{curl} \mathbf{T}_{0,j} &= \mathbf{0} \\ \oint_{\sigma_n} \mathbf{T}_{0,j} \cdot ds &= lk(\sigma_n, R^-\widehat{\sigma}_j) \quad \forall n = 1, \dots, g \\ \int_e \mathbf{T}_{0,j} \cdot \boldsymbol{\tau} &= 0 \quad \forall e \in L; \end{aligned} \quad (5.2)$$

since the matrix  $M$  with entries  $m_{i,j} = lk(\sigma_n, R^-\widehat{\sigma}_j)$  is non-singular (see Munkres [47, Sect. 71] and Seifert and Threlfall [57, point 47, p. 337]), they are linearly cohomologically independent (see Proposition 1).  $\square$

REMARK 2. *The vector fields  $\mathbf{T}_{0,j} = \boldsymbol{\eta}_{h,R^-\widehat{\sigma}_j}$  just defined depend only on the homology class  $\widehat{\sigma}_j^-$  of  $\widehat{\sigma}_j$  in  $\mathbb{R}^3 \setminus \Omega$  and not on the chosen representative  $R^-\widehat{\sigma}_j$  with support in  $\mathbb{R}^3 \setminus \overline{\Omega}$ . In fact, if  $\widehat{\sigma}'_j$  is another representative of  $\widehat{\sigma}_j^-$  with support in  $\mathbb{R}^3 \setminus \overline{\Omega}$ , then  $R^-\widehat{\sigma}_j$  and  $\widehat{\sigma}'_j$  are homologous not only in  $\mathbb{R}^3 \setminus \Omega$  but also in  $\mathbb{R}^3 \setminus \overline{\Omega}$ . This is a consequence of the fact that  $\partial\Omega$  is a locally flat surface of  $\mathbb{R}^3$ , hence it has a bicollar in  $\mathbb{R}^3$ . Now, if  $\gamma$  is a 1-cycle in  $\mathbb{R}^3$  with support in  $\overline{\Omega}$ , then  $lk(\gamma, R^-\widehat{\sigma}_j) = lk(\gamma, \widehat{\sigma}'_j)$  (see Seifert and Threlfall [57, p. 289], Rolfsen [55, p. 133]).*

*We also observe that  $lk(\gamma, R^-\widehat{\sigma}_j) = lk(\gamma', \widehat{\sigma}_j)$ , if  $\gamma'$  is any 1-cycle of  $\mathbb{R}^3$  with support in  $\Omega$  and homologous to  $\gamma$  in  $\overline{\Omega}$ . In particular, if the support of  $\gamma$  is contained in  $\partial\Omega$ , then we can write  $lk(\gamma, R^-\widehat{\sigma}_j) = lk(R^+\gamma, \widehat{\sigma}_j)$ . This can be useful for implementation, as in this way one avoids to go outside the computational domain  $\overline{\Omega}$ .*

As we already noted, formula (5.1) can be too expensive if used for all the edges of the mesh  $\mathcal{T}_h$ . It has to be employed only for computing one degree of freedom each time that STT stops.

For the sake of clarity, we report the complete algorithm for the construction of a loop field  $\mathbf{T}_{0,j}$ :

ALGORITHM 3.

1.  $D := L, N := F$
2. while  $D \neq E$ 
  - (a)  $n_D := \operatorname{card}(D)$
  - (b) for every  $f \in N$ 
    - i. if every edge of the boundary of  $f$  belongs to  $D$ , then
      - A.  $N = N \setminus \{f\}$
    - ii. if exactly one edge  $e$  of the boundary of  $f$  does not belong to  $D$

- A. compute  $\int_e \mathbf{T}_{0,j} \cdot \boldsymbol{\tau}$  from  $\oint_{\partial_{2f}} \mathbf{T}_{0,j} \cdot d\mathbf{s} = 0$
  - B.  $D = D \cup \{e\}$
- (c) for every cycle  $\sigma_n$
- i. if  $\sigma_n$  has exactly one edge  $e$  that does not belong to  $D$ 
    - A. compute  $\int_e \mathbf{T}_{0,j} \cdot \boldsymbol{\tau}$  from the homological equation (5.2)<sub>2</sub>
    - B.  $D = D \cup \{e\}$
- (d) if  $\text{card}(D) = n_D$  then
- i. take  $e \notin D$  and compute  $\int_e \mathbf{T}_{0,j} \cdot \boldsymbol{\tau} = \text{lk}(D_e, R^- \hat{\sigma}_j)$
  - ii.  $D = D \cup \{e\}$ .

**6. The construction of the homology bases.** The aim of this section is to present an algorithm for computing simultaneously a basis of  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$  and a basis of  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ . We will mainly follow the construction proposed in Hiptmair and Ostrowski [35], with some modifications in order to assure that the obtained 1-cycles have integer coefficients and to cover the case in which the boundary  $\partial\Omega$  is not connected.

First, we recall two theoretical results. The Alexander duality theorem, applied to  $\bar{\Omega}$ , asserts that the abelian groups  $\mathcal{H}_1(\bar{\Omega}, \mathbb{Z})$  and  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$  are isomorphic. Indeed, they are both isomorphic to  $\mathbb{Z}^g$ . Given a 1-cycle  $\sigma$  of  $\partial\Omega$ , denote by  $[\sigma]$  its homology class in  $\partial\Omega$ . It is quite immediate to verify that the homology classes  $\sigma^+$  in  $\bar{\Omega}$  and  $\sigma^-$  in  $\mathbb{R}^3 \setminus \Omega$  depend only on  $[\sigma]$ , and not on its representative  $\sigma$ . In this way, we can define the following homomorphism  $\varphi : \mathcal{H}_1(\partial\Omega, \mathbb{Z}) \rightarrow \mathcal{H}_1(\bar{\Omega}, \mathbb{Z}) \oplus \mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$  by setting

$$\varphi([\sigma]) := (\sigma^+, \sigma^-). \quad (6.1)$$

The Mayer–Vietoris exact sequence associated with the splitting  $\mathbb{R}^3 = \bar{\Omega} \cup (\mathbb{R}^3 \setminus \Omega)$  ensures that  $\varphi$  is an isomorphism. It follows that  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$  is isomorphic to  $\mathbb{Z}^{2g}$ . We refer the reader to Cantarella et al. [15, Sect. 6] for a friendly description of the isomorphism  $\varphi$ .

We are now in a position to present the algorithm. Recall that  $\bar{\Omega}$  is equipped with a tetrahedral triangulation  $\mathcal{T}_h = (V, E, F, T)$ .

Let us assume for a while that  $\partial\Omega$  is connected. Let  $(V', E', F')$  be the triangulation of  $\partial\Omega$  induced by  $\mathcal{T}_h$ , let  $(V', L')$  be a spanning tree of the graph  $(V', E')$  and let  $v'$  be a vertex in  $V'$ . For every  $v \in V'$  and for every  $\epsilon = [v, w] \in E'$ , we denote by  $C'_v$  the unique 1-chain in  $(V', L')$  from  $v'$  to  $v$  and by  $D'_\epsilon$  the 1-cycle  $C'_v + \epsilon - C'_w$  of  $\partial\Omega$ . In [35, Sect. 3], Hiptmair and Ostrowski describe how to find  $2g$  edges  $\epsilon_1, \dots, \epsilon_{2g}$  in  $E' \setminus L'$  in such a way that the 1-cycles  $D'_{\epsilon_1}, \dots, D'_{\epsilon_{2g}}$  represent a basis of  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$ . For simplicity, define  $\gamma_l := D'_{\epsilon_l}$  for every  $l = 1, \dots, 2g$ .

Thanks to the connectedness of  $\partial\Omega$ , it is possible to prove that, given any 1-cycle  $\sigma$  of  $\partial\Omega$ , one has  $\sigma^- = 0$ , that is,  $\sigma$  bounds in  $\mathbb{R}^3 \setminus \Omega$ , if and only if  $\text{lk}(\sigma, R^+ \gamma_k) = 0$  for all  $k = 1, \dots, 2g$  (see Hiptmair and Ostrowski [35, Corol. 4.4]). Similarly, we have that  $\sigma^+ = 0$ , that is,  $\sigma$  bounds in  $\bar{\Omega}$ , if and only if  $\text{lk}(\sigma, R^- \gamma_k) = 0$  for all  $k = 1, \dots, 2g$ . Since  $\{\gamma_l\}_{l=1}^{2g}$  represents a basis of  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$ , there exist, and are unique,  $2g$  integers  $c_1, \dots, c_{2g}$  such that  $\sigma = \sum_{l=1}^{2g} c_l \gamma_l$  in  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$  (namely,  $\sigma$  and  $\sum_{l=1}^{2g} c_l \gamma_l$  are homologous in  $\partial\Omega$ ). Denote by  $G = (g_{l,k}) \in \mathbb{Z}^{2g \times 2g}$  the matrix with entries  $g_{l,k} := \text{lk}(\gamma_l, R^+ \gamma_k)$  and by  $\mathbf{c}$  the column vector  $(c_1, \dots, c_{2g})$ . Since  $\text{lk}(\sigma, R^+ \gamma_k) = \sum_{l=1}^{2g} c_l \text{lk}(\gamma_l, R^+ \gamma_k)$  for all  $k = 1, \dots, 2g$ , it follows that  $\sigma^- = 0$  if and only if

$$G^T \mathbf{c} = \mathbf{0},$$

namely,  $\mathbf{c} \in \text{Ker } G^T$ . Similarly,  $\sigma^+ = 0$  if and only if  $\sum_{l=1}^{2g} c_l \text{lk}(\gamma_l, R^- \gamma_k) = 0$  for all  $k = 1, \dots, 2g$ . Bearing in mind that the linking number is symmetric with respect to its components (see Rolfsen [55, p. 135]), we have that  $\text{lk}(\gamma_l, R^- \gamma_k) = \text{lk}(R^+ \gamma_l, \gamma_k) = \text{lk}(\gamma_k, R^+ \gamma_l)$  and hence  $\sigma^+ = 0$  if and only if

$$G\mathbf{c} = \mathbf{0},$$

namely,  $\mathbf{c} \in \text{Ker } G$ . The existence of the isomorphism  $\varphi$  ensures that  $\text{Ker } G^T$  and  $\text{Ker } G$  are isomorphic to  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z})$  and to  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ , respectively. In particular, the rank of  $G$  (and hence of  $G^T$ ) is equal to  $g$  (see also Hiptmair and Ostrowski [35, Theorem 4.5]).

Let us perform the reduction of  $G$  to Smith normal form (see Munkres [47, Sect. 11]). We obtain two matrices  $L, R \in \mathbb{Z}^{2g \times 2g}$  and non-zero integers  $s_1, \dots, s_g$  such that  $|\det L| = |\det R| = 1$ ,  $s_j$  divides  $s_{j+1}$  for all  $j = 1, \dots, g-1$  and

$$LGR = \left[ \begin{array}{cc|cc} s_1 & 0 & & \\ & \ddots & & 0 \\ 0 & & s_g & \\ \hline & 0 & & 0 \end{array} \right].$$

Evidently, the last  $g$  columns of  $R$  form a basis of  $G$ , while the last  $g$  columns of  $L^T$  form a basis of  $\text{Ker } G^T$ . Denote by  $A = (a_{n,l})$  and  $B = (b_{n,l})$  the matrices in  $\mathbb{Z}^{g \times 2g}$  formed by the last  $g$  rows of  $L$  and by the last  $g$  rows of  $R^T$ , respectively.

Define the 1-cycles  $\{\sigma_n\}_{n=1}^g \cup \{\widehat{\sigma}_n\}_{n=1}^g$  of  $\partial\Omega$  by setting

$$\sigma_n = \sum_{l=1}^{2g} a_{n,l} \gamma_l \quad \text{and} \quad \widehat{\sigma}_n = \sum_{l=1}^{2g} b_{n,l} \gamma_l$$

for all  $n = 1, \dots, g$ . By construction,  $\{\sigma_n\}_{n=1}^g$  are representatives of a basis of  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z})$  and  $\{\widehat{\sigma}_n\}_{n=1}^g$  of a basis of  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ . Moreover, we have that  $\sigma_n^- = 0$  and  $\widehat{\sigma}_n^+ = 0$  for all  $n = 1, \dots, g$ .

It is worth noting that, by using the isomorphism  $\varphi$  again, one sees immediately that the 1-cycles  $\{\sigma_n\}_{n=1}^g \cup \{\widehat{\sigma}_n\}_{n=1}^g$  represent a basis of  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$ . In this way, the determinant of the  $(2g \times 2g)$ -matrix  $Q = [A^T | B^T]$  is  $\pm 1$ . In fact,  $Q$  is the matrix associated with the change of basis of  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$ , from the one represented by  $\{\sigma_n\}_{n=1}^g \cup \{\widehat{\sigma}_n\}_{n=1}^g$  to the one represented by  $\{\gamma_l\}_{l=1}^{2g}$ .

Let us pass now to the case in which  $\partial\Omega$  is not connected, as frequently occurs in applications. As usual, we denote by  $\{(\partial\Omega)_r\}_{r=0}^p$  the connected components of  $\partial\Omega$ . Thanks to the Jordan separation theorem (see Munkres [47, Corol. 74.2]), for each  $r = 0, \dots, p$  the set  $\mathbb{R}^3 \setminus (\partial\Omega)_r$  has exactly two connected components, both having  $(\partial\Omega)_r$  as boundary. Denote by  $D_r$  the bounded connected component of  $\mathbb{R}^3 \setminus (\partial\Omega)_r$  and by  $g_r$  the first Betti number of  $D_r$ . Clearly, it holds:  $\overline{\Omega} = \overline{D_0} \setminus \bigcup_{r=1}^p D_r$  and  $\mathbb{R}^3 \setminus \Omega = (\mathbb{R}^3 \setminus D_0) \cup \bigcup_{r=1}^p \overline{D_r}$ . Moreover, being  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$  isomorphic to  $\bigoplus_{r=0}^p \mathcal{H}_1((\partial\Omega)_r, \mathbb{Z})$ , we have that  $\sum_{r=0}^p 2g_r = 2g$ , namely  $\sum_{r=0}^p g_r = g$ .

Let us apply to each  $(\partial\Omega)_r$  the algorithm described above. For each  $r = 0, \dots, p$  we obtain a set of 1-cycles  $\{\sigma_{r,s}\}_{s=1}^{g_r} \cup \{\widehat{\sigma}_{r,s}\}_{s=1}^{g_r}$  of  $(\partial\Omega)_r$  representing a basis of  $\mathcal{H}_1((\partial\Omega)_r, \mathbb{Z})$ . Furthermore, we have that

$$\sigma_{r,s} \text{ bounds in } \mathbb{R}^3 \setminus D_r \text{ and } \widehat{\sigma}_{r,s} \text{ bounds in } \overline{D_r} \text{ for all } s = 1, \dots, g_r. \quad (6.2)$$



The next proposition completes the algorithm, giving a basis of  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z})$  and a basis of  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ . To prove such a result, we essentially follow the arguments used in the proof of Theorem 3.2.2.1 of Dey and Guha [19].

PROPOSITION 3. *The following assertions hold:*

- (1) *The set of 1-cycles  $\{\sigma_{0,s}\}_{s=1}^{g_0} \cup \{\widehat{\sigma}_{1,s}\}_{s=1}^{g_1} \cup \dots \cup \{\widehat{\sigma}_{p,s}\}_{s=1}^{g_p}$  of  $\partial\Omega$  are representatives of a basis of  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z})$ .*
- (2) *The set of 1-cycles  $\{\widehat{\sigma}_{0,s}\}_{s=1}^{g_0} \cup \{\sigma_{1,s}\}_{s=1}^{g_1} \cup \dots \cup \{\sigma_{p,s}\}_{s=1}^{g_p}$  of  $\partial\Omega$  are representatives of a basis of  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ .*

*Proof.* Since  $\mathbb{R}^3 \setminus D_0, \overline{D_1}, \dots, \overline{D_p}$  are the connected components of  $\mathbb{R}^3 \setminus \Omega$ , we have that  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$  is isomorphic to  $\mathcal{H}_1(\mathbb{R}^3 \setminus D_0, \mathbb{Z}) \oplus \mathcal{H}_1(\overline{D_1}, \mathbb{Z}) \oplus \dots \oplus \mathcal{H}_1(\overline{D_p}, \mathbb{Z})$ . Point (2) follows immediately from this fact.

Let us prove (1). Define the  $g$ -uples  $S_1$  and  $S_2$  of 1-cycles of  $\partial\Omega$  by setting

$$S_1 := (\sigma_{0,1}, \dots, \sigma_{0,g_0}, \widehat{\sigma}_{1,1}, \dots, \widehat{\sigma}_{1,g_1}, \dots, \widehat{\sigma}_{p,1}, \dots, \widehat{\sigma}_{p,g_p}),$$

$$S_2 := (\widehat{\sigma}_{0,1}, \dots, \widehat{\sigma}_{0,g_0}, \sigma_{1,1}, \dots, \sigma_{1,g_1}, \dots, \sigma_{p,1}, \dots, \sigma_{p,g_p}).$$

The 2g-uple  $(S_1, S_2)$  represents a (ordered) basis  $B$  of  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$  and, by (2),  $S_2$  represents a basis  $B_2$  of  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ . Let  $C_1$  be a fixed basis of  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z})$  and let  $\Phi$  be the matrix associated with the isomorphism  $\varphi$  defined in (6.1), with respect to the bases  $B$  of  $\mathcal{H}_1(\partial\Omega, \mathbb{Z})$  and  $(C_1, B_2)$  of  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z}) \oplus \mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ . Clearly, it has the following form:

$$\Phi = \left[ \begin{array}{c|c} X & Y \\ \hline Z & I_g \end{array} \right],$$

where  $X, Y, Z \in \mathbb{Z}^{g \times g}$  and  $I_g$  is the  $(g \times g)$ -identity matrix. Thanks to (6.2), we infer at once that  $Z = 0$ . Since  $\varphi$  is an isomorphism, we know that  $|\det \Phi| = 1$ . It follows that  $|\det X| = 1$  as well, and hence  $S_1$  represents a basis of  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z})$ . This proves (1).  $\square$

REMARK 3. *In our procedure, we have always chosen the spanning tree  $(V, L)$  of the graph  $(V, E)$  by completing the spanning tree  $(V', L')$  of the graph  $(V', E')$  induced by  $\mathcal{T}_h$  on  $\partial\Omega$ . When computing the loop fields, this allows us to initialize Algorithm 3 with  $D = L \cup \{\epsilon_1, \dots, \epsilon_{2g}\}$ , where  $\epsilon_k$  are the 2g edges on  $\partial\Omega$  provided by the algorithm of Hiptmair and Ostrowski [35]. This is possible since*

$$\int_{\epsilon_k} \mathbf{T}_{0,j} \cdot \boldsymbol{\tau} = \oint_{\gamma_k} \mathbf{T}_{0,j} \cdot ds = lk(\gamma_k, R^- \widehat{\sigma}_j).$$

*Proceeding in this way the modified algorithm reads:*

ALGORITHM 4.

1.  $D := L \cup \{\epsilon_1, \dots, \epsilon_{2g}\}$ ,  $N := F$
2. while  $D \neq E$ 
  - (a)  $n_D := \text{card}(D)$
  - (b) for every  $f \in N$ 
    - i. if every edge of the boundary of  $f$  belongs to  $D$ , then
      - A.  $N = N \setminus \{f\}$
    - ii. if exactly one edge  $e$  of the boundary of  $f$  does not belong to  $D$ 
      - A. compute  $\int_e \mathbf{T}_{0,j} \cdot \boldsymbol{\tau}$  from  $\oint_{\partial_2 f} \mathbf{T}_{0,j} \cdot ds = 0$

- B.  $D = D \cup \{e\}$   
(c) if  $\text{card}(D) = n_D$  then  
i. take  $e \notin D$  and compute  $\int_e \mathbf{T}_{0,j} \cdot \boldsymbol{\tau} = \text{lk}(D_e, R^- \hat{\sigma}_j)$   
ii.  $D = D \cup \{e\}$ .

Moreover, we note that, if all the 1-cycles  $\{\gamma_k\}_{k=1}^{2g}$  belong to the same connected component of  $\partial\Omega$  (this means that  $\partial\Omega$  has just one connected component topologically non-trivial), these degrees of freedom can be easily computed in terms of the matrices  $B$  and  $G$ , as

$$\text{lk}(\gamma_k, R^- \hat{\sigma}_j) = \sum_{l=1}^{2g} b_{j,l} \text{lk}(\gamma_k, R^- \gamma_l) = \sum_{l=1}^{2g} b_{j,l} \text{lk}(R^+ \gamma_k, \gamma_l) = \sum_{l=1}^{2g} b_{j,l} g_{l,k}.$$

**7. Numerical results.** In this section we present some numerical experiments with the aim of illustrating the efficiency of the proposed algorithms.

We will consider six different test problems. The domain  $\Omega$  is the complement in a box of: a 2-torus (Test A); the Borromean rings (Test B); a link constituted by two skeletons of a cube (topologically, two 5-tori) (Test C); a trefoil knot (Test D); the knot listed as  $4_1$  in Rolfsen [55, pp. 391] (Test E); a link constructed with two knots  $4_1$  (Test F) (see Figure 7.1).

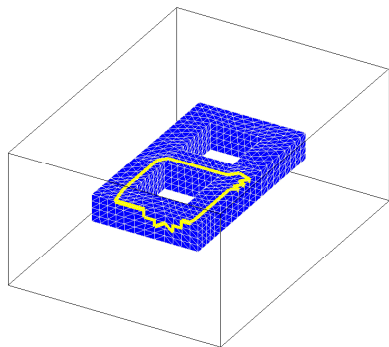
In all computations, except when explicitly stated, we use a spanning tree constructed via breadth-first search.

A preliminary step for computing loop and source fields is the construction of the bases of the homology groups  $\mathcal{H}_1(\overline{\Omega}, \mathbb{Z})$  and  $\mathcal{H}_1(\mathbb{R}^3 \setminus \Omega, \mathbb{Z})$ . Table 7.1 shows the CPU time required for the computation of all the homological cycles  $\sigma_n$  and  $\hat{\sigma}_n$  for three different meshes. Here we recall that a different mesh is only furnishing a different basis of the homology group (as well as of the cohomology group), but we are interested in the construction of a basis of  $N_h \cap H^0(\text{curl}; \Omega)$  and in the computation of the source fields, whose accuracy clearly depends on the mesh size.

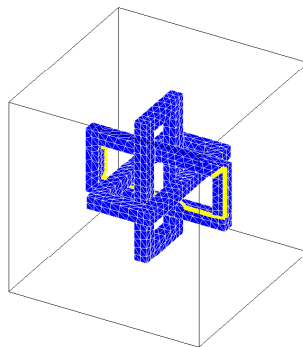
	Mesh 1		Mesh 2		Mesh 3	
	$n_e$	ms	$n_e$	ms	$n_e$	ms
Test A	42200	138	325904	868	2560416	6770
Test B	35380	93	273348	586	2147096	4397
Test C	25768	293	195256	1318	1517328	7434
Test D	15349	79	116170	294	902388	2016
Test E	34372	144	264548	749	2073688	4760
Test F	80504	310	624352	2671	4913792	12723

TABLE 7.1  
CPU time for computing all the homological 1-cycles.

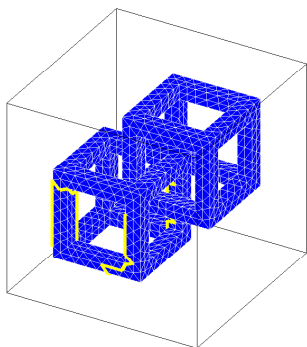
Table 7.2 shows how the number of edge unknowns decreases along the solution procedure:  $n_e$  is the number of the edges of the mesh,  $\#L$  the number of the edges of the spanning tree,  $n_e^{(1)}$  the number of unknowns left after the STT algorithm (namely, Algorithm 1 with  $D = L$ ) has stopped,  $n_e^{(2)}$  the number of unknowns not yet determined after having taken into account the homological constraints  $\oint_{\sigma_n} \mathbf{Z}_h \cdot d\mathbf{s} = \kappa_n$  for  $n = 1, \dots, g$ . Finally,  $\#CC$  is the number of the connected components of the dual graph.



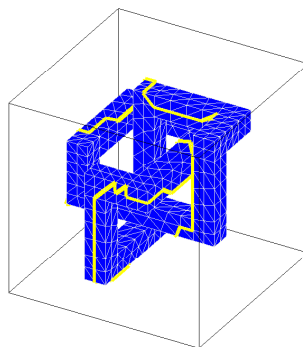
(a) Test A



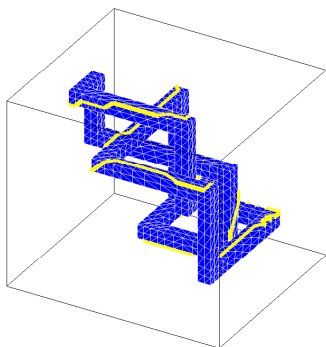
(b) Test B



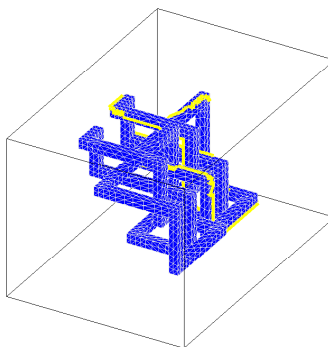
(c) Test C



(d) Test D



(e) Test E



(f) Test F

FIG. 7.1. The domain  $\Omega$  (the complement in the box of the blue set). One homological cycle  $\hat{\sigma}_j$  (yellow color) is also reported.

It can be interesting to see the structure of the linear system to solve when the overall algorithm does not terminate, namely, for cases D, E and F. In Table 7.3 we

	$n_e$	$n_e - \#L$	$n_e^{(1)}$	$n_e^{(2)}$	$\#CC$
Test A	2560416	2185729	58987	0	-
Test B	2147096	1832896	110245	0	-
Test C	1517328	1292168	124239	0	-
Test D	902388	768384	54273	34506	30
Test E	2073688	1769408	150694	98603	107
Test F	4913792	4196608	275832	212088	145

TABLE 7.2  
*Reduction of the number of unknowns.*

report the dimension of the linear system  $\text{curl } \mathbf{Z}_h = \mathbf{J}_h$  at the different steps of the reduction procedure. The first column refers to the original system, the second one to the system obtained when Algorithm 1 initialized with  $D = L$  stops, the third one to the system when the homological equations do not give additional information any longer, the last one to the system after the dual graph approach has been adopted. We denote by  $n_f$ ,  $n_f^{(1)}$ ,  $n_f^{(2)}$  the number of the faces in the different situations, and by  $\#0F$  the number of the faces for which no degree of freedom has been determined (the so-called 0-faces); the homological constraints are not counted.

	$n_f \times n_e$	$n_f^{(1)} \times n_e^{(1)}$	$n_f^{(2)} \times n_e^{(2)}$	$\#0F \times \#CC$
Test D	$1518464 \times 902388$	$134087 \times 54273$	$86186 \times 34506$	$1175 \times 30$
Test E	$3509696 \times 2073688$	$372839 \times 150694$	$246924 \times 98603$	$3372 \times 107$
Test F	$8337664 \times 4913792$	$686896 \times 275832$	$531280 \times 212088$	$7416 \times 145$

TABLE 7.3  
*Dimension of the linear system at each step.*

We have seen that the algorithm terminates in the first three cases, namely, when the domain is the complement of a non-knotted set. However, this behavior is strongly dependent on the choice of the spanning tree. Table 7.4 illustrates the influence of this choice, showing the number of remaining unknowns when the homological constraints do not give additional information, when adopting a breadth-first search or a depth-first search spanning tree.

	$n_e$	$n_e^{(2)}$ breadth-first	$n_e^{(2)}$ depth-first
Test A	42200	0	27912
Test B	35380	0	23595
Test C	25768	0	15707
Test D	15349	2092	9554
Test E	34372	6002	22776
Test F	80504	12916	53488

TABLE 7.4  
*Dependence of the reduction on the choice of the spanning tree.*

When the algorithm does not terminate (i.e.,  $n_e^{(2)} \neq 0$ ) we proceed as explained in Section 4. For the loop fields, we compute one edge unknown by means of the

explicit formula in terms of linking numbers, and restart the algorithm. This can be repeated as many times as we need: for Test D and Test E restarting once the algorithm is enough, while for Test F the procedure has been repeated four times. For the source fields, the reduced system is solved by a direct method (clearly, this approach can be used also for the determination of the loop fields). In Table 7.5 we report the CPU time for obtaining all the loop fields and one source field. We note that in the computations of the loop fields we have initialized the STT algorithm as indicated in Remark 3, namely, adopted Algorithm 4.

	$n_e$	loop fields	source field
Test A	2560416	(2) 9659	9937
Test B	2147096	(3) 9447	8822
Test C	1517328	(10) 28187	6322
Test D	902388	(1) 3759	3814
Test E	2073688	(1) 8705	8907
Test F	4913792	(2) 37338	22210

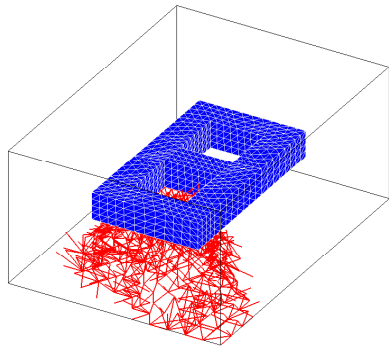
TABLE 7.5

CPU time (ms) for computing all the loop fields (their number is indicated in parenthesis) and one source field.

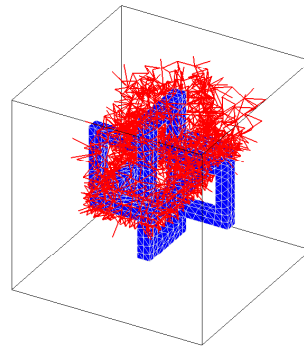
Finally, Figure 7.2 shows the support of a loop field for each test case.

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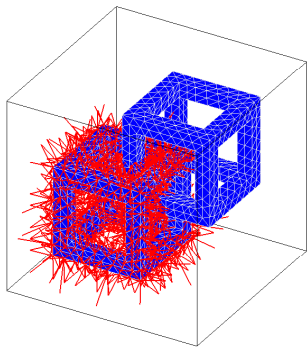
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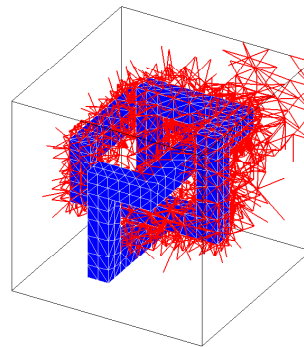
(a) Test A



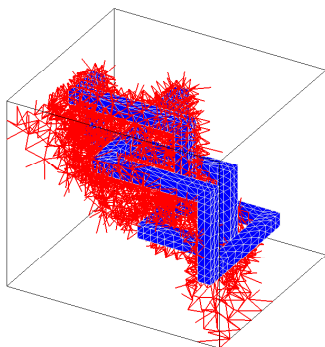
(b) Test B



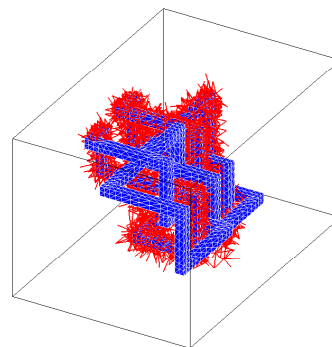
(c) Test C



(d) Test D



(e) Test E



(f) Test F

FIG. 7.2. Support of the loop field  $\mathbf{T}_{0,j}$ , associated to the yellow cycle  $\hat{\sigma}_j$  in Figure 7.1.

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