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DATA STRUCTURES FOR GEOMETRIC AND TOPOLOGICAL ASPECTS OF FINITE ELEMENT ALGORITHMS

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Abstract—This paper uses simplicial complexes and simplicial (co)homology theory to expose a foundation for data structures for tetrahedral finite element meshes. Identifying tetrahedral meshes with simplicial complexes leads, by means of Whitney forms, to the connection between simplicial cochains and fields in the region modeled by the mesh. Furthermore, lumped field parameters are tied to matrices associated with simplicial (co)homology groups. The data structures described here are sparse, and the computational complexity of constructing them is $\mathcal{O}(n)$ where n is the number of vertices in the finite element mesh. Non-tetrahedral meshes can be handled by an equivalent theory. These considerations lead to a discrete form of Poincaré duality which is a powerful tool for developing algorithms for topological computations on finite element meshes. This duality emerges naturally in the data structures. We indicate some practical applications of both data structures and underlying theory.

1. INTRODUCTION

In many algorithms for finite element applications there are computations which do not depend on the metric of the space. In these cases, once the vertex coordinates are used to ascribe an orientation (± 1) to the elements of the mesh, it is only the finite element connection matrix which is left to play a purely integer combinatorial role in the computation which handles the topological business of the algorithm. More precisely, the connection matrix alone contains a wealth of topological information about the discretized region, realizing its simplicial or cellular complex [22].

The complex is an old and venerable idea in algebraic topology and electrical circuit theory [19], but has not attracted much attention in 3-dimensional finite elements technology. Moreover, it is intimately connected to homology and cohomology theories which are an algebraic expression of how the topology of a region is tied to fields in the region and is the formalism which links fields in the continuum to lumped circuit parameters [13]. Nevertheless, the profound consequences of this algebraic structure can be seen in the computation of cuts for magnetic scalar potentials [11, 5], discretization of the magnetic helicity functional [6], and Whitney forms for finite elements [21, 9, 3]. More generally, the same data structures are related to presentations of the fundamental group of the triangulated region, sparse matrix techniques for 3-d finite elements, and, when the metric of the space is introduced, general 3-d finite element computations.

In this paper we consider finite element data structures which incarnate the simplicial chain and cochain complexes and point out a duality theorem which is a useful tool in algorithm development. The data structures tumbled out of development of finite element-based algorithms mentioned above (cuts and helicity), and this paper is a companion to [11]. Since the data structures were born in this context we make reference to it, but this does not limit their generality. In fact, the data structures are not new – some likeness of the structures described here is often found in computer graphics [4] — however we are attempting to give the motivation for their existence and a connection to the relevant physics. Furthermore, while the structures are primarily described in the context of tetrahedral discretizations, they extend to cellular discretizations (e.g. hexahedral meshes) at slightly higher time and storage complexity. That we seem to talk only about "first-order" elements is due to the fact that we are looking at the underlying connections and hence we pick the simplest and most elegant data structure. The entire discussion can be repeated for higher-order elements.

1.1. Outline

To begin, we will define the term simplicial complex. Then, noting that a finite element mesh is a simplicial complex, we will define and construct data structures which realize simplicial maps, boundary operators, and the bases of chain groups in the simplicial complex. In a sense, these will simply be a set of finite element connection matrices describing objects (simplices) in each dimension of the mesh. In Section 3 we will define the simplicial cochain complex and give realizations of the coboundary operators. This will leave us with a connection matrix from Section 2 and a coboundary operator in each dimension. In Section 4 we argue that the coboundary operators can be regarded as connection matrices for a dual complex, and underscore the duality theorem which makes sense of that notion. The rest of the paper is focused on applications in 3-d field computation. Section 4 discusses so-called Whitney forms in the context of finite elements and an application of Whitney forms to helicity in magnetic field computation. Section 5 discusses a duality theorem which is exploited in Section 6 when discussing cuts for magnetic scalar potentials. Section 6 discusses the algebra which rests on the basic structures of Sections 1–3 and relates these to lumped parameters in electrical engineering.

2. THE COMPLEX ENCODED IN THE CONNECTION MATRIX

This section begins with some definitions needed for the algebraic framework, leading to the simplicial chain complex. Since there are many good references [7, 22, 23], we do not elaborate on the technical details. Following the definitions, we show that bases for the chain groups of the complex can be constructed in a simple hierarchy of data extracted from the finite element connection matrix.

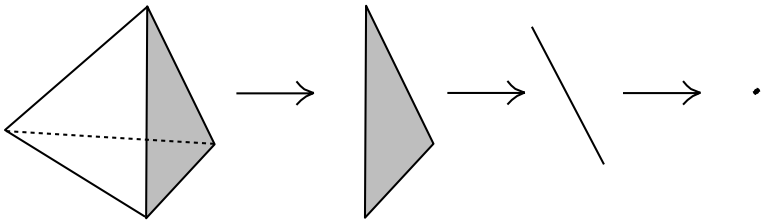

Figure 1. $3-, 2-, 1-$, and $0-$ simplices

2.1. Background and Definitions

Let $\{v_0, \ldots, v_p\}$ be an affine independent subset of points in $\mathbb{R}^n$. Affine independence means that for points $\{v_0, \ldots, v_p\}$, the set $\{v_1 - v_0, v_2 - v_0, \ldots, v_p - v_0\}$ is a linearly independent subset of $\mathbb{R}^n$. The convex set spanned by $\{v_0, \ldots, v_p\}$ is called a *p-simplex* with vertices $v_0, \ldots, v_p$ and is denoted by

$$\sigma_p =< v_0, \ldots, v_p > . \tag{1}$$

This representation is unique up to a sign which can be assigned to the permutations of the vertex indices. As illustrated in Figure 1, a tetrahedron is a 3-simplex, and its faces, edges, and nodes are 2-, 1- and 0-simplices, respectively. Note that affine independence of the vertices gives rise to barycentric coordinates on simplices so that any point in a p-simplex can be written uniquely in terms of the vertices [24, 22]. Barycentric coordinates are essential to simplex-by-simplex interpolation of functions as in the finite element method [24].

Formally, a simplex $< v_0, \ldots, v_q >$ spanned by a proper subset of $q+1$ vertices of σ_p is called a *q-face* of σ_p. A formal linear combination of p-simplices is called a *p-chain*. A simplex can be assigned an

orientation which is induced by the permutation of vertex order in $< v_0, \ldots, v_p >$, odd permutation giving negative orientation and even permutation giving positive orientation. The *boundary* of a p-simplex is the $p-1$-chain which is the following alternating sum of $p-1$-faces:

$$\partial_p \sigma_p = \partial(< v_0, \ldots, v_p >) = \sum_{i=0}^{p} (-1)^i < v_0, \ldots, v_{i-1}, v_{i+1}, \ldots, v_p > . \tag{2}$$

Note that $< v_0, \ldots, v_{i-1}, v_{i+1}, \ldots, v_p >$ is the p-face opposite vertex v_i. This definition can be used to find the boundary of a p-chain and, by (2) and direct calculation, one can verify that in general $\partial_{p-1}\partial_p(\cdot) = 0$, i.e. the boundary of the boundary of any chain is zero. The operator ∂_p determines a matrix of incidence of $p-1$-simplices with p-simplices; we will have more to say about this when discussing the coboundary operator in Section 3.2.

A *simplicial complex* K is a collection of simplices such that every face of a simplex of K is in K and the intersection of two simplices in K is a face of each of the simplices. For each $p \geq 0$, the structure formed by taking p-chains with integer coefficients in a complex K is a finitely generated free abelian group $C_p(K; \mathbb{Z})$ with basis all the p-simplices in K. This is called the p-chain group of K.

The connection between $C_p(K)$ and $C_{p-1}(K)$ is via the boundary map. Defining the boundary map on a basis of $C_p(K)$, the map extends by linearity to a map

$$\partial_p : C_p(K) \to C_{p-1}(K) \tag{3}$$

so that it is a homomorphism between the chain groups. Thus, on a complex of dimension n the collection of abelian groups $C_i(K; \mathbb{Z})$ and boundary homomorphisms give the sequence

$$0 \longrightarrow C_n(K) \xrightarrow{\partial_n} \cdots \xrightarrow{\partial_p} C_{p-1}(K) \xrightarrow{\partial_{p-1}} \cdots \longrightarrow C_1(K) \xrightarrow{\partial_1} C_0(K) \to 0. \tag{4}$$

Since Im $\partial_{p+1} \subseteq \ker \partial_p$ ($\partial_p \partial_{p+1}(\cdot) = 0$), (4) defines the *chain complex* of K, denoted by $(C_*(K), \partial)$ or simply $C_*(K)$.

As described below, the finite element connection matrix contains this basic algebraic structure. It is of interest because while Im $\partial_{p+1} \subseteq \ker \partial_p$, in general Im $\partial_{p+1} \neq \ker \partial_p$ and the part of $\ker \partial_p$ not in the inclusion contains useful information formulated concisely via homology groups and the exact homology sequence as described elsewhere [22]. However, the chain complex fits between the data which is readily available from the finite element mesh and "higher" topological structures such as the homology groups and the fundamental group of K.

2.2. From Connection Data to Chain Groups

In this paper, the prime example of the simplicial complex K is a tetrahedral finite element mesh, a tetrahedral discretization of a manifold R in $\mathbb{R}^3$ with boundary. Below we show that bases of the chain groups $C_i(K)$ related to a tetrahedral mesh can be computed from the connection matrix by "following the boundary homomorphism down the chain complex".

Consider an n-dimensional simplicial complex K with m_n n-simplices and m_0 vertices or 0-simplices. There is a total ordering of the vertices on the index set $\{0, \ldots, m_0 - 1\}$ called the global vertex ordering. There is a partial ordering of vertices such that vertices of a p-simplex are locally ordered on $\{0, \ldots, n\}$. The connection matrix is the following $m_n \times m_0$ matrix defined in terms of the global and local orderings:

$$C^i_{n,jk} = \begin{cases} 1 & \text{if global vertex } k \text{ is the } j\text{th local vertex of the } i\text{th } n\text{-simplex} \\ 0 & \text{otherwise} \end{cases} . \tag{5}$$

For a 3-d finite element mesh, C_3 is simply the connection matrix which is the output of a mesh generator. In general, (5) also defines lower dimensional subcomplexes, C_p, $0 \leq p \leq n$, or p-skeletons of a mesh. In any case, $C^i_{3,jk}$ is an $m_3 \times m_0$ matrix, but typically $m_3 = km_0$ where k is approximately 5 to 6. Since a tetrahedron has four vertices, the connection matrix C_3 has $4m_3$ nonzero entries so that the matrix is very sparse.

Because of sparsity, only the nonzero entries of the matrices C_p are stored in $m_p \times (p+1)$ arrays such that the ith row gives the (global) indices of the vertices $\sigma_{0,k}$ which define the ith p-simplex:

$$C^i_p = \{\sigma_{0,k_0}, \ldots, \sigma_{0,k_p}\} \tag{6}$$

where $0 \leq i \leq m_p - 1$ and m_p is the number of p-simplices in the mesh. This is an efficient way of storing (5), and in this form C_p also resembles a basis for the chain group $C_p(K)$ (the notation intentionally takes them to be the same). It must be emphasized that referring to the nonzero entries of the matrix in a table of pointers to the global vertex ordering gives computational efficiency and a direct link to the maps and definitions of Section 2.1.

Consider the following map which extracts the jth p-face of the kth $(p+1)$-simplex:

$$f_j(\sigma_{p+1,k}) = < \sigma_{0,0}, \ldots, \widehat{\sigma_{0,j}}, \ldots, \sigma_{0,p+1} >, \tag{7}$$

where $1 \leq i \leq m_p$, $1 \leq k \leq m_{p+1}$, $0 \leq j \leq p+1$, and $\widehat{\sigma_{0,j}}$ denotes that vertex $\sigma_{0,j}$ is omitted. Note that j and k do not uniquely specify the p-simplex since $< \sigma_{0,0}, \ldots, \widehat{\sigma_{0,j}}, \ldots, \sigma_{0,p+1} >$ may be a p-face in more than one $(p+1)$-simplex. The representation of the p-simplex by vertex ordering is unique up to orientation, but the orientation induced from the $(p+1)$-simplex can always be adopted in order to maintain consistency. In any case, the map gives the p-faces of the $p+1$-simplex when used for $0 \leq j \leq p+1$.

To build C_p, equation (7) can be used $p+2$ times on each $(p+1)$-simplex in C_{p+1} (effectively taking the boundary of each $p+1$-simplex in C_{p+1}). In each instance this requires that an algorithm which extracts the p-simplices determine from the existing data for C_p whether the result of applying (7) is a new p-simplex or one that has already been extracted. Thus, starting with C_n, it is possible to go down the complex (4) and extract all the tables C_p.

Below is an algorithm which builds C_p from C_{p+1}. The algorithm visits each p-face of every $p+1$-simplex, or $(p+2)m_{p+1}$ applications of (7).

ALGORITHM 1 (Extraction of C_p from C_{p+1})
Set C_p to be empty.
ForEach $\sigma_{p+1} \in C_{p+1}$
  ForEach p-face of σ_{p+1}
    If p-face is not in C_p *Then* add p-face to C_p.
  EndFor
Endfor

The decision at the inner loop requires a search through C_p but if implemented in an efficient data structure such as a linked list, the search is bounded by the number of times any vertex of the p-face is a vertex in a p-simplex.

2.3. Considerations for Cellular Meshes

While we focus primarily on simplicial complexes, all of the algebraic structure described is consistent for cellular complexes (e.g., hexahedral meshes). In practice, the data structures are somewhat more complicated because the vertices, while ordered on a cell, are not generally permutable. This affects the definition of (7) so that some additional information about the ordering of vertices may have to be preserved at every step of the algorithm. This also influences the way in which the algorithms are implemented — in particular, depending on application, it is most efficient to extract the 1- and

2-complexes simultaneously, 3-cell by 3-cell, in order to avoid storing extra information about vertex ordering.

3. THE COCHAIN COMPLEX

In de Rham theory, integration on manifolds in $\mathbb{R}^n$ is formulated as an algebraic structure which pairs p-chains with differential p-forms. The algebras of differential p-forms are related in a (de Rham) complex, and the related (co)homology groups are the link between lumped field parameters and topological invariants of the manifold in question [13]. An elaboration of this is given in Section 6. In the discrete setting (e.g., triangulated manifolds), cochains play a role analogous to differential forms and since simplicial (co)homology satisfies the same axioms as the de Rham cohomology, the theories are equivalent [10]. In this section we define cochains and their algebraic structure. The algebra is dual to the chain complex. Then we see how this structure also comes out of the connection matrix.

3.1. Simplicial Cochain Groups and the Coboundary Operator

Formally, the *simplicial p-cochain group* $C^p(X;\mathbb{Z})$ is the group of homomorphisms from p-chains to (for the present purpose) the integers:

$$C^p(X;\mathbb{Z}) = \hom(C_p, \mathbb{Z}). \tag{8}$$

$C^p(X;\mathbb{Z})$ is a $\mathbb{Z}$-module and not a vector space, but one can regard the homomorphisms as functionals on chains and denote the operation of a cochain $c^p \in C^p(X;\mathbb{Z})$ on a chain $c_p \in C_p(X;\mathbb{Z})$, by functional notation:

$$c^p(c_p) =< c^p, c_p > . \tag{9}$$

The *p-coboundary operator* d^p is the adjoint of the boundary operator. It is defined by

$$< d^p c^p, c_{p+1} >=< c^p, \partial_{p+1} c_{p+1} > . \tag{10}$$

so that

$$d^p = (\partial_{p+1})^T : C^p(X;\mathbb{Z}) \longrightarrow C^{p+1}(X;\mathbb{Z}). \tag{11}$$

From this point the p-coboundary operator is always written explicitly as the adjoint operator ∂^T_{p+1}. Equation (10) is simply a discrete

rendition of Stokes theorem on manifolds:

$$\int_{\Omega} d\omega = \int_{\partial\Omega} \omega \tag{12}$$

where ω is a differential p-form, $d\omega$ is a $p+1$-form, Ω is a $p+1$-chain, and $\partial\Omega$ is its boundary. This "generalized Stokes theorem" can be called the fundamental theorem of multivariable calculus. Since $\partial^2 = 0$, $\partial_{p+1}^T \partial_p^T(\cdot) = 0$, and there is a cochain complex:

$$0 \longleftarrow C^n(K) \xleftarrow{\partial_n^T} \cdots \xleftarrow{\partial_p^T} C^{p-1}(K) \xleftarrow{\partial_{p-1}^T} \cdots \longleftarrow C^1(K) \xleftarrow{\partial_1^T} C^0(K) \longleftarrow 0. \tag{13}$$

3.2. Coboundary Data Structures

Since the coboundary operator is the adjoint of the boundary operator, it can be formulated in terms of pairs of simplices (σ_p, σ_{p-1}) and their "incidence numbers. Consider a p-simplex $\sigma_p =< v_o, \ldots, v_p >$ and a $p-1$-face of σ_p, $\sigma_{p-1} =< v_0, \ldots, \widehat{v}_j, \ldots, v_p >$. Let π be a permutation function on $\{0, \ldots, p\}$, then

$$(\operatorname{sign}\pi)\sigma_p =< v_{\pi 0}, \ldots, v_{\pi p} >=< v_j, v_0, \ldots, v_{j-1}, v_{j+1}, \ldots, v_p > \tag{14}$$

where $\operatorname{sign}\pi = \pm 1$ depending on the parity of π. When $\sigma_{p-1,j}$ is a face of $\sigma_{p,i}$, $\operatorname{sign}\pi_{ij}$ is a nonzero entry in a p-simplex–$p-1$-simplex incidence matrix.

The coboundary operator ∂_p^T can be represented by storing only the nonzero entries of ∂_p^T, $\operatorname{nz}(\partial_p^T)$, and referencing each $p-1$-simplex to the p-simplices in which the $p-1$-simplex is a face in sets of pairs

$$\operatorname{nz}(\partial_p^T(\sigma_{p-1,j})) = \{(\sigma_{p,i}, \operatorname{sign}\pi_{ij}) | \sigma_p \in C_p(K)\} \tag{15}$$

where $\sigma_{p,j}$ need only be referenced by its global number j. Since a p-simplex has $p+1$ $p-1$-faces, every p-simplex is found in $p+1$ of the sets described in (15). This is equivalent to saying that there are $p+1$ nonzero entries per column in ∂_p^T.

In general (15) can be implemented efficiently in a linked list so that ∂_p^T becomes a list of linked lists. In the codimension 1 case (∂_n^T), an $n-1$-simplex is shared by at most two n-simplices and there is no need to store $\operatorname{sign}\pi_{ij}$ explicitly since the data can be indexed by the incidence number as follows:

$$\operatorname{nz}(\partial_n^T(\sigma_{n-1,j})) = \{(\sigma_{n,i} | \operatorname{sign}\pi_{ij} = 1), (\sigma_{n,l} | \operatorname{sign}\pi_{lj} = -1)\} \tag{16}$$

We will simply denote the data structure which contains (15) for all $p-1$-simplices as ∂_p^T and generate it by the following algorithm:

ALGORITHM 2. (Construction of ∂_p^T)
Set ∂_p^T to be empty.
ForEach $\sigma_{p-1} \in C_{p-1}$ (m_{p-1} $p-1$-simplices)
  ForEach σ_p such that $\operatorname{sign} \pi_{ij} \neq 0$
    augment list for σ_{p-1} with $(\sigma_p, \operatorname{sign} \pi)$.
  EndFor
EndFor

At first sight, the inner loop of algorithm 2 seems to require a search through all of the C_p data structure for each case where σ_{p-1} is a $p-1$-face. In practice the searching can be avoided by performing the augmentation procedure each time the $p-1$-simplex is encountered in the inner loop of algorithm 1. With an efficient data structure implementation, reaching the point where the ∂_p^T list is augmented is bounded by the number of times σ_p is a p-face.

4. APPLICATION: WHITNEY FORMS

Recent years have seen the growing use of so-called Whitney 1-forms or edge elements for a variety of finite element computations. The general idea comes from Whitney [27, 26] and was developed in [9, 21] to which we refer for proofs. It starts with a linear Whitney map which makes piecewise linear differential q-forms from simplicial q-cochains:

$$W : C^q(K) \to L^2\Lambda^q(X) \tag{17}$$

where X is a compact oriented C^∞ Riemannian manifold of dimension n, $L^2\Lambda^q(X)$ is the space of square-integrable de Rham C^∞ differential q-forms on X, and K is a simplicial triangulation of X. Let μ_i be barycentric coordinates corresponding to vertices v_i in K. The basic form $W\sigma \in L^2\Lambda^q(X)$ on a q-simplex σ, is defined as

$$\begin{array}{ll} W\sigma = q! \sum_{k=0}^{q} (-1)^k \mu_{i_k} \, d\mu_{i_0} \wedge \ldots \wedge \widehat{d\mu_{i_k}} \wedge \ldots \wedge d\mu_{i_q} & q > 0 \\ W(v_i) = \mu_i & q = 0 \end{array} \tag{18}$$

where $\wedge$ denotes the wedge product for differential forms and, as in Section 2.2, $\widehat{\cdot}$ denotes that the differential is excluded. Note that the construction of this q-form corresponds neatly to the process of extracting $q-1$-simplices from q-simplices in Section 2.2. We mention two properties of the Whitney map:

(i) $W\partial^T c = dWc$ for $c \in C^q(K)$ where $\partial^T c \in C^{q+1}(K)$ is the simplicial coboundary of c. The exterior derivative $d : \Lambda^q \to \Lambda^{q+1}$ applied to Wc is well-defined in this case.

(ii) Let $<,>$ denote the pairing of $C_q(K)$ and $C^q(K)$ as in (9). Then

$$\int_{c_q} Wc^q =< c^q, c_q > \tag{19}$$

for every cochain $c^q \in C^q$ and chain $c_q \in C_q(K)$.

The first property is significant because it implies that the simplicial cohomology groups of K and the de Rham cohomology group of X (see Section 6) are isomorphic.

In addition to the Whitney map (17), there is a de Rham map

$$R : L^2\Lambda^q(X) \to C^q(K) \tag{20}$$

which is defined on a basis of chains by

$$\int_{c_q} \omega =< c^q, c_q > \tag{21}$$

and the second property of the Whitney map ensures that

$$RW = I \tag{22}$$

where I is the identity map. The convergence $WR \to I$ as a mesh is refined is a special case of both finite element theory and Whitney's program, but this obvious connection does not seem to exist outside of computational electromagnetics and the work of Dodziuk [8, 9] and Müller [21].

For $c, c' \in C^q(K)$, an inner product can be defined:

$$(c, c') = \int_X Wc \wedge *Wc' = (Wc, Wc'). \tag{23}$$

This is nondegenerate by the property of the de Rham map. Although there is no obvious metric inherent to the simplicial complex K, this inner product inherits a metric from X through the Whitney map. As a mesh is refined, the inherited metric in the inner product converges to the (Riemannian) metric on X.

4.1. Example: The Helicity Functional

For finite element computations of magnetic fields, a Whitney 1-form can be used to discretize the magnetic field intensity. Namely,

$$\omega = \mathbf{H} \cdot dr. \tag{24}$$

Then, on a 1-simplex,

$$h_{ij} = \int_{v_i}^{v_j} \omega \tag{25}$$

define the variables of a 1-cochain for ω. In this formulation, it is interesting to note that the contribution of the so-called helicity density $\omega \wedge d\omega$ to the finite element "stiffness" matrix is independent of metric and constitutive laws [15]. In particular, the contribution of the helicity on a tetrahedron to the stiffness matrix is

$$\frac{1}{2}\int_{\sigma_3} \omega \wedge d\omega = \frac{1}{6}(h_{01}h_{23} - h_{02}h_{13} + h_{03}h_{12}) \tag{26}$$

The righthand side is a quadratic form which remains invariant by the action of the Lie group $SL(4, \mathbb{R})$ associated with piecewise linear volume-preserving diffeomorphisms.

5. THE DUAL COMPLEX AND DISCRETE POINCARÉ DUALITY FOR (CO)CHAINS

One reason for developing the coboundary data structures is to make use of a duality relation which relates cochains of the simplicial complex K to chains on the dual complex of K. A thorough development of the dual chain complex of K (c.f. [22]) usually starts with the first barycentric subdivision of K and construction of "blocks" in the subdivision which are dual to the p-simplices of K where the dual blocks are unions of certain sets of open simplices in the subdivision.

Although the definition of the dual complex [22] relies on some geometry, the incidence data for the dual complex can be recovered from the coboundary data structures of the simplicial complex [25], so we will formally define the dual chain complex DK with the following construction. The *dual complex* of a simplicial complex K, is a cell complex DK obtained by identifying p-simplices on K with $(n-p)$-cells. In general DK is not a simplicial complex, so it is necessary to use the terminology of cells. However it is possible to formulate a complex $C_*(DK)$ as previously done for K in (4).

In explicit terms, we identify 3-simplices with 0-cells (vertices of DK), 2-simplices with 1-cells (edges), 1-simplices with 2-cells (faces) and 0-simplices with 3-cells. Since the coboundary data structures already contain the incidence of p-simplices in $p+1$-simplices, these can be reinterpreted on the dual complex as the boundaries of $n-p$-cells. For example, the entries of (16) can be regarded as the 0-cells incident to a 1-cell in DK which passes "through" the barycenter of

$\sigma_{2,j}$. Equation (15) is interpreted as the boundaries of 2- and 3-cells (∂_1^T and ∂_2^T respectively) in DK associated with $(3-2)$- and $(3-3)$-simplices, respectively, in K.

A useful form of Poincaré duality formalizes the connection between ∂_p^T and boundaries of $(n-p)$-cells in DK seen in the data structures. It establishes a duality between cochains in K and chains in DK. While the complexes $C_p(K)$ and $C^p(K)$ are duals by definition, there exists a nondegenerate bilinear "intersection pairing"

$$I : C_p(DK) \times C^{n-p}(K) \longrightarrow \mathbb{R}. \tag{27}$$

This leads to the duality

$$C_p(DK) \cong C^{n-p}(K) \tag{28}$$

since both are duals of $C_{n-p}(K)$ [22]. Comparison of the chain complexes $C^*(K)$ and $C_*(DK)$ in light of this duality says that boundary and coboundary operators can be identified:

$$\partial_{p+1}^T = \breve{\partial}_{n-p} \tag{29}$$

where $\breve{\partial}$ denotes the boundary operator on DK. The same identification is seen in the data structures. Hence, for the price of extracting the cochain complex from the connection matrix, we have learned everything about the dual chain complex.

6. APPLICATIONS: SIMPLICIAL (CO)HOMOLOGY AND CUTS FOR SCALAR POTENTIALS

So far we have spelled out the simplicial consequences of the finite element connection matrix. In this section we look at two applications of simplicial (co)chain complexes and Poincaré duality to see how they beneficial in 3-d finite element computation.

6.1. Simplicial (Co)Homology

The chain complex is readily available from the connection matrix, but for many purposes it is merely the starting point. In this section we consider how homology groups follow from the chain complex and see how they algebraically expose the lumped parameters of electrical engineering (e.g., current, voltage, flux) which come about from integration on p-chains.

For the boundary homomorphism ∂_p in equation (3), we call $\ker \partial_p = Z_p(K)$ the *p-cycles* in K and $\operatorname{Im} \partial_{p+1} = B_p(K)$ the *p-boundaries* in K. Both $Z_p(K)$ and $B_p(K)$ are subgroups of $C_p(K)$,

and furthermore, $B_p(K) \subseteq Z_p(K) \subset C_p(K)$. This is true since if $\beta \in B_p(K)$ then $\beta = \partial_{p+1}\alpha$, for some $\alpha \in C_{p+1}(K)$, but $\partial_p \partial_{p+1}\alpha = 0$ says that $\beta \in \ker \partial_p$, i.e., $\beta \in B_p(K)$.

In general it is interesting to ask when is a p-cycle not a p-boundary. This information is summarized in the pth simplicial homology group of K, $p \geq 0$, defined as the quotient group

$$H_p(K) = \frac{Z_p(K)}{B_p(K)} = \frac{\ker \partial_p}{\text{Im } \partial_{p+1}}. \tag{30}$$

This quotient group consists of equivalence classes of cycles c such that $\partial c = 0$ but c is not a boundary. Two p-cycles a and b are in the same equivalence class if they satisfy the equivalence relation:

$$[a] \sim [b] \Longleftrightarrow a - b = \partial c_{p+1}, \tag{31}$$

where c is $p+1$-chain and $[a]$ denotes the homology class of a. The rank of $H_p(K)$ is the number of independent equivalence classes in the group and is known as the pth Betti number of K, denoted by $\beta_p(K)$; intuitively, $\beta_0(K)$ counts the number of connected components of K, and $\beta_1(K)$ counts the "number of holes in K" [20, 12, 11].

Calling $Z^p(X;\mathbb{Z}) = \ker \partial_p^T$ the group of p-cocycles, and $B^p(X;\mathbb{Z}) = \text{Im } \partial_{p-1}^T$ the group of p-coboundaries, the pth cohomology group is:

$$H^p(X;\mathbb{Z}) = \frac{Z^p(X;\mathbb{Z})}{B^p(X;\mathbb{Z})} = \frac{\ker \partial_{p+1}^T}{\text{Im } \partial_p^T}. \tag{32}$$

To make the connection with lumped parameters, we also need to introduce relative homology groups. Let L be a subcomplex of K, that is a simplicial complex contained in K. Then the pth relative simplicial homology group of K "modulo" L is

$$H_p(K, L;\mathbb{Z}) = H_p(C_*(K)/C_*(L);\mathbb{Z}), \tag{33}$$

that is, the homology of the quotient of the two complexes. In particular, if $L = \partial K$, two p-cycles from an equivalence class in $H_p(K, \partial K)$ form a p-boundary in K when taken in combination with a p-chain in ∂K. Relative cochains (with integer coefficients) are defined by

$$C^p(K, L;\mathbb{Z}) = \hom(C_p(K, L), \mathbb{Z}) \tag{34}$$

so that the pth relative cohomology group is

$$H^p(K, L;\mathbb{Z}) = \frac{\ker \partial_p^T}{\text{Im } \partial_{p+1}^T} \tag{35}$$

	Electrostatics	*Magnetostatics*
Parameter	voltage, V	flux, ϕ
Relative cohomology group	$H^1(\Omega, \partial\Omega)$	$H^2(\Omega, \partial\Omega)$
Parameter	charge, Q	current, I
Absolute cohomology group	$H^2(\Omega)$	$H^1(\Omega)$
Entries of an energy quadratic form normalized to charges or currents	$C_{ij}^{-1} = \frac{V}{Q} = \frac{\int_{c_j} \mathbf{E}_i \cdot dl}{\oint_{S_i} \mathbf{D}_i \cdot ds}$ $[S_i] \in H_2(\Omega)$ $[c_j] \in H_1(\Omega, \partial\Omega)$	$L_{ij} = \frac{\phi}{I} = \frac{\int_{S_i} \mathbf{B}_j \cdot ds}{\oint_{c_j} \mathbf{H}_j \cdot dl}$ $[S_i] \in H_2(\Omega, \partial\Omega)$ $[c_j] \in H_1(\Omega)$

Table 1. (Co)homology groups to "lumped parameters" in electro- and magnetostatics

where $\partial_p^T : C^p(K, L; \mathbb{Z}) \to C^{p+1}(K, L; \mathbb{Z})$.

Table 1 outlines the relation of these (co)homology groups to "lumped parameters" in electro- and magnetostatics. For electrostatics, Ω is the charge-free region and for magnetostatics, Ω is the region free of conduction currents.

Finally, we note that Poincaré-Lefschetz duality on chains "descends" to the (co)homology groups, that is, $H_p(DK) \cong H^{n-p}(K, \partial K)$.

6.2. Cuts for Magnetic Scalar Potentials

In "magnetoquasistatics", displacement current is ignored in Ampére's law, and the magnetic field is described by

$$\operatorname{curl} \mathbf{H} = \mathbf{J}. \tag{36}$$

In nonconducting regions $\mathbf{J} = 0$ and one may ask if $\mathbf{H} = -\operatorname{grad} \psi$ where ψ is a single-valued scalar potential defined in the nonconducting region. In general ψ is multivalued since Ampére's law shows that

$$I = \oint_{c_i} \operatorname{grad} \psi \cdot dl \neq 0 \tag{37}$$

if $I \neq 0$ and c_i is a closed path linking the current I. For reasons of computational cost and numerical analysis, it is still worthwhile to pursue the scalar potential in 3-d if one can introduce cut surfaces and impose a discontinuity across the cuts in order to make the potential single-valued. Informally, cuts are orientable surfaces embedded in the

current-free region such that when integrating $\mathbf{H} \cdot dl$ around a closed path which links current, the path must pass through the cuts. Cuts coincide with the flux measurement surfaces S_i in the right column of table 1 [11].

The existence of cuts as compact, embedded, orientable manifolds in R can be formulated via a constructive proof which gives an algorithm for computing them on finite element meshes which are triangulations of the nonconducting region [14]. There are many facets to the algorithm, but here we touch on only one. The first step to computing a set of cuts for a mesh is to compute a set of topological constraints which represent a set of generators for classes in $H_2(K, \partial K)$ [11]. By the Poincaré-Lefschetz duality of Section 4 this problem can be phrased as finding a basis for classes in $H^1(DK)$, and reduces to finding a basis of the nullspace of ∂_2^T, or a set of vectors $\{\zeta_1, \ldots \zeta_{\beta_1}\}$ satisfying

$$\partial_2^T \zeta_i = 0 \tag{38}$$

subject to Im $\breve{\partial}_0^T = 0$ [11]. The problem is motivated strictly by topological considerations at every step and requires the data structures C_3, C_2, ∂_3^T, ∂_2^T, ∂_1^T of Sections 2 and 3 and the duality of Section 4 for the computation.

7. CONCLUSION

Once a tetrahedral finite element mesh is identified as the triangulation of a 3-manifold with boundary, simplicial complexes give a systematic and general way for creating and organizing finite element data structures. The simplicial chain and cochain complexes are the bridge between the topology of the manifold, vector fields in the region, and structures from algebraic topology which are useful for finite element computation. The data structures are the most natural for using Whitney elements, in particular Whitney edge elements. Helicity functionals and cuts for magnetic scalar potentials are good examples of applications where the metric of the space and the topology can be separated. In these contexts, the data structures provide a high degree of computational efficiency.

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Table of notation

$[\cdot]$	Equivalence class of $\cdot$.
$\beta_p(R)$	pth Betti number, $\beta_p(K) = \text{Rank } H_p(R)$.
∂	Boundary operator.
∂^T	Coboundary operator.
$\breve{\partial}$	Boundary operator on dual mesh.
μ_i	Barycentric coordinates, $1 \leq i \leq 4$.
μ	Magnetic permeability.
π	Permutation map.
$\sigma_{p,i}$	ith p-simplex in simplicial complex K.
ψ	Magnetic scalar potential.
$\mathbf{B}$	Magnetic flux density vector.
B^p	p-coboundary group.
B_p	p-boundary group.
C^i_{jk}	Connection matrix, $1 \leq i \leq m_3$, $1 \leq j \leq 4$, $1 \leq k \leq m_0$.
C_p	pth chain group.
C_p	Data structure for basis of C_p.
d	Coboundary operator.
$\mathbf{D}$	Electric displacement field.
$\mathbf{E}$	Electric field.
$\mathbf{H}$	Magnetic field intensity.
$H^p(R;\mathbb{Z})$	pth cohomology group of R with coefficients in $\mathbb{Z}$.
$H_p(R;\mathbb{Z})$	pth homology group of R, coefficients in $\mathbb{Z}$.
$H^p(R,\partial R;\mathbb{Z})$	pth cohomology group of R relative to ∂R, coefficients in $\mathbb{Z}$.
$H_p(R,\partial R;\mathbb{Z})$	pth homology group of R relative to ∂R, coefficients in $\mathbb{Z}$.
$\mathbf{J}$	Current density vector.
K	Simplicial complex.
DK	Dual cell complex of simplicial complex K.
$L^2\Lambda^q(X)$	Space of square-integrable differential q-forms on manifold X.
m_p	Number of p-simplexes in a triangulation of R.
$\breve{m}_p$	Number of p-cells in dual complex.
n_p	Number of p-simplexes in a triangulation of ∂R.
$\mathcal{O}(\cdot)$	Order$(\cdot)$.
R	de Rham map, $R : L^2\Lambda^q(X) \to C^q(K)$.
v	vertex.
W	Whitney map $W : C^q(K) \to L^2\Lambda^q(X)$.
X	Riemannian manifold.
z^p	p-cocycle.
z_p	p-cycle.

REFERENCES

1. Balabanian, N. and T. A. Bickart, *Electrical Network Theory,* 80, John Wiley and Sons, New York, 1969.
2. Bamberg, P. and S. Sternberg, *A Course in Mathematics for Students of Physics: 2,* Ch. 12, Cambridge U. Press, NY, 1990.
3. Bossavit, A., *Computational Electromagnetism, Variational Formulations, Edge Elements, Complementarity,* Academic Press, Boston, 1997.
4. Brisson, E., "Representing geometric structures in d dimensions: Topology and order," *Discrete and Computational Geometry,* Vol. 9, 387–426, 1993.
5. Brown, M. L., "Scalar potentials in multiply connected regions," *Int. J. Numer. Meth. Eng.,* Vol. 20, 665–680, 1984.
6. Chammas, P. and P. R. Kotiuga, "Sparsity vis a vis Lanczos methods for discrete helicity functionals," *Proc. of the Third Int. Workshop on Electric and Magnetic Fields,* A. Nicolet and R. Belmans (eds.), 1996.
7. Croom, F. H., *Basic Concepts of Algebraic Topology,* Chaps. 2, 7.3, 4.5, Springer-Verlag, New York, 1978.
8. Dodziuk, J., "Combinatorial and continuous hodge theories," *Bull. AMS,* Vol. 80, 1014–1016, 1974.
9. Dodziuk, J., "Finite-difference approach to the hodge theory of harmonic forms," *Am. J. Math.,* Vol. 98, 79–104, 1976.
10. Eilenberg, S. and N. Steenrod, *Foundations of Algebraic Topology,* Princeton University Press, Princeton, New Jersey, 1952.
11. Gross, P. W. and P. R. Kotiuga, "Finite element-based algorithms to make cuts for magnetic scalar potentials: Topological constraints and computational complexity," this volume.
12. Gross, P. W. and P. R. Kotiuga, "A challenge for magnetic scalar potential formulations of 3-d eddy current problems: Multiply connected cuts in multiply connected regions which necessarily leave the cut complement multiply connected," *Electric and Magnetic Fields: From Numerical Models to Industrial Applications,* A. Nicolet and R. Belmans (eds.), 1–20, New York, 1995. *Proc. of the Second Int. Workshop on Electric and Magnetic Fields.*
13. Kotiuga, P. R., "Hodge decompositions and computational electromagnetics," Ph.D. thesis, 123, McGill University, Montreal, 1984.
14. Kotiuga, P. R., "An algorithm to make cuts for scalar potentials

in tetrahedral meshes based on the finite element method," *IEEE Trans. Magn.,* Vol. 25, 4129–4131, 1989.

15. Kotiuga, P. R., "Helicity functionals and metric invariance in three dimensions," *IEEE Trans. Magn.,* Vol. 25, 2813–2815, 1989.
16. Kotiuga, P. R., "Analysis of finite-element matrices arising from discretizations of helicity functionals," *J. Appl. Phys.,* Vol. 67, 5815–5817, 1990.
17. Kotiuga, P. R., "Topological duality in three-dimensional eddy-current problems and its role in computer-aided problem formulation," *J. Appl. Phys.,* Vol. 67, 4717–4719, 1990.
18. Kotiuga, P. R., "Essential arithmetic for evaluating three dimensional vector finite element interpolation schemes," *IEEE Trans. Magn.,* Vol. MAG-27, 5208–5210, 1991.
19. Kron, G., "Basic concepts of multidimensional space filters," *AIEE Trans.,* Vol. 78, 554–561, 1959.
20. Maxwell, J. C., *A Treatise on Electricity and Magnetism (1891),* Chap. 1, Art. 18–22, Dover, New York, 1954.
21. Muller, W., "Analytic torsion and r-torsion of riemannian manifolds," *Advances in Mathematics,* Vol. 28, 233–305, 1978.
22. Munkres, J. R., *Elements of Algebraic Topology,* 377–380, Addison-Wesley, Reading, MA, 1984.
23. Rotman, J. J., *An Introduction to Algebraic Topology,* Springer-Verlag, NY, 1988.
24. Silvester, P. and R. Ferrari, *Finite Elements for Electrical Engineers,* 2nd Ed., Cambridge U. Press, NY, 1990.
25. Whitney, H., "On matrices of integers and combinatorial topology," *Duke Math. J.,* Vol. 3, 35–45, 1937.
26. Whitney, H., "r-Dimensional integration in n-space," *Proc. of the Int. Congress of Mathematicians,* Vol. 1, 1950.
27. Whitney, H., *Geometric Integration Theory,* Princeton University Press, Princeton, New Jersey, 1957.