

Available online at www.sciencedirect.com



JOURNAL OF COMPUTATIONAL PHYSICS

Journal of Computational Physics 225 (2007) 1894–1918

www.elsevier.com/locate/jcp

Constitutive equations for discrete electromagnetic problems over polyhedral grids

Lorenzo Codecasa ^{a,*}, Francesco Trevisan ^b

^a Politecnico di Milano, Piazza Leonardo da Vinci 32, I-20133 Milan, Italy ^b Università di Udine, Via delle Scienze 208, I-33100 Udine, Italy

Received 11 August 2006; received in revised form 28 February 2007; accepted 28 February 2007 Available online 14 March 2007

Abstract

In this paper a novel approach is proposed for constructing discrete counterparts of constitutive equations over polyhedral grids which ensure both consistency and stability of the algebraic equations discretizing an electromagnetic field problem.

The idea is to construct discrete constitutive equations preserving the thermodynamic relations for constitutive equations. In this way, consistency and stability of the discrete equations are ensured. At the base, a purely geometric condition between the primal and the dual grids has to be satisfied for a given primal polyhedral grid, by properly choosing the dual grid.

Numerical experiments demonstrate that the proposed discrete constitutive equations lead to accurate approximations of the electromagnetic field.

© 2007 Elsevier Inc. All rights reserved.

Keywords: Discrete approach; Cell method; Constitutive equations

1. Introduction

Recently, there has been an increasing interest in the so called "Discrete Geometric Approach" for the solution of electromagnetic field problems at discrete level. Such an approach focuses directly on the geometric structure behind Maxwell equations and constitutive equations. In this respect, the works of Weiland [1,2], Tonti [3], and Bossavit [4,5] play a fundamental role. For instance, it is well known that Faraday or Ampères laws can be recast as algebraic relations between fluxes and circulations associated with surfaces and lines¹ endowed with an *inner* or *outer* orientation [6]. Then, instead of considering all the surfaces and lines, only a finite number of oriented faces and edges is considered. These faces and edges belong to a pair of dual grids according to their orientation. A grid is a collection of oriented geometric elements such as nodes, edges, faces,

^{*} Corresponding author. Tel.: +39 02 2399 3534; fax: +39 02 2399 3412.

E-mail addresses: codecasa@elet.polimi.it (L. Codecasa), trevisan@uniud.it (F. Trevisan).

¹ These lines form the boundary of those surfaces.

0021-9991/\$ - see front matter @ 2007 Elsevier Inc. All rights reserved. doi:10.1016/j.jcp.2007.02.032

and volumes; the primal grid has inner oriented geometric elements, while the outer oriented geometric elements form the dual grid. The two grids are one dual of the other; in other words, there is a one-to-one correspondence between nodes, edges, faces, and volumes of the primal grid and volumes, faces, edges and nodes of the dual grid respectively.

As a result of this discretization strategy, Maxwell's equations translate into an exact set of algebraic equations while the discrete counterparts of constitutive equations are approximate. For this reason most of the research work reported in literature, is concentrated on the construction of discrete constitutive equations.

Discrete constitutive equations are required to approximate the relation between fluxes/circulations on faces/edges of the dual grids. More specifically, the discrete constitutive equations constructed for a primal grid volume are required to exactly relate circulations/fluxes on edges/faces of the primal grid with fluxes/circulations on faces/edges of the dual grid at least when the fields involved and the material properties are uniform in such a primal grid volume. This ensures that the discrete equations are *consistent* with the continuous equations, in the sense that the discrete equations approximate the continuous equations with an error vanishing with the grain of the grid [5,7].

Besides, the matrices representing the discrete constitutive equations are required to be symmetric and positive definite. This ensures the *stability* of the discrete equations, in the sense that small perturbations in the data lead to small perturbations in the solution [8,7].

It is a matter of fact that the methods proposed in literature, in general do not ensure both consistency and stability of the discrete equations to hold simultaneously. For example in [9,10], consistency is ensured by construction, while stability is not ensured. On the contrary in [11–13], stability is ensured by construction, but consistency does not hold in general. Recently, in this last case, the authors have also shown that in some situations this approach can be extended in such a way that not only stability but also consistency is ensured [14,15].

Moreover, all these results are restricted to very particular grids, mainly composed of parallelepipeds or simplexes and mainly to scalar electric and magnetic constitutive equations. Thus no general approach has been reported in literature, at authors knowledge, for constructing discrete constitutive equations over primal polyhedral grids which ensure both consistency and stability of discrete equations. The novelty content of this paper can be summarized in the following main results.

Firstly, we relate the consistency and the stability properties to the *thermodynamic* relations for constitutive equations. Precisely, we show that the methods previously presented in literature [18] for constructing discrete constitutive equations, usually do not preserve all the thermodynamic relations for constitutive equations.

Secondly, by means of Properties 6 and 7, we show a way to construct discrete constitutive equations preserving all the thermodynamic relations for the constitutive equations. In this way we prove that consistency and stability of the discrete equations are ensured. This is possible only if the primal and the dual grids are related by a purely geometric constraint, given by Properties 3 and 4, that can be satisfied at least for primal grids of convex polyhedra, provided that the dual grid is properly chosen.

Numerical experiments show that the novel discrete constitutive equations lead to accurate approximations of the electromagnetic field.

The paper is organized as follows. In Section 2 the thermodynamic relations for constitutive equations are recalled. In Section 3 the methods reported in literature for constructing discrete constitutive equations are discussed in terms of the set of thermodynamic relations that they preserve. In Section 4 the construction of discrete constitutive equations is proposed which preserve thermodynamic relations of constitutive equations, as a way for ensuring consistency and stability of discrete equations. In Sections 5 and 6 the geometric relation between primal and dual grids is introduced and interpreted as the extension to dual grids of the relation between covariant and contravariant components. In Sections 7 and 8 the novel method for constructing discrete constitutive equations is derived. Numerical experiments are reported in Section 9. In Appendix A covariant and contravariant components are reinterpreted in terms of circulations and fluxes. In Appendix B some useful geometric relations for polygons are reported.

2. Thermodynamic relations for constitutive equations

Let us consider a linear, non-dispersive electromagnetic media.

Let *e* be the electric field, of covariant components e_i with i = 1, 2, 3. Both the electric displacement *d*, of contravariant components d^i with i = 1, 2, 3 and the electric energy density u_E can be written as a function of the electric field *e* in terms of a permittivity tensor ε , of contravariant components ε^{ij} with i, j = 1, 2, 3,

$$d = \varepsilon \cdot e, \tag{1}$$
$$u_{\rm E} = \frac{1}{2} e \cdot \varepsilon \cdot e \tag{2}$$

or equivalently, in tensorial notation,

$$d^{i} = \sum_{1}^{3} \varepsilon^{ij} e_{j},$$
$$u_{\rm E} = \frac{1}{2} \sum_{1}^{3} e_{i} \varepsilon^{ij} e_{j}.$$

From the principles of thermodynamics [16] for an electric system locally in equilibrium, the relations described in the following hold.

The electric energy density u_E is a function of the electric field *e*. The electric displacement *d* is defined from the electric energy density u_E as

$$d^{i} = \frac{\partial u_{\mathrm{E}}}{\partial e_{i}}, \quad i = 1, 2, 3.$$
(3)

The permittivity tensor is defined from the electric displacement d as

$$\varepsilon^{ij} = \frac{\partial d^i}{\partial e_j}, \quad i, j = 1, 2, 3.$$
(4)

In an equivalent way, by using (3), we can rewrite the permeability tensor ε as a function of the electric energy density $u_{\rm E}$ as

$$\varepsilon^{ij} = \frac{\partial^2 u_{\rm E}}{\partial e_j \partial e_i}, \quad i, j = 1, 2, 3 \tag{5}$$

from which, by exchanging the derivatives order, the following equations, known as *Maxwell's relations* [16], descend

$$\varepsilon^{ij} = \frac{\partial^2 u_{\rm E}}{\partial e_j \partial e_i} = \frac{\partial^2 u_{\rm E}}{\partial e_i \partial e_j} = \varepsilon^{ji}, \quad i, j = 1, 2, 3$$
(6)

or equivalently the permittivity tensor is symmetric [17].

Besides, since the local equilibrium of the electric system is stable, the electric energy density u_E is a convex function of the electric field e and the permittivity tensor ε is *positive definite* [16].

Similar considerations can be done for magnetic systems. Let **b** be the magnetic induction, of covariant components b_i with i = 1, 2, 3. Both the magnetic field **h**, of contravariant components h^i with i = 1, 2, 3, and the magnetic energy density u_M can be written as a function of the magnetic induction **b** in terms of the reluctivity tensor **v**, of contravariant components v^{ij} with i, j = 1, 2, 3,

$$\boldsymbol{h} = \boldsymbol{v} \cdot \boldsymbol{b}, \tag{7}$$
$$\boldsymbol{u}_{M} = \frac{1}{2} \boldsymbol{b} \cdot \boldsymbol{v} \cdot \boldsymbol{b}. \tag{8}$$

From the principles of thermodynamics [16] it follows:

$$h^{i} = \frac{\partial u_{M}}{\partial b_{i}}, \quad i = 1, 2, 3, \tag{9}$$

$$v^{ij} = \frac{\partial h^i}{\partial b_j}, \quad i, j = 1, 2, 3, \tag{10}$$

$$v^{ij} = \frac{\partial^2 u_M}{\partial b_j \partial b_i}, \quad i, j = 1 \dots 3.$$
(11)

Maxwell's relations [16] hold or equivalently the reluctivity tensor is *symmetric*. The local equilibrium of the magnetic system is stable, or equivalently the v reluctivity tensor is *positive definite* [16].

3. Existing approaches to discrete constitutive equations

.

The discrete geometric approach to electromagnetic problems relies on a pair of interlocked primal-dual grids introduced in the spatial region of interest. In order to compute the discrete counterparts of electric and magnetic constitutive equations, with respect to the pair of grids, various methods have been reported in literature.

In some of these methods [9,10], the discrete electric constitutive equation is represented by a matrix **E** approximating the relation between the array **v** of the circulations of *e* along the primal edges and the array $\tilde{\psi}$ of the fluxes of *d* across the dual faces as

$$\tilde{\boldsymbol{\psi}} = \mathbf{E}\mathbf{v}.$$

In this way, (12) is consistent with (1), but, in general, there is no guarantee that the matrix **E** is either symmetric or positive definite.

Analogously the discrete magnetic constitutive equation is represented by a matrix N approximating the relation between the array φ of the fluxes of **b** across the primal faces and the array $\tilde{\mathbf{f}}$ of the circulations of **h** along the dual edges as

$$\tilde{\mathbf{f}} = \mathbf{N}\boldsymbol{\varphi}.\tag{13}$$

In this way there is no guarantee that the matrix N is either symmetric or positive definite, even though it is consistent with (7).

In other methods [12,5], the discrete electric constitutive equation is represented by a matrix \mathbf{E} which defines a quadratic form approximating the relation between \mathbf{v} and electric energy U_E as

$$U_E = \frac{1}{2} \mathbf{v}^{\mathrm{T}} \mathbf{E} \mathbf{v}. \tag{14}$$

In this way (14) is consistent with (2) and matrix E can be ensured by construction to be symmetric positive definite. However, there is no guarantee that the discrete electric constitutive equation is consistent with (1).

Analogously, the discrete magnetic constitutive equation is represented by a matrix N which defines a quadratic form approximating the relation between the array φ and the magnetic energy U_M as

$$U_M = \frac{1}{2} \boldsymbol{\varphi}^{\mathrm{T}} \mathbf{N} \boldsymbol{\varphi}.$$
(15)

In this way (15) is consistent with (8) and matrix N can be ensured by construction to be symmetric, positive definite. However there is no guarantee that it is consistent with (7).

In order to ensure the consistency and stability of the resulting system of discrete equations, the following properties are sufficient conditions as proved in [5]:

- (i) consistency of the discrete constitutive equation (12), (13) with (1), (7) respectively;
- (ii) symmetry and positive definiteness of the matrices E, N.

However, neither of the previous two techniques is, in general, able to ensure these properties simultaneously.

4. Discrete constitutive equations preserving the thermodynamic relations for constitutive equations

Here we propose to combine the two previous techniques in such a way that properties (i) and (ii) hold simultaneously. Thus, we require that the discrete electric constitutive equation is consistent both with (1), and (2), being **E** a symmetric, positive definite matrix.

This can be reinterpreted as follows: all the thermodynamic relations for the electric constitutive equations at the continuous level are preserved at the discrete level. This is equivalent to saying that, from the relations for the electric system of Section 2, the relations at discrete level can be obtained by substituting $\boldsymbol{e} = [e_j]$, $\boldsymbol{d} = [d^i]$, $\boldsymbol{\varepsilon} = [\varepsilon^{ij}]$, u_E , with i, j = 1...3, with their discrete counterparts $\mathbf{v} = [v_j]$, $\tilde{\boldsymbol{\psi}} = [\tilde{\boldsymbol{\psi}}^i]$, $\mathbf{E} = [E^{ij}]$, U_E , with i, j = 1...l, respectively,² *l* being the number of edges of the primal grid.

Thus, the electric energy U_E is a function of the array \mathbf{v} . The array $\tilde{\boldsymbol{\psi}}$ of elements $\tilde{\psi}^i$ with $i = 1 \dots l$, is obtained from U_E as

$$\tilde{\psi}^i = \frac{\partial U_{\rm E}}{\partial v_i}, \quad i = 1 \dots l.$$

Matrix **E**, of elements E^{ij} with $i, j = 1 \dots l$, is obtained from ψ as

$$E^{ij} = \frac{\partial \psi^i}{\partial v_j}, \quad i, j = 1 \dots l$$

or equivalently from U_E as

$$E^{ij} = \frac{\partial^2 U_{\rm E}}{\partial v_i \partial v_i}, \quad i, j = 1 \dots l$$

from which, by exchanging the order of derivatives, Maxwell's relations hold for discrete quantities

$$E^{ij} = \frac{\partial^2 U_{\rm E}}{\partial v_j \partial v_i} = \frac{\partial^2 U_{\rm E}}{\partial v_i \partial v_j} = E^{ji}, \quad i, j = 1 \dots l$$

or equivalently the matrix **E** must be *symmetric*. U_E is a convex function of **v** or equivalently **E** must be *positive definite*.

As for the electric system, also for the magnetic system we require that the discrete magnetic constitutive equation is consistent both with (7) and (8), N being a symmetric, positive definite matrix. This can be reinterpreted as follows: all the thermodynamic relations for the magnetic constitutive equations at the continuous level are preserved at the discrete level. This is equivalent to saying that from the relations at continuous level for the magnetic system of Section 2 relations at discrete level can be obtained by substituting $\mathbf{b} = [b_j]$, $\mathbf{h} = [h^i]$, $\mathbf{v} = [v^{ij}]$, u_M , with i, j = 1...3, with their discrete counterparts $\boldsymbol{\varphi} = [\varphi_j]$, $\mathbf{\tilde{f}} = [\tilde{f}^i]$, $\mathbf{N} = [n^{ij}]$, U_M , with i, j = 1...f, respectively, f being the number of faces of the primal grid. Thus

$$\tilde{f}^{i} = \frac{\partial U_{M}}{\partial \varphi_{i}}, \quad i = 1 \dots f,$$
$$N^{ij} = \frac{\partial \tilde{f}^{i}}{\partial \varphi_{i}}, \quad i, j = 1 \dots f.$$

Maxwell's relations hold for discrete quantities, or equivalently N is symmetric. U_M is a convex function of φ , or equivalently N is positive definite.

5. Extension of the notion of covariant and contravariant components to dual grids

Hereafter we assume that the primal grid is composed of one volume Ω . Let Γ_i , with $i = 1 \dots l$, be the *l* primal edges of Ω , having edge vectors

 $^{^{2}}$ We attach subscript and superscript indexes to discrete quantities in a similar way to continuous quantities; the adoption of such a notation will be motivated in Section 5.

$$\boldsymbol{l}_i = \int_{\Gamma_i} \boldsymbol{t}(\boldsymbol{r}),$$

being $t(\mathbf{r})$ the unit tangent vector to Γ_i . Let Σ_i , with $i = 1 \dots f$, be the f primal faces of Ω , having face vectors

$$s_i = \int_{\Sigma_i} n(\mathbf{r}),$$

being n(r) the unit normal vector to Γ_i . In a similar way, but with a superscript index, we indicate with \tilde{l}^i , $i = 1 \dots f$, the edge vectors of the dual edges $\tilde{\Gamma}_i$ of Ω and with \tilde{s}^i , $i = 1 \dots l$, the face vectors of the dual faces $\tilde{\Sigma}_i$ of Ω .

In order to preserve the thermodynamic relations for the electric constitutive equations at the discrete level, (12) and (14) are required to be *exact* at least when the permittivity tensor ε is homogeneous and when the electric field e and the electric displacement d are spatially uniform in Ω .

Property 1. In order that (12) and (14) hold exactly for arbitrary, spatially uniform, electric field e and electric displacement d and for an arbitrary homogeneous, symmetric positive definite, permittivity tensor e, it is necessary that the following equation:

$$VI = \sum_{i=1}^{l} I_i \tilde{s}^i, \tag{16}$$

holds, where V is the volume of Ω , **I** is the fundamental tensor.³

Proof. Since e is spatially uniform it results in $v_i = l_i \cdot e$. Then since $d = \varepsilon \cdot e$ it results in $\tilde{\psi}^i = \tilde{s}^i \cdot \varepsilon \cdot e$. Thus from (14) it follows:

$$\sum_{i=1}^{l} (\boldsymbol{l}_{i} \cdot \boldsymbol{e})(\tilde{\boldsymbol{s}}^{i} \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{e}) = \boldsymbol{e} \cdot \left(\sum_{i=1}^{l} \boldsymbol{l}_{i} \tilde{\boldsymbol{s}}^{i}\right) \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{e} = V \boldsymbol{e} \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{e}$$

Then, since e is arbitrary, it results in⁴

$$\operatorname{sym}(\boldsymbol{A}\cdot\boldsymbol{\varepsilon})=V\boldsymbol{\varepsilon},$$

being

$$\boldsymbol{A} = \sum_{1}^{i} \boldsymbol{l}_{i} \tilde{\boldsymbol{s}}^{i}$$

Let us assume orthogonal Cartesian coordinates. Since ε is an arbitrary symmetric, positive definite tensor we can choose

$$\varepsilon = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

from which it follows that $A_{11} = A_{22} = A_{33} = V$. Alternatively by choosing

$$\varepsilon = \begin{bmatrix} 1 & \frac{1}{2} & 0\\ \frac{1}{2} & 1 & 0\\ 0 & 0 & 1 \end{bmatrix}$$

it follows $A_{12} = A_{21} = 0$. Similarly by choosing

³ In orthogonal Cartesian coordinates the fundamental tensor is represented by an identity matrix.

⁴ With "sym" we indicate the operator which transform a double tensor of components T^{ij} into the symmetric double tensor of components $(T^{ij} + T^{ji})/2$.

$$\boldsymbol{\varepsilon} = \begin{bmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & 1 \end{bmatrix}$$

it follows $A_{13} = A_{31} = 0$. Lastly by choosing

$$\varepsilon = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ 0 & \frac{1}{2} & 1 \end{bmatrix}$$

it follows $A_{23} = A_{32} = 0$. Thus

$$A = VI$$

and (16) holds. \Box

Property 1 is a geometric property relating primal edges to dual faces. It is thus independent of material properties. By taking the dot product of (16) with two arbitrary vectors a and b, it also follows:

$$V\boldsymbol{b} = \sum_{1}^{l} \tilde{B}^{i} \boldsymbol{l}_{i}, \tag{17}$$

$$V\boldsymbol{a} = \sum_{1}^{l} A_{i} \tilde{\boldsymbol{s}}^{i}, \tag{18}$$

$$V\boldsymbol{a}\cdot\boldsymbol{b} = \sum_{1}^{l} A_{i}\tilde{B}^{i}, \tag{19}$$

 A_i being the circulations of **a** along the edges of the primal grid and \tilde{B}^i being the fluxes of **b** across the faces of the dual grid. Assuming that it is $A_i = \mathbf{a} \cdot \mathbf{l}_i$ and $\tilde{B}^i = \mathbf{b} \cdot \tilde{s}^i$, it straightforwardly follows that each of Eqs. (16)–(19) implies all of the others.

Eqs. (16)–(19) have the same structure of (A.10)–(A.13) of Appendix A, relating covariant and contravariant components and bases. Thus they can be reinterpreted as extensions of the relations between covariant and contravariant components and bases rewritten as in Appendix A in terms of edges and face vectors and circulations and fluxes. In fact (16) relates primal edge vectors to dual face vectors, (17) expresses b in terms its fluxes across dual faces and primal edge vectors, (18) expresses a in terms its circulations along primal edges and dual face vectors, (19) expresses the dot product of a and b in terms of the circulations of a along primal edges and the fluxes of b across dual faces.

In a similar way, to preserve the thermodynamic relations for the magnetic constitutive equations at the discrete level, (13) and (15) are required to be *exact* when the reluctivity tensor v is homogeneous and when the magnetic induction b and the magnetic field h are spatially uniform in Ω .

Property 2. In order that (13) and (15) are exact for arbitrary, spatially uniform, magnetic field \mathbf{h} and magnetic induction \mathbf{b} and for an arbitrary homogeneous, symmetric positive definite, reluctivity tensor \mathbf{v} , it is necessary that the following equation:

$$VI = \sum_{1}^{f} s_{i} \tilde{l}^{i}, \tag{20}$$

holds, where V is the volume of Ω , **I** is the fundamental tensor.

Proof. Since **b** is spatially uniform it results in $\varphi_i = \mathbf{s}_i \cdot \mathbf{b}$. Then since $\mathbf{h} = \mathbf{v} \cdot \mathbf{b}$ it results in $\tilde{f}^i = \tilde{\mathbf{l}}^i \cdot \mathbf{v} \cdot \mathbf{b}$. Thus from (14) it results in

$$\sum_{1}^{f} (\mathbf{s}_{i} \cdot \mathbf{b})(\tilde{\mathbf{l}}^{i} \cdot \mathbf{v} \cdot \mathbf{b}) = \mathbf{b} \cdot \left(\sum_{1}^{1} s_{i} \tilde{\mathbf{l}}^{i}\right) \cdot \mathbf{v} \cdot \mathbf{b} = V \mathbf{b} \cdot \mathbf{v} \cdot \mathbf{b}$$

Then, since \boldsymbol{b} is arbitrary, it results in

$$\operatorname{sym}(\boldsymbol{A}\cdot\boldsymbol{v})=V\boldsymbol{v},$$

in which

$$\boldsymbol{A} = \sum_{1}^{f} \boldsymbol{s}_{i} \tilde{\boldsymbol{l}}^{i}.$$

Then, since v is an arbitrary symmetric, positive definite reluctivity tensor, proceeding as in the proof of Property 1, (20) follows. \Box

Property 2 is a geometric property relating the faces of the primal grid to the edges of the dual grid. By taking the dot product of (20) with two arbitrary vectors a and b, it also follows:

$$V\boldsymbol{b} = \sum_{i=1}^{J} \tilde{B}^{i} \boldsymbol{s}_{i}, \tag{21}$$

$$V\boldsymbol{a} = \sum_{i=1}^{f} A_{i} \tilde{\boldsymbol{\ell}}^{i}, \tag{22}$$

$$V\boldsymbol{a}\cdot\boldsymbol{b} = \sum_{1}^{J} A_{i}\tilde{B}^{i}, \qquad (23)$$

 A_i being the fluxes of \boldsymbol{a} across the faces of the primal grid and \tilde{B}^i being the circulations of \boldsymbol{b} along the edges of the dual grid. Assuming that it is $A_i = \boldsymbol{a} \cdot \boldsymbol{s}_i$ and $\tilde{B}^i = \boldsymbol{b} \cdot \tilde{\boldsymbol{l}}^i$, it straightforwardly follows that each of Eqs. (20)–(23) implies all of the others.

Eqs. (20)–(23) are obtained from (A.16)–(A.19) of Appendix A, relating covariant and contravariant components and bases. In fact, (20) relates primal face vectors to dual edge vectors, (21) expresses \boldsymbol{b} in terms of its circulations along dual edges and primal face vectors, (22) expresses \boldsymbol{a} in terms its fluxes across primal faces and dual edge vectors, (23) expresses the dot product of \boldsymbol{a} and \boldsymbol{b} in terms of fluxes of \boldsymbol{a} across primal faces and the circulations of \boldsymbol{b} along dual edges.

6. Constructing the dual of a polyhedral grid

We show here how the dual of a *polyhedral* primal grid can be constructed in such a way that Properties 1 and 2 are satisfied.

So let us assume that Ω is a polyhedron, shown in Fig. 1. Its faces Σ_i with $i = 1 \dots f$ are polygons and its edges Γ_j with $j = 1 \dots l$ are segments. Its nodes are points \mathbf{r}_k with $k = 1 \dots n$. The dual of Ω has volumes $\tilde{\Omega}_k$ with $i = 1 \dots n$, faces $\tilde{\Sigma}_j$ with $j = 1 \dots l$ and edges $\tilde{\Gamma}_i$ with $i = 1 \dots f$. Both the edges $\tilde{\Gamma}_i$ with $i = 1 \dots f$ and the traces of faces $\tilde{\Sigma}_j$ with $j = 1 \dots l$ on the boundary of Ω are assumed to be segments. However *dual* faces $\tilde{\Sigma}_j$ with $j = 1 \dots l$ are not required to be polygons, not being in general planar.

Let \mathbf{r}_{Ω} be the dual node of Ω . Let \mathbf{r}_{Σ_i} be the intersections of Σ_i and $\tilde{\Gamma}_i$ with $i = 1 \dots f$. Let \mathbf{r}_{Γ_j} be the intersections of Γ_j and $\tilde{\Sigma}_j$ with $j = 1 \dots l$. Besides, given the Γ_j edge and the two Σ_i faces adjacent to Γ_j , let the Σ_{Γ_j} face be the union of the two triangles having as vertices the nodes of Γ_j and \mathbf{r}_{Σ_i} .

By exploiting the geometric relations for polygons given in Appendix B, it results in

Property 3. Eq. (16) holds if and only if

$$\boldsymbol{T} = \sum_{1}^{f} \sum_{i=1}^{n} \int_{\bar{\Omega}_{k} \cap \Sigma_{i}} (\boldsymbol{r} - \boldsymbol{r}_{k}) \boldsymbol{n}(\boldsymbol{r}) \,\mathrm{d}\boldsymbol{\sigma}$$
(24)

$$= -\frac{1}{2} \sum_{i=1}^{f} s_i \left(\frac{1}{|\Sigma_i|} \int_{\Sigma_i} \mathbf{r} \, \mathrm{d}\boldsymbol{\sigma} - \mathbf{r}_{\Sigma_i} \right) - \sum_{i=1}^{l} s_{\Gamma_j} \left(\frac{1}{|\Gamma_j|} \int_{\Gamma_j} \mathbf{r} \, \mathrm{d}\boldsymbol{\gamma} - \mathbf{r}_{\Gamma_j} \right) = \mathbf{0}, \tag{25}$$



Fig. 1. A polyhedron Ω .

being $\mathbf{n}(\mathbf{r})$ a unit vector normal to Σ_i at \mathbf{r} , and being $\mathbf{s}_i, \mathbf{s}_{\Gamma_j}$ the face vectors of Σ_i and Σ_{Γ_j} respectively, outward normal to $\partial \Omega$.

Proof. If (16) holds then also (19) holds for arbitrary, spatially uniform, a and b. It is

$$\int_{\Omega} \boldsymbol{a} \cdot \boldsymbol{b} \, \mathrm{d} \boldsymbol{\omega} = \sum_{1}^{n} \int_{\bar{\Omega}_{k}} \boldsymbol{a} \cdot \boldsymbol{b} \, \mathrm{d} \boldsymbol{\omega}$$

Besides, since *a* is spatially uniform and thus it is $a = \nabla u(\mathbf{r})$ with $u(\mathbf{r}) = \mathbf{a} \cdot \mathbf{r}$, it results in

$$\int_{\tilde{\Omega}_{k}} \boldsymbol{a} \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} = \int_{\tilde{\Omega}_{k}} \nabla(\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{k})) \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} = \int_{\tilde{\Omega}_{k}} \nabla \cdot (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{k})) \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} - \int_{\tilde{\Omega}_{k}} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{k})) \nabla \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega}$$
$$= \int_{\tilde{\Omega}\tilde{\Omega}_{k}} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{k})) \boldsymbol{b} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\sigma}$$
$$= \sum_{1}^{f} \int_{\tilde{\Omega}_{k} \cap \Sigma_{i}} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{k})) \boldsymbol{b} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\sigma} + \sum_{1}^{l} \int_{\tilde{\Omega}_{k} \cap \tilde{\Sigma}_{j}} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{k})) \boldsymbol{b} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\sigma}, \tag{26}$$

n(r) being oriented as the outward normal to $\partial \tilde{\Omega}_k$. It is

$$\int_{\tilde{\Omega}_k \cap \tilde{\Sigma}_j} (u(\mathbf{r}) - u(\mathbf{r}_k)) \mathbf{b} \cdot \mathbf{n}(\mathbf{r}) \, \mathrm{d}\sigma = \int_{\tilde{\Omega}_k \cap \tilde{\Sigma}_j} (u(\mathbf{r}_{\Gamma_j}) - u(\mathbf{r}_k)) \mathbf{b} \cdot \mathbf{n}(\mathbf{r}) \, \mathrm{d}\sigma + \int_{\tilde{\Omega}_k \cap \tilde{\Sigma}_j} (u(\mathbf{r}) - u(\mathbf{r}_{\Gamma_j})) \mathbf{b} \cdot \mathbf{n}(\mathbf{r}) \, \mathrm{d}\sigma.$$

Besides

$$\sum_{1}^{l} \sum_{j=1}^{n} \int_{\tilde{\Omega}_{k} \cap \tilde{\Sigma}_{j}} (u(\mathbf{r}_{\Gamma_{j}}) - u(\mathbf{r}_{k})) \mathbf{b} \cdot \mathbf{n}(\mathbf{r}) \, \mathrm{d}\sigma = \sum_{1}^{l} A_{j} \tilde{B}^{j}.$$

$$\tag{27}$$

and

4

$$\sum_{1}^{n} \int_{\tilde{\Omega}_{k} \cap \tilde{\Sigma}_{j}} (u(\mathbf{r}) - u(\mathbf{r}_{\Gamma_{j}})) \mathbf{b} \cdot \mathbf{n}(\mathbf{r}) \, \mathrm{d}\sigma = 0.$$
⁽²⁸⁾

Thus, using (19) together with (26)–(28), it follows:

$$\sum_{1}^{n} \sum_{i=1}^{J} \int_{\tilde{\Omega}_{k} \cap \Sigma_{i}} \boldsymbol{a} \cdot (\boldsymbol{r} - \boldsymbol{r}_{k}) \boldsymbol{n}(\boldsymbol{r}) \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\sigma} = 0$$

or equivalently since *a* and *b* are arbitrary,

$$\sum_{1}^{f} \sum_{1}^{n} \sum_{1}^{k} \int_{\tilde{\Omega}_{k} \cap \Sigma_{i}} (\boldsymbol{r} - \boldsymbol{r}_{k}) \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\sigma} = \boldsymbol{0}.$$

By applying Lemma 5 of Appendix B to each face Σ_i , (24) follows.

Besides

Property 4. Eq. (20) holds if and only if

$$\widetilde{\boldsymbol{T}} = \sum_{1}^{J} \int_{\Sigma_{i}} (\boldsymbol{r} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{n}(\boldsymbol{r}) \,\mathrm{d}\omega$$

$$= \sum_{1}^{J} s_{i} \left(\frac{1}{|\Sigma_{i}|} \int_{\Sigma_{i}} \boldsymbol{r} \,\mathrm{d}\sigma - \boldsymbol{r}_{\Sigma_{i}} \right) = \boldsymbol{0},$$
(30)

being $\mathbf{n}(\mathbf{r})$ a unit vector normal to Σ_i at \mathbf{r} .

Proof. If (20) holds then also (23) holds for arbitrary, spatially uniform, a and b. Since b is spatially uniform and thus it is $b = \nabla u(\mathbf{r})$ with $u(\mathbf{r}) = b \cdot \mathbf{r}$, it results in

$$\int_{\Omega} \boldsymbol{a} \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} = \int_{\Omega} \boldsymbol{a} \cdot \nabla(\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Omega})) \, \mathrm{d}\boldsymbol{\omega} = \int_{\Omega} \nabla \cdot (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Omega})) \boldsymbol{a} \, \mathrm{d}\boldsymbol{\omega} - \int_{\Omega} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Omega})) \nabla \cdot \boldsymbol{a} \, \mathrm{d}\boldsymbol{\omega}$$
$$= \int_{\partial\Omega} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Omega})) \boldsymbol{a} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\omega}$$
$$= \sum_{1}^{f} \int_{\Sigma_{i}} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Sigma_{i}})) \boldsymbol{a} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\omega} + \sum_{1}^{f} \int_{\Sigma_{i}} (\boldsymbol{u}(\boldsymbol{r}_{\Sigma_{i}}) - \boldsymbol{u}(\boldsymbol{r}_{\Omega})) \boldsymbol{a} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\omega}, \tag{31}$$

n(r) being oriented as the outward normal to $\partial \Omega$. It is

$$\sum_{1}^{f} \int_{\Sigma_{i}} (u(\mathbf{r}_{\Sigma_{i}}) - u(\mathbf{r}_{\Omega})) \mathbf{a} \cdot \mathbf{n}(\mathbf{r}) \,\mathrm{d}\omega = \sum_{1}^{f} A_{i} \tilde{B}^{i}.$$
(32)

Thus by using (23) together with (31), (32), it results in

$$\sum_{1}^{f} \int_{\Sigma_{i}} \boldsymbol{b} \cdot (\boldsymbol{r} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{n}(\boldsymbol{r}) \cdot \boldsymbol{a} \, \mathrm{d}\omega = 0$$

or equivalently, since *a* and *b* are arbitrary,

$$\sum_{1}^{f} \int_{\Sigma_{i}} (\boldsymbol{r} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\omega} = \boldsymbol{0}$$

from which (29) follows. \Box

From Properties 3 and 4 it descends that the validity of (16), (20) depends only on the *trace* of the dual of Ω on $\partial\Omega$. Thus it is completely *independent* on the position of \mathbf{r}_{Ω} . As a consequence the dual of Ω is *not* completely fixed. But the main question is: for a polyhedron Ω , can the trace of the dual of Ω on $\partial\Omega$ be chosen in such a way that (16) and (20) hold?

Firstly, it can be observed that in some cases there are different ways to choose the trace of the dual of Ω on $\partial\Omega$ in order to satisfy (16) and (20). For instance, it can be straightforwardly verified that for an oblique parallelepiped Properties 3, 4 hold if its faces are subdivided by the dual grid *parallely* to its edges as shown in Fig. 2(a).

Secondly, from Properties 3, 4, it follows that (16) and (20) hold if and only if the trace of the dual of Ω on $\partial\Omega$ is such that



Fig. 2. Dual grid for different choices \mathbf{r}_{Ω} , \mathbf{r}'_{Ω} of the dual node and for different choices of the polyhedron Ω : (a) parallelepiped; (b) tetrahedron.

$$\sum_{i=1}^{J} s_i \left(\frac{1}{|\Sigma_i|} \int_{\Sigma_i} \mathbf{r} \, d\sigma - \mathbf{r}_{\Sigma_i} \right) = \mathbf{0},\tag{33}$$

$$\sum_{j=1}^{l} s_{\Gamma_j} \left(\frac{1}{|\Gamma_j|} \int_{\Gamma_j} \mathbf{r} \, \mathrm{d}\gamma - \mathbf{r}_{\Gamma_j} \right) = \mathbf{0}. \tag{34}$$

From (33) and (34) we note that there is a *unique* choice of the trace of the dual of Ω on $\partial\Omega$ such that its restriction to each edge and to each face is *independent* of its restrictions on all other edges and faces. This choice is such that

$$\mathbf{r}_{\Sigma_i} = \frac{1}{|\Sigma_i|} \int_{\Sigma_i} \mathbf{r} \, \mathrm{d}\sigma, \quad i = 1 \dots f, \tag{35}$$

$$\mathbf{r}_{\Gamma_j} = \frac{1}{|\Gamma_j|} \int_{\Gamma_j} \mathbf{r} \, \mathrm{d}\gamma, \quad j = 1 \dots l.$$
(36)

or equivalently such that \mathbf{r}_{Σ_i} are the barycenters of faces Σ_i , with $i = 1 \dots f$, and \mathbf{r}_{Γ_j} are the barycenters of edges Γ_j , with $j = 1 \dots l$. Thus a simple construction of the trace of the dual of Ω on $\partial\Omega$, such that (33) and (34) hold can be obtained by means of a *barycentric subdivision of* $\partial\Omega$ [18]. This can be done at least in the case in which the Σ_i faces with $i = 1 \dots f$ are *convex* polygons, since then the barycentric subdivision of $\partial\Omega$ is ensured to be contained in $\partial\Omega$. In particular cases, such as with a tetrahedron Ω show in Fig. 2(b), the barycentric subdivision of $\partial\Omega$ is also the only choice of the trace of the dual of Ω on $\partial\Omega$ such that (33) and (34) hold, as it can be directly verified.

Thus by arbitrarily choosing a position vector r_{Ω} as in Fig. 2 within Ω , a dual grid such that (16) and (20) hold is obtained. This can be done at least in the case in which the Ω polyhedron is *convex*, since then the dual grid is ensured to be contained in Ω .

We note that the convexity of the polyhedron Ω is just a sufficient condition and not a necessary condition for constructing a dual grid in such a way that (16) and (20) hold.

7. Reinterpreting known constitutive equations which preserve all thermodynamics relations

Lately the present authors have proposed a method [14,15] for generating electric and magnetic discrete constitutive equations preserving all the thermodynamic relations for constitutive equations. This method is

limited to the case of a primal grid composed of tetrahedra, (oblique) triangular prisms and (oblique) parallelepipeds and of a dual grid obtained by barycentric subdivision of the primal grid [18]. The method has been presented in terms of piece-wise uniform edge elements and piece-wise uniform face elements. It is here reinterpreted in a different manner.

Let the Ω primal grid be either a tetrahedron, an (oblique) triangular prism or an (oblique) parallelepiped and let the dual grid be the barycentric subdivision of Ω , as shown in Fig. 3.

Let $\tilde{\Omega}_k$, with $k = 1 \dots n$, be a dual volume of Ω . Let $I_{1k} = \tilde{I}^{1k}$, $I_{2k} = \tilde{I}^{2k}$ and $I_{3k} = \tilde{I}^{3k}$, be the edge vectors of the intersections of the primal edges of Ω incident in node r_k with $\tilde{\Omega}_k$. These edge vectors identify the edges of a parallelepiped. Let $\tilde{s}^{1k} = s_{1k}$, $\tilde{s}^{2k} = s_{2k}$ and $\tilde{s}^{3k} = s_{3k}$ be the face vectors of the faces of the parallelepiped opposite to and positively oriented with respect to these edges.

Let

 $\mathbf{v}_k = \begin{bmatrix} v_{1k} \\ v_{2k} \\ v_{3k} \end{bmatrix}$

be the array of the circulations of *e* along the edges of edge vectors I_{1k}, I_{2k}, I_{3k} , with $k = 1 \dots n$. For an electric field *e*, spatially uniform in Ω , such circulations are fractions of the circulations of *e* along the +3 primal edges of Ω incident in node r_k , so that

$$\mathbf{v}_k = \mathbf{T}_k \mathbf{v},$$

in which \mathbf{T}_k are $d \times l$ matrices. Let \mathbf{E}_k be the matrices which transform the circulations of e along the edges of edge vectors $\mathbf{l}_{1k}, \mathbf{l}_{2k}, \mathbf{l}_{3k}$ into the fluxes of $\mathbf{d} = \mathbf{\epsilon} \cdot \mathbf{e}$ across the faces of face vectors $\tilde{\mathbf{s}}^{1k}, \tilde{\mathbf{s}}^{2k}, \tilde{\mathbf{s}}^{3k}$. These matrices are defined by (A.15) of Appendix A by assuming $\mathbf{t} = \mathbf{\epsilon}$ and $\tilde{\mathbf{s}}^1 = \tilde{\mathbf{s}}^{1k}, \tilde{\mathbf{s}}^2 = \tilde{\mathbf{s}}^{2k}$ and $\tilde{\mathbf{s}}^3 = \tilde{\mathbf{s}}^{3k}$, with $k = 1 \dots n$. As proved in [14,15], matrix

$$\mathbf{E} = K \sum_{1}^{n} \mathbf{T}_{k}^{\mathrm{T}} \mathbf{E}_{k} \mathbf{T}_{k}^{\mathrm{T}}$$

in which K is 1/3, 2/3 and +1 respectively for tetrahedra, (oblique) triangular prisms and (oblique) parallelepipeds, defines a discrete electric constitutive equation, preserving the thermodynamic relations for the electric constitutive equations at the continuous level.



Fig. 3. A tetrahedral volume Ω .

Let

$$arphi_k = egin{bmatrix} arphi_{1k} \ arphi_{2k} \ arphi_{2k} \ arphi_{3k} \end{bmatrix}$$

be the arrays of the fluxes of **b** across the faces whose face vectors are s_{1k}, s_{2k}, s_{3k} , with $k = 1 \dots n$. For a magnetic induction **b**, spatially uniform in Ω , such fluxes are fractions of the fluxes of **b** across the +3 primal faces of Ω incident in node r_k , so that

$$\boldsymbol{\varphi}_k = \mathbf{P}_k \boldsymbol{\varphi},$$

in which \mathbf{P}_k are $d \times f$ matrices. Let \mathbf{N}_k be the matrices, which transform the fluxes of \boldsymbol{b} across the faces of face vectors $\boldsymbol{s}_{1k}, \boldsymbol{s}_{2k}, \boldsymbol{s}_{3k}$ into the circulations of $\boldsymbol{h} = \boldsymbol{v} \cdot \boldsymbol{b}$ along the edges of edge vectors $\tilde{\boldsymbol{l}}^{1k}, \tilde{\boldsymbol{l}}^{2k}, \tilde{\boldsymbol{l}}^{3k}$. These matrices are defined by (A.21) of Appendix A by assuming $\boldsymbol{t} = \boldsymbol{v}$ and $\tilde{\boldsymbol{l}}^1 = \tilde{\boldsymbol{l}}^{1k}, \tilde{\boldsymbol{l}}^2 = \tilde{\boldsymbol{l}}^{2k}$ and $\tilde{\boldsymbol{l}}^3 = \tilde{\boldsymbol{l}}^{3k}$, with $k = 1 \dots n$. As proved in [14,15], matrix

$$\mathbf{N} = K \sum_{1}^{n} \mathbf{P}_{k}^{\mathrm{T}} \mathbf{N}_{k} \mathbf{P}_{k}$$

is a discrete magnetic constitutive equation, preserving the thermodynamic relations for the magnetic constitutive equation at the continuous level.

8. Constitutive equations over polyhedral grids

In Section 5, Properties 1 and 2 were shown to be necessary conditions for the construction of discrete constitutive equations preserving the thermodynamic relations for constitutive equations. Such Properties are here proved to be also sufficient conditions. In fact discrete constitutive equations preserving the thermodynamic relations for constitutive equations are here deduced by extending the method described in Section 7, when Properties 1 and 2 hold.

Thus let the dual grid satisfy (33) and (34). The polyhedron Ω can be naturally subdivided into tetrahedra τ_h , with $h = 1 \dots 2l$, as shown in Fig. 4. Each tetrahedron has as vertices the dual node \mathbf{r}_{Ω} the two extrema of one edges Γ_j and point \mathbf{r}_{Σ_i} of a primal face Σ_i adjacent to Γ_j . Let \mathbf{l}_{1h} be the edge vector of Γ_j . Let \mathbf{l}_{2h} be the edge vector of the intersection of Σ_i with $\tilde{\Sigma}_j$, oriented from \mathbf{r}_{Γ_j} to \mathbf{r}_{Σ_i} . Let \mathbf{l}_{3h} be the edge vector of $\tilde{\Gamma}_i$, oriented as the outward normal to $\partial\Omega$. As in Appendix A, $\mathbf{l}_{1h} = \tilde{\mathbf{l}}^{1h}$, $\mathbf{l}_{2h} = \tilde{\mathbf{l}}^{2h}$, $\mathbf{l}_{3h} = \tilde{\mathbf{l}}^{3h}$ are the edge vectors of edges identifying



Fig. 4. The subdivision of the Ω polyhedron into the τ_h tetrahedra, with $h = 1 \dots 2l$.

1907

a parallelepiped. Let $\tilde{s}^{1h} = s_{1h}$, $\tilde{s}^{2h} = s_{2h}$ and $\tilde{s}^{3h} = s_{3h}$ be the face vectors of the faces of the parallelepiped opposite to and positively oriented with respect to these edges.

The following Lemmas 1-4 lead to Property 5.

Lemma 1. The following relation holds:

$$\widetilde{\boldsymbol{T}} - \boldsymbol{T} = \sum_{1}^{f} \sum_{k=1}^{n} (\boldsymbol{r}_{k} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{f}^{ik},$$
(37)

 f^{ik} being the vector face of the intersection of Σ_i with $\tilde{\Omega}_k$, outward normal to $\partial\Omega_i$.

Proof. From (24), (29), it results in

$$\widetilde{\boldsymbol{T}} - \boldsymbol{T} = \sum_{1}^{f} \int_{\Sigma_{i}} (\boldsymbol{r} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\omega - \sum_{1}^{f} \sum_{1}^{n} \int_{\Sigma_{i} \cap \tilde{\Omega}_{k}} (\boldsymbol{r} - \boldsymbol{r}_{k}) \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\sigma = \sum_{1}^{f} \sum_{1}^{n} \int_{\Sigma_{i} \cap \tilde{\Omega}_{k}} (\boldsymbol{r}_{k} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\omega$$

from which (37) follows. \Box

Lemma 2. The following relation holds:

$$\frac{1}{2}\sum_{1}^{2l} \mathbf{I}_{2h}\tilde{\mathbf{s}}^{2h} = \sum_{1}^{l} \mathbf{e}_{j}\mathbf{f}^{j} - \frac{1}{2}\sum_{1}^{2l} \mathbf{I}_{2h}\tilde{\mathbf{s}}^{3h},$$
(38)

in which \mathbf{e}_j is the edge vector of the trace of $\tilde{\Sigma}_j$ on $\partial \Omega$, arbitrarily oriented, and \mathbf{f}^j is the face vector of the triangle whose vertices are \mathbf{r}_{Ω} and the extrema of Γ_j , positively oriented with respect to \mathbf{e}_j .

Proof. Let τ_{h_1} and τ_{h_2} be the pair of tetrahedra adjacent to the Γ_j edge, as shown in Fig. 5. It results in

$$\tilde{s}^{2h_1} = I_{3h_1} \times I_{1h_1} = (I_{3h_1} - I_{2h_1}) \times I_{1h_1} + I_{2h_1} \times I_{1h_1} = 2f^j - \tilde{s}^{3h_1}.$$

Similarly

$$\tilde{s}^{2h_2} = -l_{3h_2} \times l_{1h_2} = (-l_{3h_2} + l_{2h_2}) \times l_{1h_2} - l_{2h_2} \times l_{1h_2} = -2f^j - \tilde{s}^{3h_2}.$$

Thus

$$l_{2h_1}\tilde{s}^{2h_1} = 2l_{2h_1}f^j - l_{2h_1}\tilde{s}^{3h_1},$$

$$l_{2h_2}\tilde{s}^{2h_2} = -2l_{2h_2}f^j - l_{2h_2}\tilde{s}^{3h_2}.$$
(39)
(40)



Fig. 5. Elements e_i and f^j , with $j = 1 \dots l$.

By summing (39) and (40) over all edges Γ_i and by observing that

 $\boldsymbol{l}_{2h_1}-\boldsymbol{l}_{2h_2}=\boldsymbol{e}_j,$

then (38) follows. \Box

Lemma 3. The following relation holds:

$$\frac{1}{2}\sum_{1}^{2l} \boldsymbol{l}_{2h} \tilde{\boldsymbol{s}}^{3h} = -3\,\widetilde{\boldsymbol{T}} + \sum_{1}^{f} \sum_{1}^{n} (\boldsymbol{r}_{k} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{f}^{ik}.$$

$$\tag{41}$$

Proof. From Property 4 and Lemma 6 of Appendix B, it follows:

$$\widetilde{\boldsymbol{T}} = \sum_{1}^{f} \int_{\Sigma_{i}} (\boldsymbol{r} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{n}(\boldsymbol{r}) \,\mathrm{d}\omega = \frac{1}{3} \sum_{1}^{f} \sum_{1}^{n} \sum_{1}^{n} (\boldsymbol{r}_{k} - \boldsymbol{r}_{\Sigma_{i}}) \boldsymbol{f}^{ik} - \frac{1}{6} \sum_{1}^{2l} \boldsymbol{I}_{2h} \widetilde{\boldsymbol{s}}^{3h}$$

and (41) follows. \Box

Lemma 4. The following relation holds:

$$VI = \sum_{1}^{l} e_{j} f^{j} + \widetilde{T}.$$
(42)

Proof. Let a, b be spatially uniform fields, so that $a = \nabla u(\mathbf{r})$ with $u(\mathbf{r}) = \mathbf{a} \cdot \mathbf{r}$. Let ρ_i be the pyramid whose base is the Σ_i face and has vertex \mathbf{r}_{Ω} , with $i = 1 \dots f$ (Fig. 6). Let the lateral faces of these pyramids be π_j with $j = 1 \dots l$. It results in

$$\begin{split} \int_{\rho_i} \boldsymbol{a} \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} &= \int_{\rho_i} \nabla (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Sigma_i})) \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} = \int_{\rho_i} \nabla \cdot (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Sigma_i})) \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} - \int_{\rho_i} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Sigma_i})) \nabla \cdot \boldsymbol{b} \, \mathrm{d}\boldsymbol{\omega} \\ &= \int_{\partial \rho_i} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Sigma_i})) \boldsymbol{b} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\sigma} \\ &= \int_{\Sigma_i} (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Sigma_i})) \boldsymbol{b} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\sigma} + \sum_{1}^l \int_{\partial \rho_i \cap \pi_j} ((\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}_{\Gamma_j})) + (\boldsymbol{u}(\boldsymbol{r}_{\Gamma_j}) - \boldsymbol{u}(\boldsymbol{r}_{\Sigma_i}))) \boldsymbol{b} \cdot \boldsymbol{n}(\boldsymbol{r}) \, \mathrm{d}\boldsymbol{\sigma}. \end{split}$$



Fig. 6. A pyramid ρ_i of base Σ_i .

Since, for each $j = 1 \dots l$,

$$\sum_{1}^{f} \int_{\partial \rho_i \cap \pi_j} (u(\mathbf{r}) - u(\mathbf{r}_{\Gamma_j})) \mathbf{b} \cdot \mathbf{n}(\mathbf{r}) \, \mathrm{d}\sigma = 0,$$

$$\sum_{1}^{f} \int_{\partial \rho_i \cap \pi_j} (u(\mathbf{r}_{\Gamma_j}) - u(\mathbf{r}_{\Sigma_i})) \mathbf{b} \cdot \mathbf{n}(\mathbf{r}) \, \mathrm{d}\sigma = (\mathbf{a} \cdot \mathbf{e}_j) (\mathbf{f}^j \cdot \mathbf{b}),$$

it results in

$$V\boldsymbol{a}\cdot\boldsymbol{b} = \sum_{1}^{f} \int_{\rho_{i}} \boldsymbol{a}\cdot\boldsymbol{b}\,\mathrm{d}\omega = \sum_{1}^{l} (\boldsymbol{a}\cdot\boldsymbol{e}_{j})(\boldsymbol{f}^{j}\cdot\boldsymbol{b}) + \sum_{1}^{f} \int_{\Sigma_{i}} (u(\boldsymbol{r}) - u(\boldsymbol{r}_{\Sigma_{i}}))\boldsymbol{b}\cdot\boldsymbol{n}(\boldsymbol{r})\,\mathrm{d}\sigma.$$

Because a, b are arbitrary, (42) follows. \Box

From previous Lemmas 1-4 the following result is deduced.

Property 5. The following relation holds:

$$\frac{1}{2}\sum_{1}^{2l} l_{2h}\tilde{s}^{2h} = \frac{1}{2}\sum_{1}^{2l} \tilde{l}^{2h}s_{2h} = VI + T + \tilde{T}.$$
(43)

Proof. From Lemmas 1 and 3, it is

$$\frac{1}{2}\sum_{j=1}^{2l}\boldsymbol{I}_{2h}\tilde{\boldsymbol{s}}^{3h}=-3\,\tilde{\boldsymbol{T}}+(\tilde{\boldsymbol{T}}-\boldsymbol{T})=-2\,\tilde{\boldsymbol{T}}-\boldsymbol{T}.$$

Then from Lemma 2 it follows:

$$\frac{1}{2}\sum_{1}^{2l}\boldsymbol{I}_{2h}\widetilde{\boldsymbol{s}}^{2h} = \sum_{1}^{l}\boldsymbol{e}_{j}\boldsymbol{f}^{j} + 2\widetilde{\boldsymbol{T}} + \boldsymbol{T}.$$

Thus from Lemma 4, (43) follows. \Box

The dual grids are here assumed to be such that (33) and (34) hold. As a particular case (35) and (36) hold, that is the trace of the dual of $\partial \Omega$ on Ω is the barycentric subdivision of $\partial \Omega$. The approach of Section 7 for constructing discrete constitutive equations is extended to such dual grids, as follows.

Let

$$\mathbf{v}_h = \begin{bmatrix} v_{1h} \\ v_{2h} \\ v_{3h} \end{bmatrix}$$

- -

be the arrays with the circulations of *e* along edges I_{1h} , I_{2h} , I_{3h} , with $h = 1 \dots 2l$. From (18), for an electric field *e*, spatially uniform in Ω , such circulations can be expressed as

$$\mathbf{v}_h = \mathbf{T}_h \mathbf{v},$$

where

$$\mathbf{T}_{h} = \begin{bmatrix} 0 & \cdots & 1 & \cdots & 0 \\ \boldsymbol{I}_{2h} \cdot \frac{\tilde{s}^{1}}{V} & \cdots & \boldsymbol{I}_{2h} \cdot \frac{\tilde{s}^{j}}{V} & \cdots & \boldsymbol{I}_{2h} \cdot \frac{\tilde{s}^{j}}{V} \\ \boldsymbol{I}_{3h} \cdot \frac{\tilde{s}^{1}}{V} & \cdots & \boldsymbol{I}_{3h} \cdot \frac{\tilde{s}^{j}}{V} & \cdots & \boldsymbol{I}_{3h} \cdot \frac{\tilde{s}^{j}}{V} \end{bmatrix}.$$

Let \mathbf{E}_h be the matrices which transform the circulations of e along the edges of edge vectors $\mathbf{I}_{1h}, \mathbf{I}_{2h}, \mathbf{I}_{3h}$ into the fluxes of $\mathbf{d} = \boldsymbol{\varepsilon} \cdot \mathbf{e}$ across the faces of face vectors $\tilde{\mathbf{s}}^{1h}, \tilde{\mathbf{s}}^{2h}, \tilde{\mathbf{s}}^{3h}$. These matrices are defined by (A.15) of Appendix A by assuming $\mathbf{t} = \boldsymbol{\varepsilon}$ and $\tilde{\mathbf{s}}^1 = \tilde{\mathbf{s}}^{1h}, \tilde{\mathbf{s}}^2 = \tilde{\mathbf{s}}^{2h}$ and $\tilde{\mathbf{s}}^3 = \tilde{\mathbf{s}}^{3h}$, with $h = 1 \dots 2l$.

Now, using Property 5, we can prove the following main result.

Property 6. Matrix

$$\mathbf{E} = \frac{1}{6} \sum_{1}^{2l} \mathbf{T}_{h}^{\mathrm{T}} \mathbf{E}_{h} \mathbf{T}_{h}$$
(44)

is a discrete electric constitutive equation preserving the thermodynamic relations for electric constitutive equations at the continuous level.

Proof. For an electric field e, spatially uniform in Ω , it is

$$\mathbf{T}_{h}\mathbf{v} = \begin{bmatrix} \mathbf{I}_{1h} \cdot \mathbf{e} \\ \mathbf{I}_{2h} \cdot \mathbf{e} \\ \mathbf{I}_{3h} \cdot \mathbf{e} \end{bmatrix}$$

and

$$\mathbf{E}_{h}\mathbf{T}_{h}\mathbf{v} = \begin{bmatrix} \widetilde{s}^{1h} \cdot d \\ \widetilde{s}^{2h} \cdot d \\ \widetilde{s}^{3h} \cdot d \end{bmatrix},$$

being $d = \varepsilon \cdot e$. Then

$$\mathbf{E}\mathbf{v} = \frac{1}{6} \sum_{1}^{2l} \mathbf{T}_{h}^{\mathrm{T}} \begin{bmatrix} \tilde{\mathbf{s}}^{1h} \cdot \mathbf{d} \\ \tilde{\mathbf{s}}^{2h} \cdot \mathbf{d} \\ \tilde{\mathbf{s}}^{3h} \cdot \mathbf{d} \end{bmatrix} = \begin{bmatrix} \frac{1}{6} \frac{\tilde{\mathbf{s}}^{1}}{V} \cdot \left(2V\mathbf{I} + \sum_{1}^{2l} \mathbf{l}_{2h} \tilde{\mathbf{s}}^{2h} + \sum_{1}^{2l} \mathbf{l}_{3h} \tilde{\mathbf{s}}^{3h} \right) \cdot \mathbf{d} \\ \vdots \\ \frac{1}{6} \frac{\tilde{\mathbf{s}}^{l}}{V} \cdot \left(2V\mathbf{I} + \sum_{1}^{2l} \mathbf{l}_{2h} \tilde{\mathbf{s}}^{2h} + \sum_{1}^{2l} \mathbf{l}_{3h} \tilde{\mathbf{s}}^{3h} \right) \cdot \mathbf{d} \end{bmatrix}.$$
(45)

Thus since, from Property 5 it is

$$\sum_{1}^{2l} \boldsymbol{l}_{2h} \tilde{\boldsymbol{s}}^{2h} = 2V \boldsymbol{l}$$

and from Property 2 it is

$$\sum_{1}^{2l} \mathbf{I}_{3h} \tilde{\mathbf{s}}^{3h} = \sum_{1}^{2l} \tilde{\mathbf{I}}^{3h} \mathbf{s}_{3h} = 2 \sum_{1}^{f} \tilde{\mathbf{I}}^{i} \mathbf{s}_{i} = 2V \mathbf{I},$$

from (45) it results in

$$\mathbf{E}\mathbf{v} = \begin{bmatrix} \tilde{\mathbf{s}}^1 \cdot \mathbf{d} \\ \vdots \\ \tilde{\mathbf{s}}^l \cdot \mathbf{d} \end{bmatrix}$$

and \mathbf{E} is consistent with (1).

Also it is

$$\frac{1}{2}\mathbf{v}^{\mathrm{T}}\mathbf{E}\mathbf{v} = \frac{1}{12}\sum_{h}^{2l}\mathbf{v}_{h}^{\mathrm{T}}\mathbf{E}_{h}\mathbf{v}_{h} = \frac{1}{2}\sum_{h}^{2l}|\tau_{h}|\boldsymbol{e}\cdot\boldsymbol{d} = \frac{1}{2}V\boldsymbol{e}\cdot\boldsymbol{d}$$

and **E** is consistent with (2).

Since $\mathbf{E}_{h}^{\mathrm{T}} = \mathbf{E}_{h}$, for each $h = 1 \dots 2l$, it results in

$$\mathbf{E}^{\mathrm{T}} = \left(\sum_{1}^{2l} \mathbf{T}_{h}^{\mathrm{T}} \mathbf{E}_{h} \mathbf{T}_{h}\right)^{\mathrm{T}} = \sum_{1}^{2l} \mathbf{T}_{h}^{\mathrm{T}} \mathbf{E}_{h}^{\mathrm{T}} \mathbf{T}_{h} = \sum_{1}^{2l} \mathbf{T}_{h}^{\mathrm{T}} \mathbf{E}_{h} \mathbf{T}_{h} = \mathbf{E}$$

and E is symmetric.

Since $\mathbf{v}_h^{\mathrm{T}} \mathbf{E}_h \mathbf{v}_h \ge 0$, for each $h = 1 \dots 2l$, it results in

$$\frac{1}{2}\mathbf{v}^{\mathrm{T}}\mathbf{E}\mathbf{v} = \frac{1}{12}\sum_{h=1}^{2l}\mathbf{v}^{\mathrm{T}}\mathbf{T}_{h}^{\mathrm{T}}\mathbf{E}_{h}\mathbf{T}_{h}\mathbf{v} = \frac{1}{12}\sum_{h=1}^{2l}\mathbf{v}_{h}^{\mathrm{T}}\mathbf{E}_{h}\mathbf{v}_{h} \ge 0$$

Also $\mathbf{v}^{\mathrm{T}}\mathbf{E}\mathbf{v} = 0$ implies $\mathbf{v}_{h}^{\mathrm{T}}\mathbf{E}_{h}\mathbf{v}_{h} = 0$ and thus $\mathbf{v}_{h} = \mathbf{T}_{h}\mathbf{v} = \mathbf{0}$ for all $h = 1 \dots 2l$. Then $v_{1h} = 0$ for all $h = 1 \dots 2l$, or equivalently $v_{j} = 0$ for all $j = 1 \dots l$ that is $\mathbf{v} = \mathbf{0}$. Thus \mathbf{E} is *positive definite*. \Box

In a similar way let

$$\boldsymbol{\varphi}_h = \begin{bmatrix} \varphi_{1h} \\ \varphi_{2h} \\ \varphi_{3h} \end{bmatrix}$$

be the fluxes of **b** across faces s_{1h} , s_{2h} , s_{3h} , with $h = 1 \dots 2l$. From (22), for a magnetic induction **b**, spatially uniform in Ω , such fluxes can be expressed as

$$\boldsymbol{\varphi}_h = \mathbf{P}_h \boldsymbol{\varphi},$$

where

$$\mathbf{P}_{h} = \begin{bmatrix} \mathbf{s}_{1h} \cdot \frac{\tilde{l}^{1}}{V} & \cdots & \mathbf{s}_{1h} \cdot \frac{\tilde{l}^{i}}{V} & \cdots & \mathbf{s}_{1h} \cdot \frac{\tilde{l}^{i}}{V} \\ \mathbf{s}_{2h} \cdot \frac{\tilde{l}^{1}}{V} & \cdots & \mathbf{s}_{2h} \cdot \frac{\tilde{l}^{i}}{V} & \cdots & \mathbf{s}_{2h} \cdot \frac{\tilde{l}^{i}}{V} \\ \mathbf{0} & \cdots & \boldsymbol{\xi}_{i} & \cdots & \mathbf{0} \end{bmatrix}$$

and $\xi_i = \mathbf{s}_{3h} \cdot \mathbf{s}_i / |\mathbf{s}_i|^2$.

Let \mathbf{N}_k be the matrices, which transform the fluxes of \boldsymbol{b} across the faces of face vectors \boldsymbol{s}_{1h} , \boldsymbol{s}_{2h} , \boldsymbol{s}_{3h} into the circulations of $\boldsymbol{h} = \boldsymbol{v} \cdot \boldsymbol{b}$ along the edges of edge vectors $\tilde{\boldsymbol{l}}^{1h}$, $\tilde{\boldsymbol{l}}^{2h}$, $\tilde{\boldsymbol{l}}^{3h}$. These matrices are defined by (A.21) of Appendix B by assuming $\boldsymbol{t} = \boldsymbol{v}$ and $\tilde{\boldsymbol{l}}^1 = \tilde{\boldsymbol{l}}^{1h}$, $\tilde{\boldsymbol{l}}^2 = \tilde{\boldsymbol{l}}^{2h}$ and $\tilde{\boldsymbol{l}}^3 = \tilde{\boldsymbol{l}}^{3h}$, with $h = 1 \dots 2l$.

Using again Property 5, the following main result is now proved:

Property 7. Matrix

$$\mathbf{N} = \frac{1}{6} \sum_{1}^{2l} \mathbf{P}_{h}^{\mathrm{T}} \mathbf{N}_{h} \mathbf{P}_{h}$$
(46)

is a discrete magnetic constitutive equation, preserving the thermodynamic relations for magnetic constitutive equations at the continuous level.

Proof. For a magnetic field \boldsymbol{b} , spatially uniform in Ω , it is

$$\mathbf{P}_h oldsymbol{arphi} = egin{bmatrix} oldsymbol{s}_{1h} \cdot oldsymbol{b} \ oldsymbol{s}_{2h} \cdot oldsymbol{b} \ oldsymbol{s}_{3h} \cdot oldsymbol{b} \end{bmatrix}$$

and

$$\mathbf{N}_{h}\mathbf{P}_{h}\boldsymbol{\varphi} = \begin{bmatrix} \tilde{\boldsymbol{l}}^{1h} \cdot \boldsymbol{h} \\ \tilde{\boldsymbol{l}}^{2h} \cdot \boldsymbol{h} \\ \tilde{\boldsymbol{l}}^{3h} \cdot \boldsymbol{h} \end{bmatrix},$$

being $h = v \cdot b$. Then

$$\mathbf{N}\boldsymbol{\varphi} = \frac{1}{6} \sum_{1}^{2l} \mathbf{P}_{h}^{\mathrm{T}} \begin{bmatrix} \tilde{\boldsymbol{I}}^{1h} \cdot \boldsymbol{h} \\ \tilde{\boldsymbol{I}}^{2h} \cdot \boldsymbol{h} \\ \tilde{\boldsymbol{I}}^{3h} \cdot \boldsymbol{h} \end{bmatrix} = \begin{bmatrix} \frac{1}{6} \frac{\tilde{l}^{l}}{V} \cdot \left(\sum_{1}^{2l} \tilde{\boldsymbol{I}}^{1h} \boldsymbol{s}_{1h} + \sum_{1}^{2l} \tilde{\boldsymbol{I}}^{2h} \boldsymbol{s}_{2h} + 2V\boldsymbol{I} \right) \cdot \boldsymbol{h} \\ \vdots \\ \frac{1}{6} \frac{\tilde{l}^{l}}{V} \cdot \left(\sum_{1}^{2l} \tilde{\boldsymbol{I}}^{1h} \boldsymbol{s}_{1h} + \sum_{1}^{2l} \tilde{\boldsymbol{I}}^{2h} \boldsymbol{s}_{2h} + 2V\boldsymbol{I} \right) \cdot \boldsymbol{h} \end{bmatrix}.$$
(47)

Thus since, from Property 5 it is

$$\sum_{1}^{2l} \tilde{\boldsymbol{l}}^{2h} \boldsymbol{s}_{2h} = 2V \boldsymbol{l}$$

and from Property 1 it is

$$\sum_{1}^{2l} \tilde{\boldsymbol{l}}^{1h} \boldsymbol{s}_{1h} = \sum_{1}^{2l} \boldsymbol{l}_{1h} \tilde{\boldsymbol{s}}^{1h} = \sum_{1}^{l} \boldsymbol{l}_{j} \tilde{\boldsymbol{s}}^{j} = 2V \boldsymbol{I},$$

from (47) it results in

$$\mathbf{N}\boldsymbol{\varphi} = \begin{bmatrix} \boldsymbol{l}^1 \cdot \boldsymbol{h} \\ \vdots \\ \tilde{\boldsymbol{l}}^f \cdot \boldsymbol{h} \end{bmatrix}$$

and N is consistent with (2).

Also it is

$$\frac{1}{2}\boldsymbol{\varphi}^{\mathrm{T}}\mathbf{N}\boldsymbol{\varphi} = \frac{1}{12}\sum_{1}^{2l} \boldsymbol{\varphi}_{h}^{\mathrm{T}}\mathbf{N}_{h}\boldsymbol{\varphi}_{h} = \frac{1}{2}\sum_{1}^{2l} |\tau_{h}|\boldsymbol{b}\cdot\boldsymbol{h} = \frac{1}{2}V\boldsymbol{b}\cdot\boldsymbol{h}$$

and N is consistent with (8). Since $\mathbf{N}_{h}^{\mathrm{T}} = \mathbf{N}_{h}$, for each $h = 1 \dots 2l$, it results in

$$\mathbf{N}^{\mathrm{T}} = \left(\sum_{1}^{2l} \mathbf{P}_{h}^{\mathrm{T}} \mathbf{N}_{h}^{\mathrm{T}} \mathbf{P}_{h}\right)^{\mathrm{T}} = \sum_{1}^{2l} \mathbf{P}_{h}^{\mathrm{T}} \mathbf{N}_{h}^{\mathrm{T}} \mathbf{P}_{h} = \sum_{1}^{2l} \mathbf{P}_{h}^{\mathrm{T}} \mathbf{N}_{h} \mathbf{P}_{h} = \mathbf{N}$$

and N is symmetric.

Since $\boldsymbol{\varphi}_h^{\mathrm{T}} \mathbf{N}_h \boldsymbol{\varphi}_h \ge 0$, for each $h = 1 \dots 2l$, it results in

$$\frac{1}{2}\boldsymbol{\varphi}^{\mathrm{T}}\mathbf{N}\boldsymbol{\varphi} = \frac{1}{12}\sum_{1}^{2l} \boldsymbol{\varphi}^{\mathrm{T}}\mathbf{P}_{h}^{\mathrm{T}}\mathbf{N}_{h}\mathbf{P}_{h}\boldsymbol{\varphi} = \frac{1}{12}\sum_{1}^{2l} \boldsymbol{\varphi}_{h}^{\mathrm{T}}\mathbf{N}_{h}\boldsymbol{\varphi}_{h} \ge 0.$$

Also $\varphi^{\mathsf{T}} \mathbf{N} \varphi = 0$ implies $\varphi_h^{\mathsf{T}} \mathbf{N}_h \varphi_h = 0$ and thus $\varphi_h = \mathbf{P}_h \varphi = \mathbf{0}$ for all $h = 1 \dots 2l$. Then $\varphi_{1h} = 0$ for all $h = 1 \dots 2l$, or equivalently $\varphi_i = 0$ for all $i = 1 \dots f$ that is $\varphi = \mathbf{0}$. Thus \mathbf{N} is *positive definite*. \Box

Remark 1. Property 1 implies that also (A.14) and (A.15) of Appendix A can be extended to dual grids. Thus the following relation holds:

$$\tilde{\psi} = \mathbf{E}'\mathbf{v}$$

with

$$\mathbf{E}' = \left[\frac{\tilde{\mathbf{s}}^i \cdot \mathbf{\varepsilon} \cdot \tilde{\mathbf{s}}^j}{V}\right].$$

Such E' matrix is a natural candidate for a discrete electric constitutive equation. However, as it can be straightforwardly verified, even though \mathbf{E}' is consistent with (4) and (5) and is symmetric, it is positive **Remark 2.** Property 2 implies that also (A.20) and (A.21) of Appendix A can be extended to dual grids. Thus the following relation holds

$$\tilde{\mathbf{f}} = \mathbf{N}' \boldsymbol{\varphi}$$

with

$$\mathbf{N}' = \left[\frac{\tilde{\boldsymbol{l}}^i \cdot \boldsymbol{v} \cdot \tilde{\boldsymbol{l}}^j}{V}\right].$$

Such \mathbf{N}' matrix is a natural candidate for a discrete magnetic constitutive equation. However, as it can be straightforwardly verified, even though \mathbf{N}' is consistent with (10) and (11) and is symmetric, it is positive semi-definite and *not* positive definite being *singular*. Thus it does *not* preserve the thermodynamic relations for magnetic constitutive equations at the continuous level.

9. Numerical experiments

As working example, we consider an electromagnetic wave propagation problem formulated in the frequency domain, where the constitutive equations previously introduced can be naturally used. The field along a short-circuited section of a coaxial transmission line has been computed, the analytical solution being well known [20]. The transmission line has internal radius r = 2 cm, external radius R = 4 cm and length l = 8 cm. The numerical analysis has been performed both on a grid of tetrahedra and of hexahedra. The constitutive equations have been constructed using the method here proposed. The per cent error of the computed electric field, in the energy norm, with respect to the analytical solution [20] is plotted in Fig. 7, versus the maximum grid diameter h_{max} , at frequency

$$f = 1.1 \frac{l}{\sqrt{\mu_0 \varepsilon_0}},$$

being μ_0 and ε_0 vacuum permeability and permittivity respectively. The error with respect to the analytical solution appears to be limited and to decrease with grid size. As a reference, the per cent error with respect



Fig. 7. Percent error of the computed electric field with respect to the analytical solution, in the energy norm, versus maximum grid diameter.

to the analytical solution is reported also when for a grid of tetrahedra the constitutive equations are constructed by means of edge elements using Whitney's functions [13].

10. Conclusions

In the paper, we proved a way to construct discrete counterparts of constitutive equations over polyhedral grids, preserving the thermodynamic relations for constitutive equations as a mean to ensure consistency and stability of the resulting equations at discrete level.

Numerical experiments demonstrate that the obtained discrete constitutive equations lead to accurate approximations of the electromagnetic field.

Appendix A. Reinterpreting covariant and contravariant components in terms of circulations and fluxes

Let v_i , with i = 1...3, be a triple of non-coplanar vectors, defining the covariant basis of a coordinate system [19]. The *covariant* components of vector **a** are then

$$a_i = \boldsymbol{a} \cdot \boldsymbol{v}_i \quad i = 1 \dots 3. \tag{A.1}$$

The contravariant components b^i of a vector **b**, with i = 1...3, are defined by

$$\boldsymbol{b} = \sum_{i=1}^{d} b^{i} \boldsymbol{v}_{i}. \tag{A.2}$$

By solving (A.2) for b^i with $i = 1 \dots 3$, it results in

$$b^i = \boldsymbol{b} \cdot \boldsymbol{v}^i \quad i = 1 \dots 3, \tag{A.3}$$

where

$$\mathbf{v}^{i} = \frac{\mathbf{v}_{i-1} \times \mathbf{v}_{i+1}}{\mathbf{v}_{i-1} \times \mathbf{v}_{i+1} \cdot \mathbf{v}_{i}}, \quad i = 1 \dots 3$$
 (A.4)

the operations on indexes being modulo 3.

The vectors v^i with i = 1...3 define the contravariant basis of the coordinate system and are solutions of equation

$$I = \sum_{1}^{3} v_i v^i. \tag{A.5}$$

By taking the dot product of (A.5) by *a* it also follows:

$$\boldsymbol{a} = \sum_{i=1}^{3} a_i \boldsymbol{v}^i \tag{A.6}$$

and by taking the scalar product of (A.6) with b,

$$\boldsymbol{a} \cdot \boldsymbol{b} = \sum_{1}^{3} a_{i} b^{i}. \tag{A.7}$$

By assuming (A.1) and (A.3), it follows that each of Eqs. (A.2), (A.5), (A.6), (A.7) implies all of the others.

Covariant and contravariant components can be applied also to tensors. For instance for a double tensor t, its contravariant components

$$t^{ij} = \mathbf{v}^i \cdot \mathbf{t} \cdot \mathbf{v}^j \quad i, j = 1 \dots 3 \tag{A.8}$$

transform the covariant components a_i of a vector **a** into the contravariant components b^i of a vector **b** as follows

$$b^{i} = \sum_{1}^{3} t^{ij} a_{j} \quad i = 1 \dots 3.$$
 (A.9)

Now let l_i with i = 1...3 be the edge vectors of 3 segments identifying a parallelepiped of volume $V = |l_{i-1} \times l_i \cdot l_{i+1}|$. Let \tilde{s}^i , with i = 1...3, be the face vectors of the faces of the parallelepiped opposite to and positively oriented with respect to these edges. By assuming $v_i = l_i$ it straightforwardly results in $v^i = \tilde{s}^i/V$, with i = 1...3.

Let A_i be the circulations of a vector \mathbf{a} along the edge of edge vector \mathbf{l}_i and let \tilde{B}^i be the flux of a vector \mathbf{b} across the face of face vector \tilde{s}^i , with $i = 1 \dots 3$. Then it results in $a_i = A_i$, $b^i = \tilde{B}^i/V$. Moreover (A.5), (A.2), (A.6), (A.7) can be rewritten as

$$VI = \sum_{i=1}^{3} l_i \tilde{s}^i, \tag{A.10}$$

$$V\boldsymbol{b} = \sum_{i=1}^{3} \widetilde{B}^{i} \boldsymbol{l}_{i}, \tag{A.11}$$

$$V\boldsymbol{a} = \sum_{i=1}^{3} A_i \tilde{\boldsymbol{s}}^i, \tag{A.12}$$

$$V\boldsymbol{a}\cdot\boldsymbol{b} = \sum_{1}^{3} A_{i}\widetilde{B}^{i}.$$
(A.13)

Thus covariant components a_i of vector a and contravariant components b^i of vector b can be equivalently represented in terms of circulations A_i of vector a and fluxes \tilde{B}^i of vector b. Similarly covariant basis vectors v_i and contravariant basis vectors v^i can be equivalently represented in terms of edge vectors l_i and face vectors \tilde{s}^i . Analogously (A.8) and (A.9) can be rewritten as

$$\widetilde{B}^i = \sum_{j=1}^{3} T^{ij} A_j \quad i = 1 \dots 3$$
(A.14)

in which

$$T^{ij} = V t^{ij} = \frac{\tilde{s}^i \cdot t \cdot \tilde{s}^j}{V} \quad i, j = 1...3.$$
(A.15)

Alternatively the role of circulations and fluxes can also be exchanged. In fact let s_i with $i = 1 \dots 3$ be the face vectors of +3 parallelograms identifying a parallelepiped of volume $V = \sqrt{|s_{i-1} \times s_i \cdot s_{i+1}|}$ and let \tilde{l}^i , with $i = 1 \dots 3$, be the edge vectors of the edges opposite to and positively oriented with respect to these faces. By assuming $v_i = s_i$ it results in $v^i = \tilde{l}^i / V$, with $i = 1 \dots 3$.

Let A_i be the flux of a vector \boldsymbol{a} across the face of face vector \boldsymbol{s}_i and let \tilde{B}^i be the circulation of a vector \boldsymbol{b} along the edge of edge vector $\tilde{\boldsymbol{l}}^i$, with i = 1...3. It results in $a_i = A_i$ and $b^i = \tilde{B}^i/V$. Moreover (A.5), (A.2), (A.6), (A.7) can be rewritten as

$$VI = \sum_{i=1}^{3} s_i \tilde{l}^i, \tag{A.16}$$

$$V\boldsymbol{b} = \sum_{i=1}^{3} \widetilde{B}^{i} \boldsymbol{s}_{i}, \tag{A.17}$$

$$V\boldsymbol{a} = \sum_{i=1}^{3} A_i \tilde{\boldsymbol{l}}^i, \tag{A.18}$$

$$V\boldsymbol{a}\cdot\boldsymbol{b} = \sum_{1}^{3} A_{i}\widetilde{B}^{i}.$$
(A.19)

Thus covariant components a_i of vector a and contravariant components b^i of vector b can be equivalently represented in terms of fluxes A_i of vector a and circulations \tilde{B}^i of vector b. Similarly covariant basis vectors v_i and contravariant basis vectors v^i can be equivalently represented in terms of face vectors s_i and edge vectors \tilde{l}^i . Analogously (A.8), (A.9) can be rewritten as

$$\widetilde{B}^{i} = \sum_{1}^{3} T^{ij} A_{j} \quad i = 1 \dots 3$$
(A.20)

in which

$$T^{ij} = \mathcal{W}^{ij} = \frac{l^i \cdot t \cdot l^j}{V} \quad i, j = 1...3.$$
(A.21)

Appendix B. Geometric relations for polygons

Let Σ be a generic polygon. Let \mathbf{r}_k be the nodes of Σ , with $k = 1 \dots n$. Let Γ_k be the edges of Σ , with $k = 1 \dots n$. Nodes are assumed to be numbered counterclockwise. Edges Γ_k are assumed to be oriented from node \mathbf{r}_k to node \mathbf{r}_{k+1} . Operations on indexes are modulo n (Fig. B.1).

The dual grid of Σ has faces $\tilde{\Sigma}_k$ and edges $\tilde{\Gamma}_k$ with $k = 1 \dots n$. Edges $\tilde{\Gamma}_k$ are assumed to be segments. Let \mathbf{r}_{Σ} be the dual node of Σ and let \mathbf{r}_{Γ_k} be the intersection of Γ_k and $\tilde{\Gamma}_k$, with $k = 1 \dots n$.

Dual face $\tilde{\Sigma}_k$ is the union of triangle $\tilde{\Sigma}_k^-$ (having vertices \mathbf{r}_{Σ} , \mathbf{r}_k , $\mathbf{r}_{\Gamma_{k-1}}$) and triangle $\tilde{\Sigma}_k^+$ (having vertices \mathbf{r}_{Σ} , \mathbf{r}_k , \mathbf{r}_{Γ_k}). The union of faces $\tilde{\Sigma}_k^+$ and $\tilde{\Sigma}_{k+1}^-$ is referred to as Σ_{Γ_k} . It follows:

Lemma 5.

$$-\sum_{1}^{n} \int_{\tilde{\Sigma}_{k}} (\boldsymbol{r} - \boldsymbol{r}_{k}) \, \mathrm{d}\boldsymbol{\sigma} = \frac{1}{2} |\boldsymbol{\Sigma}| \left(\frac{1}{|\boldsymbol{\Sigma}|} \int_{\boldsymbol{\Sigma}} \boldsymbol{r} \, \mathrm{d}\boldsymbol{\sigma} - \boldsymbol{r}_{\boldsymbol{\Sigma}} \right) + \sum_{1}^{n} |\boldsymbol{\Sigma}_{\Gamma_{k}}| \left(\frac{1}{|\Gamma_{k}|} \int_{\Gamma_{k}} \boldsymbol{r} \, \mathrm{d}\boldsymbol{\gamma} - \boldsymbol{r}_{\Gamma_{k}} \right)$$
(B.1)

Proof.

$$-\sum_{1}^{n} \int_{\tilde{\Sigma}_{k}} (\mathbf{r} - \mathbf{r}_{k}) \, \mathrm{d}\sigma = -\int_{\Sigma} (\mathbf{r} - \mathbf{r}_{\Sigma}) \, \mathrm{d}\sigma + \sum_{1}^{n} \int_{\tilde{\Sigma}_{k}} (\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) \, \mathrm{d}\sigma$$
$$= -|\Sigma| \left(\frac{1}{|\Sigma|} \int_{\Sigma} \mathbf{r} \, \mathrm{d}\sigma - \mathbf{r}_{\Sigma} \right) + \sum_{1}^{n} |\tilde{\Sigma}_{k}| (\mathbf{r}_{k} - \mathbf{r}_{\Sigma}). \tag{B.2}$$



Fig. B.1. Geometric elements of the Σ polygon.

Moreover

$$\begin{split} \sum_{1}^{n} |\tilde{\Sigma}_{k}|(\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) &= \sum_{1}^{n} |\tilde{\Sigma}_{k}^{+}|(\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) + |\tilde{\Sigma}_{k+1}^{-}|(\mathbf{r}_{k+1} - \mathbf{r}_{\Sigma}) \\ &= \sum_{1}^{n} \frac{1}{2} (|\tilde{\Sigma}_{k}^{+}| + |\tilde{\Sigma}_{k+1}^{-}|)((\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) + (\mathbf{r}_{k+1} - \mathbf{r}_{\Sigma})) + \sum_{1}^{n} \frac{1}{2} (|\tilde{\Sigma}_{k}^{+}| - |\tilde{\Sigma}_{k+1}^{-}|)(\mathbf{r}_{k} - \mathbf{r}_{k+1}). \end{split}$$

Thus, since it is

$$\frac{1}{2}(|\tilde{\Sigma}_k^+|+|\tilde{\Sigma}_{k+1}^-|)((\boldsymbol{r}_k-\boldsymbol{r}_{\Sigma})+(\boldsymbol{r}_{k+1}-\boldsymbol{r}_{\Sigma}))=\frac{3}{2}\int_{\Sigma_+^k\cup\Sigma_-^{k+1}}(\boldsymbol{r}-\boldsymbol{r}_{\Sigma})\,\mathrm{d}\sigma,$$

and also

$$\frac{1}{2}(|\Sigma_{+}^{k}| - |\Sigma_{-}^{k+1}|)(\mathbf{r}_{k} - \mathbf{r}_{k+1}) = \frac{1}{2}|\Sigma_{\Gamma_{k}}|((\mathbf{r}_{k} - \mathbf{r}_{\Gamma_{k}}) + (\mathbf{r}_{k+1} - \mathbf{r}_{\Gamma_{k}})) = |\Sigma_{\Gamma_{k}}|\left(\frac{1}{|\Gamma_{k}|}\int_{\Gamma_{k}}\mathbf{r}\,\mathrm{d}\gamma - \mathbf{r}_{\Gamma_{k}}\right)$$

it also results in

$$\sum_{1}^{n} |\tilde{\Sigma}_{k}|(\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) = \frac{3}{2} |\Sigma| \left(\frac{1}{|\Sigma|} \int_{\Sigma} \mathbf{r} \, \mathrm{d}\sigma - \mathbf{r}_{\Sigma} \right) + \sum_{1}^{n} |\Sigma_{\Gamma_{k}}| \left(\frac{1}{|\Gamma_{k}|} \int_{\Gamma_{k}} \mathbf{r} \, \mathrm{d}\gamma - \mathbf{r}_{\Gamma_{k}} \right). \tag{B.3}$$

By substituting (B.3) into (B.2), (B.1) follows. \Box

Lemma 6.

$$\int_{\Sigma} (\boldsymbol{r} - \boldsymbol{r}_{\Sigma}) \, \mathrm{d}\boldsymbol{\sigma} = \frac{1}{3} \sum_{1}^{n} |\tilde{\Sigma}_{k}| (\boldsymbol{r}_{k} - \boldsymbol{r}_{\Sigma}) + \frac{1}{3} \sum_{1}^{n} |\Sigma_{\Gamma_{k}}| (\boldsymbol{r}_{\Gamma_{k}} - \boldsymbol{r}_{\Sigma}) \tag{B.4}$$

Proof. From the formula of the barycenter of a triangle it results in

$$\begin{split} \int_{\Sigma} (\mathbf{r} - \mathbf{r}_{\Sigma}) \, \mathrm{d}\sigma &= \frac{1}{3} \sum_{1}^{n} |\tilde{\Sigma}_{k}^{+}| ((\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) + (\mathbf{r}_{\Gamma_{k}} - \mathbf{r}_{\Sigma})) + \frac{1}{3} \sum_{1}^{n} |\tilde{\Sigma}_{k}^{-}| ((\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) + (\mathbf{r}_{\Gamma_{k-1}} - \mathbf{r}_{\Sigma})) \\ &= \frac{1}{3} \sum_{1}^{n} (|\tilde{\Sigma}_{k}^{-}| + |\tilde{\Sigma}_{k}^{+}|) (\mathbf{r}_{k} - \mathbf{r}_{\Sigma}) + \frac{1}{3} \sum_{1}^{n} (|\tilde{\Sigma}_{k}^{+}| + |\tilde{\Sigma}_{k+1}^{-}|) (\mathbf{r}_{\Gamma_{k}} - \mathbf{r}_{\Sigma}) \end{split}$$

from which (B.4) follows. \Box

It can be straightforwardly concluded that Lemmas 5, 6 hold also with arbitrary numerations and orientations of edges and nodes of Σ .

References

- T. Weiland, A numerical method for the solution of the eigenvalue problem of longitudinally homogeneous waveguides, Electronics and Communication (AEÜ) 31 (1977) 308–311.
- [2] T. Weiland, On the unique numerical solution of Maxwellian eigenvalue problems in three dimensions, Particle Accelerators 17 (1985) 227–242.
- [3] E. Tonti, Finite formulation of the electromagnetic field, IEEE Transactions on Magnetics 38 (2) (2002) 333-336.
- [4] A. Bossavit, How weak is the Weak Solution in finite elements methods? IEEE Transactions on Magnetics 34 (5) (1998) 2429– 2432.
- [5] A. Bossavit, L. Kettunen, Yee-like schemes on staggered cellular grids: A synthesis between FIT and FEM approaches, IEEE Transactions on Magnetics 36 (4) (2000) 861–867.
- [6] E. Tonti, Algebraic topology and computational electromagnetism, in: 4th International Workshop on Electric and Magnetic Fields, Marseille (Fr) 12–15 May, 1998, pp. 284–294.
- [7] M. Marrone, Properties of constitutive matrices for electrostatic and magnetostatic problems, IEEE Transactions on Magnetics 40 (2004) 1516–1520.
- [8] R. Schuhmann, T. Weiland, Stability of the FDTD algorithm on non-orthogonal grids related to the spatial interpolation scheme, IEEE Transactions on Magnetics 34 (5) (1998) 2751–2754.

- [9] M. Marrone, Computational aspects of the cell method in electrodynamics, Progress in Electromagnetic Research 32 (2001) 317–356.
- [10] F. Trevisan, L. Kettunen, Geometric interpretation of discrete approaches to solving Magnetostatics, IEEE Transactions on Magnetics 40 (2) (2004) 361–365.
- [11] P. Dular, J.Y. Hody, A. Nicolet, A. Genon, W. Legros, Mixed finite elements associated with a collection of tetrahedra, hexahedra and prisms, IEEE Transactions on Magnetics 30 (5) (1994) 2980–2983.
- [12] Man-Fai Wong, O. Picon, V.F. Hanna, A finite element method based on Whitney forms to solve Maxwell equations in the time domain, IEEE Transactions on Magnetics 31 (3) (1995) 1618–1621.
- [13] T. Tarhasaari, L. Kettunen, A. Bossavit, Some realizations of a discrete Hodge operator: a reinterpretation of finite element techniques, IEEE Transactions on Magnetics 35 (3) (1999) 1494–1497.
- [14] L. Codecasa, V. Minerva, M. Politi, Use of Barycentric dual grids for the solution of frequency domain problems by FIT, IEEE Transactions on Magnetics 40 (2) (2004) 1414–1419.
- [15] L. Codecasa, F. Trevisan, Piecewise uniform bases and energetic approach for discrete constitutive matrices in electromagnetic problems, International Journal of Numerical Methods and Engineering 65 (4) (2006) 548–565.
- [16] H.B. Callen, Thermodynamics and an Introduction to Thermostatistics, second ed., Wiley, New York, 1985.
- [17] L.D. Landau, E.M. Lifshitz, Electrodynamics of Continuous Media, Pergamon Press, Oxford, 1960.
- [18] A. Bossavit, Computational Electromagnetism, Academic Press, 1998.
- [19] R. Abraham, J.E. Marsden, T.S. Ratiu, Manifolds, Tensor Analysis, and Applications, second ed., Springer-Verlag, 1991.
- [20] R.E. Collin, Foundations of Microwave Engineering, second ed., McGraw-Hill, 1992.