

GEOMETRIC ASPECTS OF THE SIMPLICIAL DISCRETIZATION OF MAXWELL'S EQUATIONS

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Abstract—Aspects of the geometric discretization of electromagnetic fields on simplicial lattices are considered. First, the convenience of the use of exterior differential forms to represent the field quantities through their natural role as duals (cochains) of the geometric constituents of the lattice (chains = nodes, edges, faces, volumes) is briefly reviewed. Then, the use of the barycentric subdivision to decompose the (ordinary) simplicial primal lattice together with the (twisted) non-simplicial barycentric dual lattice into simplicial elements is considered. Finally, the construction of lattice Hodge operators by using Whitney maps on the first barycentric subdivision is described. The objective is to arrive at a discrete formulation of electromagnetic fields on general lattices which better adheres to the underlying physics.

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1. INTRODUCTION

Like most equations of physics, Maxwell's equations are extremely rich in symmetries and (hence) conservation laws. In the continuum, many conservation laws follow directly from invariances of the Lagrangian (Noether symmetries) such as energy or momentum conservation, while others have an inherent topological aspect, such as magnetic charge. However, when Maxwell's equations are discretized on a lattice, a number of symmetries of the continuum theory are modified or broken. Still, many conservation laws may be trivially preserved on a discrete setting. This is because they often relate a quantity on certain region of space to an associated quantity on the boundary of the region. Because the boundary is a topological invariant, such conservation laws should not depend on the metric of the space (i.e., they are invariant under homeomorphisms). As a result they are also scale invariant and should not depend (in a consistent discrete model of the theory) whether a continuum limit is taken. A natural mathematical language that explore this aspect is the calculus of exterior differential forms [1–45] and associated algebraic topological structures [1–12, 15–21, 23–29, 32, 35–38, 40–45].

This is partly because, when cast in such language, Maxwell's equations are factorized into a purely topological (i.e., metric-free) part

$$dE = -\frac{\partial}{\partial t}B \quad (1)$$

$$dH = \frac{\partial}{\partial t}D + J \quad (2)$$

$$dB = 0 \quad (3)$$

$$dD = \rho \quad (4)$$

and a metric dependent part

$$D = \star_{\epsilon}E \quad (5)$$

$$B = \star_{\mu}H \quad (6)$$

In the above, E and H are electric and magnetic field intensity 1-forms, D and B are electric and magnetic flux density 2-forms, J is the electric current density 2-form, and ρ is the electric charge density 3-form. The metric-free operator d is the exterior derivative, which simultaneously plays the role of the grad, curl, and div operators of vector calculus, distilled from their metric structure. Constitutive parameters of a given medium in Eqs. (5) and (6) relate the 1-forms E , H to the 2-forms D , B and are given in terms of the so-called *Hodge operators*, $\star_\epsilon$ and $\star_\mu$, which also include all metric information [13, 26, 28, 32, 33, 36, 38–40, 48].

This is unlike the vector calculus formalism, where metric and topological structures are intertwined in the equations. As alluded, such factorization has important consequences (even in the topologically trivial manifolds of interest) if the objective is to arrive at a consistent discretization scheme for Maxwell's equations in general lattices. There are many reasons for that. First, the topological equations (1)–(4) admit an *exact* discrete spatial rendering [40]. Therefore, many theorems (such as charge conservation alluded before) are automatically fulfilled after discretization, without the need to involve metric concepts. Second, because the metric is completely encoded into Eqs. (5) and (6), the treatment of curved boundaries and material interfaces [also entirely encoded in Eqs. (5) and (6)] can be done in a more systematic manner, without affecting, e.g., conservation laws related to the topological equations. Third, once discretized, the topological (spatial) part of the equations often comprises integer arithmetic only and are more efficiently handled by a computer if a priori recognized as such¹.

Besides this natural factorization, the language of forms also sheds light in a number of issues faced by various discretization methods. Among them are rationale for the use of edge (Whitney) elements in finite element methods [19, 23, 35] (related with the correct interpolation of the electric and magnetic field intensities 1-forms E and H) and for the dual grid construction in finite difference and finite volume methods [10, 32, 40] (related with the concept of external and internal orientations of differential forms).

1.1. Outline

In this paper, we first review the terminology and basic concepts of the spatial discretization of Maxwell's equations using discrete differential forms (cochains), with special emphasis on the factorization

¹ Exceptions to this last point are lattices involving some sort of spatial interpolation for the boundary stencil, such as in many subgridding or locally conformal grid situations.

of the topological and metric problems. We then discuss more specific geometric aspects of the discretization using a simplicial primal lattice and a non-simplicial barycentric dual lattice as starting point, followed by a barycentric subdivision (decomposition) of both these lattices. Motivated by the results in [45] and through the representation of the cochains (electromagnetic fields) via Whitney forms, the first barycentric subdivision is then used as the actual tool for discretization. The objectives are to arrive at a coordinate-free, discrete version of Maxwell's equations for general lattices with fewer ad-hoc interpolatory rules, and to have the geometric structure of the continuum theory mirrored, to a maximum extent, by its discrete counterpart.

2. DISCRETIZATION OF THE TOPOLOGICAL EQUATIONS

2.1. Simplicial Lattices and Complexes

Simplicial lattices will be considered here not only because of their flexibility in dealing with complex geometries, but also because they are more fundamental in the sense that any lattice can be built by assembling simplicial elements. For our purposes, the term *simplicial lattice* will refer to a *simplicial complex* embedded on a Euclidean, E^3 space (i.e., with a metric structure associated to it).

For completeness, we will next briefly sketch the definition of simplicial complex. More detailed descriptions can be found elsewhere, e.g., [1, 4, 5, 6, 7, 40, 45].

Given $x_0, x_1, \dots, x_M$ affine points in an abstract space, a M -simplex, σ^M , is the set of points (convex hull) given by $x = \sum_{i=0}^M \lambda_i x_i$ where λ_i are the *barycentric* coordinates such that $\sum_{i=0}^M \lambda_i = 1$ and $\lambda_i \geq 0$. We write $\sigma^M = [x_0, x_1, \dots, x_M]$. In a three-dimensional space, a 0-simplex is a point, a 1-simplex is an edge (line segment), a 2-simplex is a face (triangle), and a 3-simplex is a volume (tetrahedron). An *oriented* M -simplex changes sign under a change of orientation, i.e., if $\sigma^M = [x_0, x_1, \dots, x_M]$ and a permutation of the indices is carried out, then $[x_{\tau(0)}, x_{\tau(1)}, \dots, x_{\tau(M)}] = (-1)^\tau \sigma^M$, where τ denotes the total number of permutations needed to restore the original index order (odd or even permutations). The j -face of a simplex is the set defined by $\lambda_j = 0$. The faces of a 1-simplex $[x_0, x_1]$ are the points $[x_0]$ and $[x_1]$ (0-simplices), the faces of a 2-simplex $[x_0, x_1, x_2]$ are its three edges, i.e., $[x_0, x_1]$, $[x_1, x_2]$, and $[x_0, x_2]$ (1-simplices), and so forth. We denote the simplex σ_i^M as being a face of the simplex $\sigma_j^{M'}$, with $M < M'$, by

$$\sigma_i^M \subset \sigma_j^{M'}.$$

A *simplicial complex* χ is a collection of simplices such that (i) for all σ^M belonging to χ , its faces also belong to χ , and (ii) for any two simplices their intersection is either empty or it is a common face of both. We note that the concept of simplicial complex (and of barycentric coordinates) is independent of a metric and therefore will constitute the general structure over which the discretized version of Eqs. (1)–(4) will be cast. Only Eqs. (5) and (6) will make use of the metric structure to be introduced a posteriori. When the elements are not necessarily simplicial (e.g., Yee's tetrahedral cells), we have a *cell complex*, and its elements are called *cells*. A simplicial complex is therefore a particular case of a cell complex.

In the continuum, a natural duality exists between exterior differential forms and regions of integration (points, lines, surfaces, volumes) [1, 2, 13, 15, 23, 40, 60]. Indeed, integrals can be thought as a pairing (contraction) of differential forms with these geometrical objects which gives a scalar as a result. On a lattice or cell complex, the geometrical objects will be formal sums of simplices, called *chains*. A M -chain is a linear combination of M -simplices in χ through $\Omega^M = \sum_i \alpha_i \sigma_i^M \in \chi$, with coefficients α_i over the reals (for our purposes). From this definition, a 0-chain is a linear combination of points, a 1-chain is a linear combination of edges (lines), etc. A chain is always one of these types (there are no mixed chains) and the M -simplices σ^M (or M -cells in general) form a basis for the space of M -chains, C_M .

2.2. Pairing and Incidence Matrices

Given an arbitrary simplicial complex, Eqs. (1)–(4) are easily discretized through a pairing with corresponding elements of two complexes χ and $\tilde{\chi}$, and by using the adjoint of the exterior derivative d . On a lattice, the operator d is referred as the *coboundary* operator whose adjoint is called the *boundary* operator ∂ [32, 40, 45]. The boundary operator carries its usual intuitive meaning [14]. Eqs. (3) and (4) are trivially verified on a lattice from the nilpotency of the boundary operator, $\partial^2 = 0$ (i.e., the topological fact that the boundary of a boundary is zero). The topological Eqs. (1)–(4) on a complex are written as

$$\sum_j \beta_{ij} \langle \sigma_j^1, E \rangle = -\frac{\partial}{\partial t} \langle \sigma_i^2, B \rangle \quad (7)$$

$$\sum_j \tilde{\beta}_{ij} \langle \tilde{\sigma}_j^1, H \rangle = -\frac{\partial}{\partial t} \langle \tilde{\sigma}_i^2, D \rangle + \langle \tilde{\sigma}_i^2, J \rangle \quad (8)$$

$$\sum_j \gamma_{ij} \langle \sigma_j^2, B \rangle = 0 \quad (9)$$

$$\sum_j \tilde{\gamma}_{ij} \langle \tilde{\sigma}_j^2, D \rangle = \langle \tilde{\sigma}_i^3, \rho \rangle \quad (10)$$

The *incidence matrices* $\alpha_{ij}, \beta_{ij}, \gamma_{ij}$ (and $\tilde{\alpha}_{ij}, \tilde{\beta}_{ij}, \tilde{\gamma}_{ij}$) in the above equations are the discrete representation of the operator ∂ in a given complex χ (and $\tilde{\chi}$). The incidence matrices are operationally defined by the action of the boundary operator on a basis of 1-, 2- and 3-chains (i.e., simplices), $\{\sigma_i^1\}$, $\{\sigma_i^2\}$, $\{\sigma_i^3\}$, respectively, through $\partial\sigma_i^1 = \sum_j \alpha_{ij} \sigma_j^0$, $\partial\sigma_i^2 = \sum_j \beta_{ij} \sigma_j^1$, $\partial\sigma_i^3 = \sum_j \gamma_{ij} \sigma_j^2$, $\partial\tilde{\sigma}_i^1 = \sum_j \tilde{\alpha}_{ij} \tilde{\sigma}_j^0$, $\partial\tilde{\sigma}_i^2 = \sum_j \tilde{\beta}_{ij} \tilde{\sigma}_j^1$, and $\partial\tilde{\sigma}_i^3 = \sum_j \tilde{\gamma}_{ij} \tilde{\sigma}_j^2$ [40]. These matrices are the discrete counterparts to the grad, curl, and div operators, respectively, distilled from their metric structure. In the case of simplicial complexes (or any cell complex where the definition of the boundary stencil does not involve spatial interpolations), the elements of those matrices are integers having the values ± 1 (depending on the relative orientation) when $\sigma_j^{(k-1)} \in \partial\sigma_i^k$, and zero otherwise (hence it involves only integer arithmetic).

The incidence matrices should obey a number of (consistency) properties as discussed, e.g., in [40]. These properties are important to assure that key theorems of the continuum theory (e.g., charge conservation, reciprocity) are preserved in the discrete setting. Violation of those properties often result in clear nonphysical behavior and harmful numerical artifacts such as unconditional instabilities. Because any metric structure is still irrelevant at this level of description, these properties are classified as topological consistency properties. For simple, regular lattices, they are almost automatically fulfilled in the most usual discretization schemes. However, in lattices with more involved topological structures, e.g., those involving some form of subgridding or conformal gridding, special care should be taken to avoid violation of these properties under naive discretization schemes [40].

The discrete fields in Eqs. (7)–(10), counterpart to the differential forms fields in Eqs. (1)–(4), are called *cochains* to stress that they belong to the dual space of the chains of the cell complex, i.e., C^M . Cochains therefore constitute the discrete representation of the electromagnetic fields. The map from the space of M-forms Φ^M to the space of M-cochains, C^M is called the *de Rham map*, $Rh : \Phi^M \rightarrow C^M$. In the following, we will often use the terms cochains and forms interchangeably to reflect that cochains are just discrete differential forms.

2.3. Complexes and Orientation

The choice of two distinct complexes, χ for Eqs. (7) and (9) and $\tilde{\chi}$ for Eqs. (8) and (10), is not arbitrary. Instead, it is rooted on distinct geometrical properties of the differential forms in Eqs. (1) and (3) versus those in Eqs. (2) and (4), and related to the concept of orientation [32, 40]. This is because while E and B (associated with energy) possess *internal* orientation (*ordinary* forms or cochains), D and H (associated with sources J and ρ) possess *external* orientation (*twisted* forms or cochains) [3, 40]. Because of this difference on geometric properties, they are associated with different complexes inheriting these two types of orientation (i.e., ordinary forms to a ordinary complex, and twisted forms to a twisted complex). This is indeed the geometrical reason behind the dual lattice construction in many finite volume and finite difference methods [32]. Here, we will choose the simplicial primal complex as the ordinary complex and the dual cell complex as the twisted complex. The reciprocal choice could be made as well.

3. DISCRETIZATION OF THE METRIC EQUATIONS

The discretization of the topological equations provide a *counterpart* to the continuum equations, Eqs. (1)–(4). In contrast, the discretization of the metric equations provides an *approximation* of the continuum equations, Eqs. (5), (6). Error analysis may focus on the metric part of the equations.

3.1. Discrete Hodge Operators

Equations (5) and (6) generalize the constitutive equations and incorporate all metric information about a particular lattice. In the continuum, the Hodge operators relate M -forms with $(N - M)$ forms, where N is the dimension of the space. It establishes an isomorphism between these two spaces. In the discrete case, the discrete version of the Hodge operators $\star_\epsilon$ and $\star_\mu$ establish a map between the M -cochains on the primal, ordinary complex χ with the $(N - M)$ -cochains on the dual, twisted complex $\tilde{\chi}$ and vice-versa, i.e.,

$$\begin{aligned} [\star_\epsilon] : C^1(\chi) &\rightarrow C^2(\tilde{\chi}) \\ \langle \tilde{\sigma}_i^2, D \rangle &= \sum_j [\star_\epsilon]_{ij} \langle \sigma_j^1, E \rangle \end{aligned} \quad (11)$$

$$[\star_\mu] : C^1(\tilde{\chi}) \rightarrow C^2(\chi)$$

$$\langle \sigma_i^2, B \rangle = \sum_j [\star_\mu]_{ij} \langle \tilde{\sigma}_j^1, H \rangle \quad (12)$$

Discrete Hodge operators approximate the continuum Hodge operators [26]. Discretization methods usually yield procedural equivalent ‘Hodge operators’ through quadratures rules and interpolations. From the material properties of the background medium and from the metric properties of the lattice (or equivalently, of the manifold where the lattice is assumed embedded), the discrete Hodge operators should exhibit some key basic properties in order to lead to a consistent (in the sense of [40]) discrete theory. For example, in the case of a reciprocal medium and on the usual Euclidean space, the discrete Hodge operators should necessarily be symmetric, positive definite operators [40].

In order to obtain an explicit time-update scheme in the case of a time domain method, at least one of the matrices in Eqs. (11), (12) needs to be diagonal. In the Yee’s FDTD scheme, this is achieved by the dual orthogonal hexahedral grid construction. For an arbitrary simplicial lattice, however, this is not possible in general (some particular tetrahedral and dual grid constructions, such as the Delaunay-Voronoi grid [46], are mutually orthogonal by construction and therefore produce diagonal Hodge operators at the expense geometric flexibility). In general, the matrices in Eqs. (11) and (12) will be only sparse, but not diagonal. In those cases however, it is still possible to approximate those sparse matrices (at least one of them) by diagonal matrices through *mass lumping* and arrive at an explicit scheme [48].

3.2. Whitney and de Rham Maps

As mentioned before, it is possible to associate a differential M -form field, ω^M , to a cochain by using the de Rham map $\Omega_M, Rh : \Phi^M \rightarrow C^M$. The ‘inverse’ process of associating Ω_M to ω^M is called the *Whitney map*, $Wh : C^M \rightarrow \Phi^M$ [26, 43]. Furthermore, from the natural pairing between a chain in C_M and a cochain in C^M (isomorphism between dual spaces), it is possible to further associate a Whitney form to a given simplex, i.e., to define a map, $\varphi : C_M \rightarrow \Phi^M$. Given a M -simplex, σ^M , this pivotal map (note that we will also call it a Whitney map) is given by

$$\varphi(\sigma^M) = \omega^M = M! \sum_{i=0}^M (-1)^i \lambda_i d\lambda_0 \wedge \dots d\lambda_{i-1} \wedge d\lambda_{i+1} \dots d\lambda_M \quad (13)$$

where $\lambda_i, i = 0, \dots, M$ are the barycentric coordinates associated with σ^M . Both de Rham and Whitney maps do *not* depend on a metric. Note also that the de Rham and Whitney maps do not necessarily commute, and hence the error in the discretization [26].

Equations (11) and (12) implicitly incorporate the metric of the background manifold by assuming lengths, areas and volumes for the lattice elements (they can also be thought as ‘defining’ the metric). Maxwell’s system of eqs. (1)–(6) is fully discretized once the matrices in Eqs. (11) and (12) are obtained. This can be done, e.g., by first introducing an inner product and using a modified Whitney map which incorporates this background metric through the canonical isomorphism between forms and vectors (defined by the metric itself). Then, from this (metric dependent) representation for the cochains, a modified de Rham map on the dual lattice could be used to obtain the matrices in Eqs. (11) and (12) explicitly for any lattice. A fundamental problem with this (otherwise natural) approach, however, is that the dual lattice of a simplicial primal lattice is not simplicial anymore and hence the Whitney and de Rham maps are not applicable as defined before (i.e., on a simplicial lattice). This problem can be overcome by using a barycentric dual lattice $\tilde{\chi}$, and modified Whitney and de Rham maps on the first barycentric subdivision of χ and $\tilde{\chi}$ [43–45, 47, 48]. This is the topic of the next section.

4. DUAL LATTICES AND BARYCENTRIC SUBDIVISION

4.1. Hodge Duality in Topological Field Theories

A simple geometric construction exists such that the dual lattice to *any* (primal) simplicial lattice can be decomposed into simplicial elements [43–45, 47, 48]. This construction is based on the concept of a barycentric dual lattice and its barycentric subdivision.

In the context of the Abelian Chern-Simons (CS) theory (an extensively used model for 2+1 gauge theories), it was recently demonstrated that by using a barycentric subdivision (and a field-doubling procedure not relevant here²), the resulting discretization scheme is capable of completely capturing the *topological* features of the theory even before taking the continuum limit [45]. Among the unique aspects of the barycentric subdivision is that it is affine invariant (the

² Through this field doubling, the original gauge field and a new gauge field are made to belong to dual spaces (dual cell complexes). In the electromagnetic case, the field doubling is unnecessary because the explicit presence of the Hodge operator in Eq. (15) below already *forces* the presence of the dual complex from the start.

barycenter construction is metric-free). We will next consider this scheme in connection with the simplicial discretization of eqs. (1)–(6).

In the case of the Abelian CS theory considered in [45], the action of the theory is given by

$$S_{CS} = \int_{D^3} A \wedge dA \quad (14)$$

where A is the gauge field (potential 1-form) and D^3 the domain of interest (a three-dimensional compact manifold). In contrast, the action for Eqs. (1)–(6) is written as

$$S_{EM} = \int_{D^4} F \wedge *F = \int_{D^4} dA \wedge *dA \quad (15)$$

where F is the electromagnetic (strength) 2-form, $F = E \wedge dt + B$, and, A is the electromagnetic four-potential 1-form (gauge field) [2]. In the electromagnetic case, the domain D^4 in the equation above is the flat four-dimensional (Minkowski) space-time.

Conspicuous in Eq. (15) (apart from the dimensionality) is the appearance of the four-dimensional spatio-temporal Hodge $*$, which is responsible for the metric structure of Maxwell’s equations [the $*$ operator is related to the previously considered Hodge operators (on each spatial slice) of Eqs. (5) and (6) through $*F = -\mu^{-1} \star_\mu B \wedge dt + \epsilon^{-1} \star_\epsilon E$]. In contrast, Eq. (14) is entirely metric-free, constituting a celebrated example of a topological field theory [49–53]. To capture the topological features of the CS theory, a discrete duality operator was introduced in [45]. Such operator [dubbed ‘discrete Hodge star’ but not quite so in the sense of the (metric dependent) operators of Eqs. (5) and (6)] is also metric-free. It defines a Hodge duality through a pairing in C_p which does not reproduce (in general) the metric structure of a general lattice. This is not a issue for the CS theory because of the metric-free character of Eq. (14)³. For the electromagnetic field, we use the same barycentric subdivision, but we must necessarily incorporate the presence of the metric structure associated with the Hodge operator. This is detailed in the next section.

4.2. Whitney Maps on the Dual Lattice via Barycentric Subdivision

Analogously to [45], the construction here relies also on the concept of a barycentric dual lattice and its barycentric subdivision. The

³ Because of this, the Hodge star in [45] always appears in conjunction with an inner product so that the end result does not depend on the metric used to construct both.

barycenter of a simplex $\sigma^M = [x_0, x_1, \dots, x_M]$ is defined by

$$b(\sigma^M) = \frac{1}{M+1} \sum_{i=0}^M x_i \quad (16)$$

A barycentric dual lattice $\tilde{\chi}$ can be constructed by joining barycenters of the primal lattice, see [45]. This dual lattice is not simplicial anymore⁴.

The vertices of the barycentric *subdivision* of the simplicial complex χ are given by $b(\sigma^M)$ for *all* σ^M in χ , $M = 0, 1, \dots, N$. We denote the first barycentric subdivision (or barycentric subdivision, for short) as $\hat{\chi}$. The important point here is that $\hat{\chi}$ *is always* a simplicial complex. The oriented $(M-p)$ -simplices of $\hat{\chi}$ are given by $[b(\sigma_i^p), b(\sigma_j^{p+1}), \dots, b(\sigma_k^{p+M})]$ for all combinations where $\sigma_i^p \subset \sigma_j^{p+1} \subset \dots \subset \sigma_k^{p+M}$. In other words, the vertices of the barycentric subdivision are the barycenters of a sequence of successively higher dimensional simplices, where each successive simplex is a face of the next one. Because both the primal χ and barycentric dual $\tilde{\chi}$ complexes are subsets of the barycentric subdivision complex $\hat{\chi}$, a Whitney map on $\tilde{\chi}$ can be defined by *identifying* elements (cells) of $\tilde{\chi}$ with a corresponding chain on $\hat{\chi}$, $B_{\tilde{\chi}} : C_p(\tilde{\chi}) \rightarrow C_p(\hat{\chi})$ (barycentric map), using the natural pairing $C_p(\hat{\chi}) \rightarrow C^p(\hat{\chi})$, and the Whitney map on the cochains of $\hat{\chi}$ (union of simplices), $Wh : C^p(\hat{\chi}) \rightarrow \Phi^p(\hat{\chi})$. A lattice Hodge operator in the sense of Eqs. (11), (12) can then be constructed on a simplicial lattice and its dual by using the following composition

$$\begin{aligned} [\star]_{\tilde{\chi}\chi} &: C_p(\tilde{\chi}) \rightarrow C_p(\chi) \\ [\star]_{\tilde{\chi}\chi} &= (B_{\chi})^{-1} \circ (Rh) \circ (\star) \circ (Wh) \circ (B_{\tilde{\chi}}) \end{aligned} \quad (17)$$

and analogously for reverse map

$$\begin{aligned} [\star]_{\chi\tilde{\chi}} &: C_p(\chi) \rightarrow C_p(\tilde{\chi}) \\ [\star]_{\chi\tilde{\chi}} &= (B_{\tilde{\chi}})^{-1} \circ (Rh) \circ (\star) \circ (Wh) \circ (B_{\chi}) \end{aligned} \quad (18)$$

Note that such discrete Hodge $\star$ operators are in general not local anymore: The matrices $[\star]_{\tilde{\chi}\chi}$ and $[\star]_{\chi\tilde{\chi}}$ are sparse but not necessarily diagonal. This non-locality turns out to be a general feature in the case of arbitrary (non-orthogonal) lattices. Diagonal matrices are obtained only in particular cases by an explicit construction of orthogonal dual lattices (such as the Yee cell [54–61] or the Voronoi-Delaunay cell

⁴ Also, this is not equivalent to the standard Poincaré dual complex construction often found in the literature, which is carried out by joining barycenters of the N -dimensional simplices *only*, where N is the dimension of the space.

mentioned before [46, 61, 62]). A similar non-local character is also present (this time on the definition of discrete spatial operators or their adjoints) in discretization schemes which do not resort to a dual lattice construction [63–65].

For the B_χ and $B_{\tilde{\chi}}$ maps, we write $\sigma_i^M = \sum_k \eta_{ik}^M \hat{\sigma}_k^M$, $\tilde{\sigma}_i^M = \sum_k \tilde{\eta}_{ik}^M \hat{\sigma}_k^M$, respectively, where $M = 0, \dots, 3$, and the coefficients η_{ik}^M and $\tilde{\eta}_{ik}^M$ are equal to zero or unity (chain projections on $\hat{\chi}$). For $M = 0, 1$ we have that $\eta_{ik}^M \tilde{\eta}_{jk}^M = 0$ for any i, j, k (i.e., χ and $\tilde{\chi}$ map into disjoint subspaces of $\hat{\chi}$), but this is not true anymore for $M = 2, 3$. Both η_{ik}^M and $\tilde{\eta}_{ik}^M$ are sparse matrices. For the B_χ map (decomposition of simplices on χ into ‘smaller’ simplices on $\hat{\chi}$), there is a total of $(M+1)!$ nonzero entries on each row of the matrix η_{ik}^M . For the $B_{\tilde{\chi}}$ map (decomposition of non-simplicial cells on $\tilde{\chi}$ into simplices on $\hat{\chi}$), we still have the same total of nonzero entries on each row of $\tilde{\eta}_{ik}^M$ for the 0-cells and 1-cells ($M = 0, 1$) cases, but for the higher dimensional cells, the number of non-zero entries of $\tilde{\eta}_{ik}^M$ in general will vary (since the number of vertices on each 2-cell or 3-cell on $\tilde{\chi}$ may vary).

Using Eqs. (17)-(18), the discrete Hodge operators are written as

$$[\star_\epsilon]_{ij} = \sum_k \tilde{\eta}_{ik}^2 \int_{\hat{\sigma}_k^2} \sum_{k'} \eta_{jk'}^1 [\star_\epsilon \varphi(\hat{\sigma}_{k'}^1)] \quad (19)$$

$$[\star_\mu]_{ij} = \sum_k \eta_{ik}^2 \int_{\hat{\sigma}_k^2} \sum_{k'} \tilde{\eta}_{jk'}^1 [\star_\mu \varphi(\hat{\sigma}_{k'}^1)] \quad (20)$$

Or, in vector calculus language,

$$\begin{aligned} [\star_\epsilon]_{ij} &= \sum_k \tilde{\eta}_{ik}^2 \int_{\hat{\sigma}_k^2} \epsilon \hat{n} dS \cdot \sum_{k'} \eta_{jk'}^1 g_E [\varphi(\hat{\sigma}_{k'}^1)] = \\ &\quad \sum_k \tilde{\eta}_{ik}^2 \int_{\hat{\sigma}_k^2} \epsilon \hat{n} dS \cdot g_E [\varphi(\sigma_j^1)] \end{aligned} \quad (21)$$

$$\begin{aligned} [\star_\mu]_{ij} &= \sum_k \eta_{ik}^2 \int_{\hat{\sigma}_k^2} \mu \hat{n} dS \cdot \sum_{k'} \tilde{\eta}_{jk'}^1 g_E [\varphi(\hat{\sigma}_{k'}^1)] = \\ &\quad \int_{\sigma_i^2} \mu \hat{n} dS \cdot \sum_{k'} \tilde{\eta}_{jk'}^1 g_E [\varphi(\hat{\sigma}_{k'}^1)] \end{aligned} \quad (22)$$

where dS is the area element, $\hat{n}$ its unit normal vector, and the operator g_E represents the (canonical) isomorphism between forms and vectors given by a metric [40]. For instance, in the Euclidean case and for the

1-forms ($M = 1$) in Eqs. (21)–(22), g_E replaces the exterior derivative d in Eq. (13) by the nabla operator ∇ (this, together with the inner product with the area element dS , represents the metric in the vector calculus picture). The (arbitrary) choice of the ordinary complex (E and B) as the primal (simplicial) and the twisted complex (D and H) as the dual (non-simplicial) is evident from the above equations.

The expressions on the right of Eqs. (21)–(22) (containing a single summation) result from the fact that the primal lattice χ is already simplicial. However, these shortened expressions involve two spaces (χ and $\hat{\chi}$) instead of a single one $\hat{\chi}$, and lack the symmetry of the middle expressions with double summation which fully utilize the barycentric subdivision and where the simplicial primal lattice does not play any special role. Furthermore, they allow the elimination of any reference to χ and $\hat{\chi}$, once the coefficients η_{ik}^M and $\tilde{\eta}_{ik}^M$ are fixed, as also evident in Eqs. (19)–(20).

Another property of the barycentric subdivision important to mention here and demonstrated in [47] is that, in conjunction with Whitney interpolations on the primal lattice, the chains of the barycentric dual lattice are the assembling pieces of the surfaces for which flux conservation (2-forms) can be verified. This suggests a ‘granular’ divergence-free condition at a discrete, interelement level. Recall that the divergence-free condition is not true in general for arbitrary surfaces because of the inter-element flux leaks (note also that this aspect involves both the primal and the dual lattices simultaneously, and therefore it does not follow from $\partial^2 = 0$ on χ or $\hat{\chi}$). This also indicates that such flux leaks are irrelevant if a certain granularity is assumed for the spatial domain according to the barycentric subdivision. Integrations over domains which do not comprise chains of the barycentric subdivision are in this sense just rendered meaningless.

5. CONCLUSIONS

Aspects of the discretization of Maxwell’s equations for general simplicial lattices using differential forms and algebraic topological concepts have been discussed.

First, the treatment of the discrete counterpart to the topological part of Maxwell’s equations was reviewed. This treatment employs the known pairing between the dual spaces of cochains (discrete differential forms) and chains (geometrical elements) on a cell complex.

Then, the role of the first barycentric subdivision to establish an isomorphism between the simplicial primal complex and the non-simplicial dual complex was stressed. A key property of the barycentric

dual complex and the barycentric subdivision complex is that they are both metric-free constructions.

Under this rationale, we have shown that Whitney maps, defined on the first barycentric subdivision lattice, can be used to build discrete Hodge operators (i.e., the discretization of the metric part of Maxwell's equations encoded in the constitutive equations) for general simplicial lattices.

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