Notes on Discrete Exterior Calculus

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These notes are aimed at mathematics graduate students familiar with introductory algebraic and differential topology. The notes were written under the guidance of Dr. John Luecke and Dr. Jennifer Mann as part of NSF Research Training Grant DMS-0636643 at the University of Texas at Austin.

Contents

1 Introduction

1.1 Differential Forms for Physical Models

Differential forms are often presented to mathematicians as the underpinning of modern calculus. The dx familiar to calculus students, for example, is revealed to be the most basic type of 1-form. Higher order forms such as the 2-form dA and the 3-form dV are often thought of in terms of their composite 1-forms, suggesting that 1-forms are the essential building blocks of differential calculus. Delving into applied mathematics, however, one discovers that certain physical phenomena are most accurately described by differential forms of specific dimensions and to treat them as products of 1-forms or as anything else would greatly complicate their analysis.

While this has been acknowledged for some time in theoretical circles (including, for example, works by both Maxwell and Kelvin in the late 1800s) it has only recently gained traction in the modeling and simulation communities. With the advent of high-speed computing and high-level programming languages, engineers are now incorporating more differential topology concepts into their programs so that their models can benefit from a rigorous theoretical foundation.

The importance of differential forms is perhaps most evident in electromagnetics research where the main quantities of interest - potential, electric fields, magnetic fields, and current density - are best described as forms of dimension 0, 1, 2, and 3, respectively. (For those unfamiliar with these terms, a useful review of electromagnetics is the textbook [21] by Griffiths.) To see why these are truly different-dimensional phenomena, we can begin by looking at their units as shown in Table 1.

Table 1: Units Used in Electromagnetics

Quantity	Symbol	Unit	Dimension
Electric Potential	ϕ	V	0
Electric Field	$\mathbf{E}$	V/m	1
Magnetic Field	$\mathbf{B}$	$(V \cdot s)/m^2$	2
Current Density (3D)	ρ	A/m^3	3

Each variable is quantified relative to a different dimensional unit: ϕ is per point, $\mathbf{E}$ is per length, $\mathbf{B}$ is per area, and ρ is per volume. This dimensionality analysis extends to the auxiliary magnetic field $\mathbf{H}$ which is measured in A/m, a per length measurement, reflecting its complementary relationship to $\mathbf{B}$.

Dimensionality, however, is only a component of differential form based modeling. We take $\mathbf{E}$ as an example of how forms can more faithfully represent physical phenomena than, for example, vector fields. When a charge at a point x moves to point $x + v(x)$, energy is transferred by $\mathbf{E}$ depending on the displacement $v(x)$. This energy transfer is called work and experiments show that the work done is proportional to $v(x)$. Therefore, the value of $\mathbf{E}$ at x should be a linear function of $v(x)$. In the language of differential forms, this is the same as saying $\mathbf{E}$ should be a linear functional on the tangent space at x, i.e. a 1-form.[1]

We note that the information encoded by a 1-form can be captured by a vector field in a canonical way. The flat operator $\flat$ converts vector fields to forms and the sharp operator $\sharp$ does the reverse [1]. In our example, the vector representing $\mathbf{E}$ at x is defined to be $\vec{w}(x)$ such that the work done by $\mathbf{E}$ on a charge with displacement $v(x)$ is given by $w(x) \cdot v(x)$. The linear functional representing E at x is defined to be $(w(x), -)$ where $(-, -)$ indicates the dot product.

The motivation of using forms for modeling is thus based on the mathematical relationships

[1] For a primer on differential geometry applied to electromagnetism, see [11].

implied by differential topology that cannot be expressed in the language of vector fields alone. Since computational modeling must be done in a discrete manner, we turn to discrete exterior calculus to guide the discretization of form models.

1.2 What is Discrete Exterior Calculus?

Discrete Exterior Calculus (DEC) is an attempt to create from scratch a discrete theory of differential geometry and topology whose definitions and theorems mimic their smooth counterparts. A manifold is discretized as a simplicial complex and discrete k-forms are defined to be cochains on the k-dimensional simplices. The exterior derivative operator d is discretized as ∂^T, the transpose of the adjacency matrix in the appropriate dimension. Other discrete operators have more elaborate discretizations.

The main application of DEC, aside from any theoretical interest, is the creation of discrete operators for use in numerical methods for Partial Differential Equations (PDEs). While discrete operators have appeared in the literature for some time, DEC offers a unified approach to their construction, backed by the rigor of differential topology. The main steps in such an approach are as follows.

1. Write out the PDE in terms of smooth differential operators.
2. Replace the smooth domain, variables, and operators by their DEC counterparts.
3. Use DEC-based analysis to set up an appropriate linear system of equations.

The resulting linear system can then be solved by existing numerical methods to approximate solutions to the PDE.

1.3 Relevance to Biological Modeling

While DEC-based methods are useful to many modeling problems involving PDEs, they are especially relevant to PDEs arising in biological modeling at the molecular scale. Today, many methods exist for imaging molecules at scales as small as an Angstrom (1 Å$= 10^{-10}$ m) and creating computational models of them. These discrete 2- and 3-manifolds then become the domains used in simulations of biological activity not observable by any direct method. Events such as protein construction and folding, virus capsid assembly, and DNA knotting and unknotting occur at such small physical scales and rapid time scales that no known or theoretical device can record them as they are happening. However, these types of activity are governed by various PDEs, depending on the scale and context, hence a rigorous analysis suitable to large datasets and undulating shapes is required. DEC provides the theoretical backing to move these types of computational models from ad hoc approximations to robust error-analyzed algorithms.

1.4 History of Discrete Exterior Calculus

As mentioned previously, it was recognized for some time that certain physical phenomena, such as those observed in electromagnetics, are well described by differential forms. In the 1980s, researchers began to consider how this characterization could or should be used in computational models [19, 6]. As individual techniques advanced, attempts were made to unify various discretization methods, such the work of Hyman and Shashkov [28, 27, 29] on natural discretizations of the div, curl, and grad operators. Work by Hiptmair [23] and Bossavit [11, 13, 14] began to lay the foundation in computational electromagnetics for a more unified theory.

Treating discretization of differential operators entirely through the lens of exterior calculus, however, is a more recent development. For a thorough introduction to DEC theory, as well as more expansive descriptions of prior work, see Hirani [25] and Desbrun et al. [17]. DEC theory has been employed by an increasing number of authors in recent years to create mimetic operators [8, 34], develop multigrid solvers [7], solve Darcy flow problems [26], discretize Einstein's equations for general relativity [20], and geometrize elasticity [36]. Additionally, Lawrence Livermore National Laboratory has recongized DEC as the essential underpinning to its next-generation numerical methods and released a lengthy report detailing their initial implementation [16].

1.5 Comparison to Finite Element Methods

To put DEC-based PDE solvers in context, we compare them to finite element methods (FEMs), now an industry standard in applications and an area of active research. We illustrate the similarities and differences between the methods on the following general PDE problem. Given a bounded domain $\Omega \subset \mathbb{R}^n$, find $u \in V$ such that

$$Lu = f \qquad \text{on } \Omega, \tag{1}$$

where L is a linear operator, $f \in L^2(\Omega)$, and V is the appropriate solution space for the problem. For the moment, we do not specify boundary conditions. The Galerkin finite element method begins by putting (1) into a weak form. Observe that for any $v \in V$ we can compute

$$\int_\Omega (Lu)v = \int_\Omega fv.$$

Define a bilinear form $a : V \times V \to \mathbb{R}$ capturing the computation of the integral on the left and treat f as a functional $(f, \cdot)_{L^2}$ on V. Then the weak form of (1) is to find $u \in V$ such that

$$a(u, v) = (f, v)_{L^2} \quad \forall v \in V. \tag{2}$$

We clarify this reduction by a brief example.

Example 1.1. *(from [15])* Consider the PDE

$$-\frac{d^2u}{dx^2} = f \quad \text{in } (0,1) \subset \mathbb{R}^1 \text{ with } u(0) = 0.$$

The solution space is

$$V := \{v \in W_2^1(0,1) : v(0) = 0\},$$

where $W_2^1(\Omega)$ is the Sobolev space of functions in $L^2(\Omega)$ whose first derivative is also in $L^2(\Omega)$. Integrating against $v \in V$ gives

$$\int_0^1 u''v dx = \int_0^1 fv dx,$$

which after integration by parts and the boundary condition becomes

$$\int_0^1 u'v' dx = \int_0^1 fv dx.$$

Therefore, we set the bilinear form $a : V \times V \to \mathbb{R}$ in this case to be

$$a(u, v) := \int_0^1 u'v' dx.$$

It can be shown that a is a symmetric bilinear form on $W_2^1(0,1)$ and coercive on V. It is not, however, an inner product on $W_2^1(0,1)$ since $a(1,1) = 0$ (where 1 denotes the function which is identically 1 on $(0,1)$). $\Diamond$

To discretize this problem, we choose an appropriate finite dimensional subspace $V_h \subset V$ and seek an answer to the following problem: find $u \in V_h$ such that

$$a(u,v) = (f,v)_{L^2} \quad \forall v \in V_h. \tag{3}$$

Since V_h is finite-dimensional, we can fix a basis $\{\phi_i : 1 \leq i \leq n\}$ of V_h. Write $u = \sum_{j=1}^{n} U_j \phi_j$, $K_{ij} = a(\phi_j, \phi_i)$ and $F_i = (f, \phi_i)$. Set $\mathbf{U} = (U_j)$, $\mathbb{K} = (K_{ij})$ $\mathbf{F} = (F_i)$. Then solving (3) is the same as solving the matrix equation

$$\mathbb{K}\mathbf{U} = \mathbf{F}. \tag{4}$$

A proof and detailed discussion of this reduction can be found in [15].

A significant amount of care goes into the selection of V_h to ensure that the method is both well-posed and stable. **Well-posed** means the system (3) has a unique solution u_h. The more subtle question of stability asks whether u_h bears any relation to the true solution u. The method is called **stable** if there exists a constant $C > 0$ independent of h such that

$$||u - u_h||_V \leq C \inf_{w_h \in V_h} ||u - w_h||_V.$$

In other words, a method is stable if the error between the solution u to (2) and the solution u_h to (3) is bounded above uniformly by a constant multiple of the minimal approximation error for V_h. The famous Babuska inf-sup condition [5] is often used to simultaneously prove both well-posedness and stability of a finite element method and hence provide an a priori bound on solver error. Many papers have been published proving this condition for a specific finite element scheme or class of schemes. Recently, Arnold, Falk and Winther [3] have presented a unified characterization of stable solution spaces for certain classes of PDEs using the theory of differential forms.

The method of Discrete Exterior Calculus is an alternative approach which focuses on correctly discretizing the operator L instead of the solution space V. The viewpoint provided by differential geometry and topology reveals how this ought to be done. Common operators such as grad, curl, and div are all manifestations of the exterior derivative operator d in dimensions 1, 2, and 3, respectively. Equations relating quantities of complementary dimensions, such as the constitutive relations in Maxwell's equations, involve a Hodge star operator $*$ which provides the canonical mapping. The Laplacian operator Δ can be written as $\delta d + d\delta$ where δ is the coderivative operator, defined by $\delta := *d*$. Each operator has a discrete version designed to mimic the properties of its smooth counterpart. The discrete versions of the operators are written as matrices whose entries depend only on the topology and geometry of the mesh of Ω. We will give the formulation of these matrices in detail in Section 2.

To solve (1), an analysis is made as to the dimension of u as a k-form based on either the problem context (as described in Section 1.1) or the type of operator acting on u. The div operator in 3D, for example, acts on 2-forms while grad acts on 0-forms. The variable u is replaced by a vector $\vec{u}$ with one entry for each k-simplex in the mesh of Ω and the operator L is replaced by its discrete counterpart, written as a matrix $\mathbb{L}$. The load data f is converted to a vector $\vec{f}$ accordingly. This yields the equation

$$\mathbb{L}\vec{u} = \vec{f}, \tag{5}$$

which can then be solved by linear methods. The Whitney interpolant (see Section 2.8) is commonly used to compute values for u away from the k-simplices in the simplicial complex approximating Ω.

Discrete Exterior Calculus can also be used to solve (2), the weak version of the problem. Suppose that the domain Ω is a primal mesh[2] with N vertices $w_1, \dots, w_N$. Let $u_i := u(w_i)$. For any $v \in V$, let $v_i := v(w_i)$. Then we can write

$$a(u, v) = \sum_{k,m=1}^{N} \mathbb{L}_{km} u_k v_m$$

where $\mathbb{L}$ is a real symmetric matrix constructed based on the same methodology described above. We also need to approximate the right side of equation (2), that is, the L^2 inner product. For this, we need a matrix $\mathbb{M}$ such that

$$(u, v)_{L^2} \approx \sum_{k,m} \mathbb{M}_{km} u_k v_m. \tag{6}$$

Let χ denote the characteristic function of Ω so that $\chi_i = \chi(w_i) = 1$. If (6) is to hold, then in particular we should have

$$\sum_{k,m} \mathbb{M}_{km} = \sum_{k,m} \mathbb{M}_{km} \chi_k \chi_m \approx (\chi, \chi)_{L^2} = \int_{\Omega} 1 = |\Omega|$$

where $|\Omega|$ is the Lebesgue measure of Ω. Since $|\Omega|$ indicates the "quantity" or "size" of Ω in some sense, the matrix $\mathbb{M}$ is often referred to as the *mass matrix.* Combining the above statements and letting $f_i := f(w_i)$, we find that the discrete analogue of (2) is

$$\sum_{k,m} \mathbb{L}_{km} u_k v_m = \sum_{k,m} \mathbb{M}_{km} f_k v_m \quad \forall v \in V.$$

Remark 1.2. This formulation of discrete operators is only applicable when u and v are characterized by their values on the vertices of the mesh Ω. In some instances, it may be more appropriate to characterize u or v by their values on edges, faces, or some other combinatorial subset of Ω. In Section 3, we discuss such an example in detail that arises from modeling Darcy flow. $\Diamond$

2 Notation and Background

2.1 Manifold-like Simplicial Complexes

In algebraic topology, manifolds are discretized using simplicial complexes, a notion which guides the entire theory of DEC. We state the definition of simplicial complex here, along with supporting definitions to be used throughout. These definitions can be found in algebraic topology texts such as Armstrong [2] or Hatcher [22] or in Hirani's thesis [25].

Definition 2.1. A ***p*-simplex** σ^p is the convex hull of $p+1$ geometrically independent points $v_0, \dots, v_p \in \mathbb{R}^N$. That is

$$\sigma^p = \left\{ x \in \mathbb{R}^N : x = \sigma_{i=0}^{p} \mu_i v_i \quad \text{where } \mu_i \geq 0 \text{ and } \sum_{i=0}^{n} \mu_i = 1 \right\}.$$

Any simplex spanned by a (proper) subset of $\{v_0, \dots, v_p\}$ is called a **(proper) face** of σ^p. The union of the proper faces of σ^p is called its **boundary** and denoted $\mathrm{Bd}(\sigma^p)$. The **interior** of σ^p is $\mathrm{Int}(\sigma^p) = \sigma^p \backslash \mathrm{Bd}(\sigma^p)$. Note that $\mathrm{Int}(\sigma^0) = \sigma^0$. The **volume** of σ^p is denoted $|\sigma^p|$. Define $|\sigma^0| = 1$. $\Diamond$

[2] See Definition 2.9.

We will indicate that a simplex has dimension p with a superscript, e.g. σ^p, and will index simplices of any dimension with subscripts, e.g. σ_i.

Definition 2.2. A **simplicial complex** K in $\mathbb{R}^N$ is a collection of simplices in $\mathbb{R}^N$ such that

1. Every face of a simplex of K is in K.
2. The intersection of any two simplices of K is either a face of each of them or it is empty

The union of all simplices of K treated as a subset of $\mathbb{R}^N$ is called the underlying space of K and is denoted by $|K|$. $\Diamond$

Definition 2.3. A simplicial complex of dimension n is called a **manifold-like simplicial complex** if and only if $|K|$ is a C^0-manifold, with or without boundary. More precisely

1. All simplices of dimension k with $0 \leq k \leq n-1$ must be a face of some simplex of dimension n in K.
2. Each point on $|K|$ has a neighborhood homeomorphic to $\mathbb{R}^n$ or n-dimensional half-space.

$\Diamond$

Remark 2.4. Since DEC is meant to treat discretizations of manifolds, we will assume all simplicial complexes are manifold-like from here forward. We note that $|K|$ is thought of as a piecewise linear approximation of a smooth manifold M. Formally, this is taken to mean that there exists a homeomorphism h between $|K|$ and M such that h is isotopic to the identity. This homeomorphism will become relevant when we discuss different methods for defining a discrete Hodge Star in Section 2.7. In applications, however, knowing h or M explicitly may be irrelevant or impossible as K often encodes everything known about M. This emphasizes the usefulness of DEC as a theory built for discrete settings. $\Diamond$

2.2 Orientation of Simplicial Complexes

We now review how to orient a simplicial complex K. The definitions and conventions adopted here are taken from Hirani [25].

Definition 2.5. Define two orderings of the vertices of a simplex σ^p ($p \geq 1$) to be equivalent if they differ by an even permutation. Thus, there are two equivalence classes of orderings, each of which is called an **orientation** of σ^p. If σ^p is written as $[v_0, \ldots, v_p]$, the orientation of σ^p is understood to be the equivalence class of this ordering. $\Diamond$

Definition 2.6. Let $\sigma^p = [v_0, \ldots, v_p]$ be an oriented simplex with $p \geq 2$. This gives an **induced orientation** on each of the $(p-1)$-dimensional faces of σ^p as follows. Each face of σ^p can be written uniquely as $[v_0, \ldots, \hat{v}_i, \ldots, v_p]$, where $\hat{v}_i$ means v_i is omitted. If i is even, the induced orientation on the face is the same as the oriented simplex $[v_0, \ldots, \hat{v}_i, \ldots, v_p]$. If i is odd, it is the opposite. $\Diamond$

We note that this formal definition of induced orientation agrees with the notion of orientation induced by the boundary operator to be defined later. In that setting, a 0-simplex can also receive an induced orientation.

Remark 2.7. We will need to be able to compare the orientation of two oriented p-simplices σ^p and τ^p. This is possible only if at least one of the following conditions holds:

1. There exists a p-dimensional affine subspace $P \subset \mathbb{R}^N$ containing both σ^p and τ^p.

2. σ^p and τ^p share a face of dimension $p-1$.

In the first case, write $\sigma^p = [v_0, \ldots, v_p]$ and $\tau^p = [w_0, \ldots, w_p]$. Note that $\{v_1 - v_0, v_2 - v_0, \ldots, v_p - v_0\}$ and $\{w_1 - w_0, w_2 - w_0, \ldots, w_p - w_0\}$ are two ordered bases of P. We say σ^p and τ^p have the same orientation if these bases orient P the same way. Otherwise, we say they have opposite orientations. In the second case, σ^p and τ^p are said to have the same orientation if the induced orientation on the shared $p-1$ face induced by σ^p is *opposite* to that induced by τ^p. $\Diamond$

Definition 2.8. Let σ^p and τ^p with $1 \leq p \leq n$ be two simplices whose orientations can be compared, as explained in Remark 2.7. If they have the same orientation, we say the simplices have a **relative orientation** of $+1$, otherwise -1. This is denoted as $\operatorname{sgn}(\sigma^p, \tau^p) = +1$ or -1, respectively. $\Diamond$

Definition 2.9. A manifold-like simplicial complex K of dimension n is called an **oriented manifold-like simplicial complex** if adjacent n-simplices agree on the orientation of their shared face. Such a complex will be called a **primal mesh** from here forward. $\Diamond$

2.3 Dual Complexes

Dual complexes are defined relative to a primal mesh. While they represent the same subset of $\mathbb{R}^N$ as their associated primal mesh, they create a different data structure for the geometrical information and become essential in defining the various operators needed for DEC. Circumcentric subdivision is the preferred method for defining a dual complex as it best supports the theoretical constructs. We will look at an example in Section 2.13 to see how the choice of subdivision method impacts numerical calculation.

Definition 2.10. The **circumcenter** of a p-simplex σ^p is given by the center of the unique p-sphere that has all $p+1$ vertices of σ^p on its surface. It is denoted $c(\sigma^p)$. A simplex σ^p is said to be **well-centered** if $c(\sigma^p) \in \operatorname{Int}(\sigma^p)$. A **well-centered simplicial complex** is one in which all simplices (of all dimensions) in the complex are well-centered. $\Diamond$

Definition 2.11. Let K be a well-centered primal mesh of dimension n and let σ^p be a simplex in K. The **circumcentric dual cell** of σ^p, denoted $D(\sigma^p)$, is given by

$$D(\sigma^p) := \bigcup_{r=0}^{n-p} \bigcup_{\sigma^p \prec \sigma_1 \prec \cdots \prec \sigma_r} \operatorname{Int}(c(\sigma^p)c(\sigma_1)\ldots c(\sigma_r)).$$

To clarify, the inner union is taken over all sequences of r simplices such that σ^p is the first element in the sequence and each sequence element is a proper face of its successor. For $r = 0$, this is to be interpreted as the sequence σ_p only. The closure of the dual cell of σ^p is denoted $\bar{D}(\sigma^p)$ and called the **closed dual cell**. We will also use the notation $\star$ to indicate dual cells, i.e.

$$\star\sigma := \bar{D}(\sigma).$$

Each $(n-p)$-simplex on the points $c(\sigma^p), c(\sigma_1), \ldots, c(\sigma_r)$ is called an **elementary dual simplex** of σ^p. The collection of dual cells is called the **dual cell decomposition** of K and denoted $D(K)$ or $\star K$. $\Diamond$

Some examples of dual cells are shown in Figure 1 and discussed in its caption. Note that the dual cell decomposition forms a CW complex (see Munkres [31] for more on this).

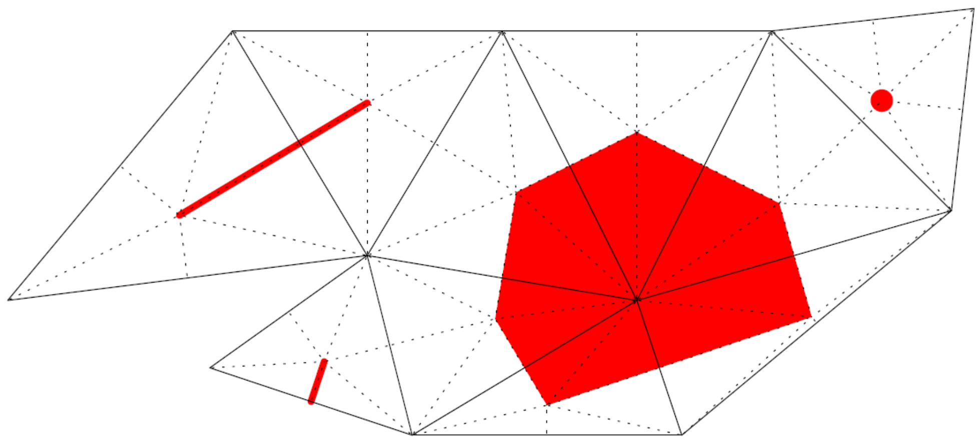

Figure 1: Figure 2.3 from Hirani [25]. The solid black lines form a simplicial complex K of dimension 2. The dotted lines show how subdivision refines the complex. A few dual cells are shown in red. The red line segments are the duals of the black 1-simplices they intersect. The red region is the dual cell of the vertex it surrounds. The red vertex is the dual of the triangle in which it sits.

2.4 Orientation of Dual Complexes

Orientation of the dual complex must be done in a such a way that it "agrees" with the orientation of the primal context. This can be done canonically since a primal simplex and any of its elementary dual simplices have complementary dimension and live in orthogonal affine subspaces of $\mathbb{R}^N$. We make this more precise and fix the necessary conventions with the following definitions.

Definition 2.12. Let K be a primal mesh with simplices $\sigma^0 \prec \sigma^1 \prec \cdots \prec \sigma^n$ and let σ^p be one of these simplices with $1 \le p \le n-1$. The **orientation** of the elementary dual simplex with vertices $c(\sigma^p), \ldots, c(\sigma^n)$ is $s[c(\sigma^p), \ldots, c(\sigma^n)]$ where $s \in \{-1, +1\}$ is given by the formula

$$s := \operatorname{sgn}\left([c(\sigma^0), \ldots, c(\sigma^p)], \sigma^p\right) \times \operatorname{sgn}\left([c(\sigma^0), \ldots, c(\sigma^n)], \sigma^n\right).$$

The sgn function was defined in Definition 2.8. For $p = n$, the dual element is a vertex which has no orientation. For $p = 0$, define $s := \operatorname{sgn}\left([c(\sigma^0), \ldots, c(\sigma^n)], \sigma^n\right)$. $\Diamond$

The above definition serves to orient all the elementary dual simplices associated to σ^p and hence all simplices in a dual cell decomposition. Further, the orientations on the elementary dual simplices induce orientations on the boundaries of dual cells in the same manner as given in Definition 2.6.

2.5 Discrete Differential Forms

Definition 2.13. Let K be a primal mesh of a smooth compact n-manifold Ω. Let K_k denote the k-simplices of K. A **k-chain** c is a linear combination of the elements of K_k:

$$c = \sum_{\sigma \in K_k} c_\sigma \sigma,$$

where $c_\sigma \in \mathbb{R}$. The set of all such chains form the **vector space of k-chains** is denoted $\mathcal{C}_k$. It has dimension $|\mathcal{C}_k|$ equal to the number of elements of K_k. A k-chain c is represented as column vector of length $|\mathcal{C}_k|$. The chains of the dual complex $\star K$ are, similarly, linear combinations of k-cells of $\star K$. $\Diamond$

Definition 2.14. A k**-cochain** ω is the dual of a k-chain:

$$\omega : \mathcal{C}_k \to \mathbb{R} \quad \text{via} \quad c \mapsto \omega(c),$$

where ω is a linear mapping. It is represented as a column vector of length $|\mathcal{C}_k|$ so that the action of ω on a k-chain c is the matrix multiplication $\omega^T c$, yielding the scalar $\omega(c)$. The set of all cochains is denoted $\mathcal{C}^k$. $\diamondsuit$

Cochains are the discrete analogues of differential forms as they can be evaluated over any k-dimensional subspace. To make this precise, we define the integration of a cochain over a chain to be the evaluation of the cochain as a function.

Definition 2.15. The **integral** of a k-cochain ω over a k-chain c is defined to be

$$\int_c \omega := \omega^T c = \omega(c).$$

Hence, the integration of ω over c is exactly the same as the evaluation of ω on c. We will also denote this pairing of cochain with chain using bracket notation:

$$< \omega, c >:= \omega(c).$$

$\diamondsuit$

2.6 Discrete Exterior Derivative

To define a discrete version of the various differential operators, we first need a discrete exterior derivative. We will use the alternative definition of the smooth exterior derivative to motivate our discrete definition. First we define the boundary operator in the discrete case.

Definition 2.16. The k**th boundary operator** denoted by ∂ takes a k-chain to its $(k-1)$-chain boundary. It is defined by its action on an oriented k-simplex:

$$\partial[v_0, v_1, \cdots, v_k] := \sum_{i=0}^{k} (-1)^i [v_0, \cdots, \widehat{v_i}, \cdots, v_k]$$

where $\widehat{v_i}$ indicates that v_i is omitted. The boundary operator is represented as a matrix of size $|\mathcal{C}_{k-1}| \times |\mathcal{C}_k|$ so that the action of ∂ on a k-chain c is the usual matrix multiplication ∂c. $\diamondsuit$

Definition 2.17. Let ω be a k-cochain. The k**th discrete exterior derivative** of ω is the transpose of the $(k+1)$st boundary operator:

$$\mathbb{D}_k = \partial^T.$$

This is also referred to in the literature as the **coboundary operator**. It is represented as a matrix of size $|\mathcal{C}_{k+1}| \times |\mathcal{C}_k|$ so that the action of $\mathbb{D}_k$ on a k-chain c is the usual matrix multiplication $\mathbb{D}c := \partial^T c$. $\diamondsuit$

The discrete exterior derivative satisfies the discrete version of Stokes' theorem.

Lemma 2.18. *Let ω be a k-cochain and $c \in \mathcal{C}_{k+1}$ any $(k+1)$-chain. Then*

$$\int_c \mathbb{D}_k \omega = \int_{\partial c} \omega.$$

Proof. By definition 2.15 we see that

$$\int_{\partial c} \omega = \omega^T \partial c = (\partial^T \omega)^T c = (\mathbb{D}_k \omega)^T c = \int_c \mathbb{D}_k \omega.$$

□

Remark 2.19. The discrete exterior derivative d as defined operates on primal cochains, however we will need to understand how it acts on dual cochains as well. According to [18] (Section 4.5), the relationship is the following:

$$\mathbb{D}_{n-k}^{Dual} = (-1)^k (\mathbb{D}_{k-1}^{Primal})^T.$$

The negative sign comes from the orientation on the dual mesh induced by the orientation on the primal mesh. ♢

2.7 Projection and Interpolation of Discrete Forms

To pass the rest of our theory between smooth and discrete settings, we will need a homeomorphism $h : K \to \Omega$ between our smooth and discrete spaces as well as maps between the smooth k-forms Λ^k and the discrete k-forms $\mathcal{C}^k$. These maps are denoted

$$\mathcal{R}_k : \Lambda^k \to \mathcal{C}^k \quad \text{and} \quad \mathcal{I}_k : \mathcal{C}^k \to \Lambda^k$$

which we will now define.

Definition 2.20. Fix a primal mesh K of an n-manifold Ω with an accompanying homeomorphism $h : K \to \Omega$. The **kth deRham map** $\mathcal{R}_k : \Lambda^k \to \mathcal{C}^k$ is defined as follows. Given $\omega \in \Lambda^k$ and $c \in \mathcal{C}_k$ a chain, define

$$(\mathcal{R}_k \omega)(c) := \int_{h(c)} \omega.$$

♢

In words, the evaluation of the k-cochain $\mathcal{R}_k \omega$ on k-chain $c \in K$ is the integral of the k-form ω over $h(c)$, the image of the c in Ω.

Lemma 2.21. *The map $\mathcal{R}$ satisfies $\mathcal{R}d = \mathbb{D}\mathcal{R}$, i.e. the following is a commutative diagram:*

$$\begin{tikzcd}
\Lambda^k \arrow[r, "d_k"] \arrow[d, "\mathcal{R}_k"] & \Lambda^{k+1} \arrow[d, "\mathcal{R}_{k+1}"] \\
\mathcal{C}^k \arrow[r, "\mathbb{D}_k"] & \mathcal{C}^{k+1}
\end{tikzcd}$$

The map $\mathcal{I}_k : \mathcal{C}^k \to \Lambda^k$ is called an interpolation map and has no canonical choice since $\mathcal{R}$ is not invertible. We can require, however, that $\mathcal{I}_k$ be chosen such that:

- $\mathcal{R}\mathcal{I} = \text{id}$ (consistency)
- $\mathcal{I}\mathcal{R} = \text{id} + O(h^s)$ (approximation)

where $h \in \mathbb{R}_{>0}$ is the partition size of the mesh and $s \in \mathbb{R}_{>0}$ is the approximation order. Note that for the Whitney interpolation maps we define next, $s = 1$.

2.8 Whitney Interpolatory Forms

The Whitney map is a commonly used interpolation operator. The idea is to construct a basis of k-forms whose support is defined relative to a particular k-simplex. The namesake of these forms is Hassler Whitney, who first described them in 1957 in [35] (page 139). Bossavit explains the relevance of Whitney forms to "mixed methods" of finite elements in [9]. We will state the general definition of a Whitney form first (as given in [10]) and then give the specific definitions for Whitney forms on subsets of a tetrahedron.

Given a primal mesh K of Ω, fix a vertex i in the mesh and let x be a point in one of the tetrahedra that shares vertex i. Let $\lambda_i(x)$ be the barycentric weight of the point x in its tetrahedron with respect to vertex i. Note that λ_i is continuous and defined on shared edges and faces with vertex i and can be extended to a function on all of Ω by defining it to be zero outside the tetrahedra containing x.

Definition 2.22. Let $\tau := [v_0, \dots, v_k]$ denote a k-simplex and $\lambda_0, \dots, \lambda_k$ the barycentric coordinate functions of τ. The **Whitney form** $\eta_\tau \in \Lambda^k$ associated to this simplex is defined by

$$\eta_\tau := k! \sum_{i=0}^{k} (-1)^i \lambda_i d\lambda_0 \wedge \dots \wedge \widehat{d\lambda_i} \wedge \dots \wedge d\lambda_k$$

where $\widehat{d\lambda_i}$ indicates that $d\lambda_i$ is omitted. Given a k-cochain $\omega \in \mathcal{C}^k$, its **Whitney interpolant** $\mathcal{I}(\omega)$ is

$$\mathcal{I}(\omega) := \sum_{\tau \in \mathcal{C}_k} \omega(\tau)\eta_\tau$$

$\diamondsuit$

We compute examples of Whitney forms in Section 2.13.

2.9 Discrete Hodge Star

Next we want to define a discrete Hodge Star. Recall that in the smooth setting, $*$ maps k-forms to $(n-k)$-forms and satisfies the relationship $\alpha \wedge *\beta = (\alpha, \beta)\mu$ where μ is the volume form. Thus, in the discrete setting, $*$ should map k-cochains to $(n-k)$-cochains and satisfy a similar relationship. We therefore have two choices on how to proceed in our definitions:

1. Define an inner product of two cochains and induce a discrete Hodge Star.
2. Define a discrete Hodge Star and induce an inner product.

We will examine each in turn. First we consider how one could define an inner product of two cochains and induce a discrete Hodge Star.

Definition 2.23. Let $a, b \in \mathcal{C}^k$. The **inner product of k-cochains** is defined by $(a, b)_{\mathcal{C}^k} := (\mathcal{I}a, \mathcal{I}b)_{\Lambda^k}$. $\diamondsuit$

This definition allows for two possible discrete Hodge stars.

Definition 2.24. The **natural** discrete $*$ is given by $\overset{\mathrm{N}}{*} := \mathcal{R} * \mathcal{I}$ so that

$$(a, \overset{\mathrm{N}}{*}\, b)_{\mathcal{C}^k} = (\mathcal{I}a, \mathcal{I}\mathcal{R} * \mathcal{I}b)_{\Lambda^k}$$

which implies $\overset{\mathrm{N}}{*}\mathcal{R} = \mathcal{R}*$. The **derived** discrete $*$ is induced by $\int a\wedge \overset{\mathrm{D}}{*} b := \int \mathcal{I}a \wedge *\mathcal{I}b$ so that

$$(a, \overset{\mathrm{D}}{*} b)_{\mathcal{C}^k} = (\mathcal{I}a, *\mathcal{I}b)_{\Lambda^k}$$

which implies $\int a\wedge \overset{\mathrm{D}}{*} a = (a,a)$ for $a \in \mathcal{C}^k$. $\Diamond$

Unfortunately, the implied property listed after each definition is not implied by the other definition. That is, $\overset{\mathrm{D}}{*}\mathcal{R} = \mathcal{R}* + O(h^s)$ and $\int a\wedge \overset{\mathrm{N}}{*} a = (a,a) + O(h^s)$. This is elucidated further by Bochev and Hyman [8]. The difficulty in this approach from a computational standpoint is in defining an inner product that can be evaluated over non-flat triangulations.

The alternative option to this route is to define a discrete Hodge Star such that an inner product can be induced. Observe that an $(n-k)$-cochain is defined by its action on $(n-k)$-chains, however there is no canonical way to associate a k-simplex to an $(n-k)$-simplex in the same primal mesh. On the other hand, there is a very natural way to associate a k-simplex in a primal mesh to an $(n-k)$-cell in the dual complex and vice versa. Hence the discrete Hodge star will be a map from discrete primal k-forms to discrete dual $(n-k)$-forms.

Definition 2.25. The **kth discrete Hodge Star** for a primal mesh K is a map from $\mathcal{C}^k(K)$ to $\mathcal{C}^{n-k}(\star K)$ represented by a matrix $\mathbb{M}_k$ of size $|\mathcal{C}_k| \times |\mathcal{C}_k|$. The formulation of the entries of $\mathbb{M}_k$ depends on the problem. $\Diamond$

Example 2.26. A general purpose definition of the Hodge Star follows. Let $1 \le k \le n-1$.[3] For a k-simplex σ^k and a discrete k-form α, suppose we wish to enforce the relationship

$$\frac{1}{|\star\sigma^k|} < *\alpha, \star\sigma^k > = \frac{1}{|\sigma^k|} < \alpha, \sigma^k > .$$

Let $\{\sigma_i^k\}$ be the k-simplices of K. Then the kth Hodge star is a diagonal matrix with

$$(\mathbb{M}_k)_{ii} := |\star\sigma_i^k| / |\sigma_i^k|. \tag{7}$$

In words, the value of $*\alpha$ on the dual cell of σ is the value of α on σ, scaled by some weight coefficient. Here the weight coefficient is the simple ratio of volumes of σ and its dual. For the Darcy Flow example in Section 3, however, we will see that a more subtle weighting choice is preferable. Note that $\mathbb{M}_k$ is computed without specifying an interpolant, as opposed to $\overset{\mathrm{D}}{*}$ and $\overset{\mathrm{N}}{*}$ which require one. $\Diamond$

We would like our discrete Hodge star to mimic the property

$$**\alpha = (-1)^{k(n-k)}\alpha$$

which holds for any smooth k-form α. We enforce this property in our discrete setting via definition.

Definition 2.27. The **kth discrete inverse Hodge Star** for a primal mesh K of dimension n is the map from $\mathcal{C}^{n-k}(\star K)$ to $\mathcal{C}^k(K)$ represented by the matrix

$$(-1)^{k(n-k)}\mathbb{M}_k^{-1}$$

$\Diamond$

[3] For $k = 0$ or n, the definition is modified only slightly to ensure consistent orientation. See [25] page 41.

2.10 Discrete Coderivative

Definition 2.28. Let ω be a k-cochain. The **discrete coderivative** of ω is the composition $*d*$ using the discrete versions of each of these operators. Hence

$$\begin{aligned}\delta_k &= (-1)^{(k-1)(n-k+1)}\mathbb{M}_{k-1}^{-1}\mathbb{D}_{n-k}^{Dual}\mathbb{M}_k \\ &= (-1)^{n(k-1)-1}\mathbb{M}_{k-1}^{-1}\mathbb{D}_{k-1}^{T}\mathbb{M}_k\end{aligned}$$

Here we have used Remark 2.19 for the definition of $\mathbb{D}_{n-k}^{Dual}$ and Definition 2.27 for the inverse Hodge star operation. The operator δ is represented as a matrix of size $|\mathcal{C}_{k-1}| \times |\mathcal{C}_k|$ so that the action of δ on a k-chain c is the usual matrix multiplication. $\diamondsuit$

We note that δ decreases form order by 1 while the exterior derivative increases form order by 1.

2.11 Discrete Vector Fields

We now address the question of how vector fields will be modeled in our discrete setting. Recall that k-cochains are valued on k-simplices and have their values elsewhere given by interpolation. Discrete vector fields will be valued on either primal or dual 0-simplices and have their values elsewhere given by interpolation.

Definition 2.29. A **discrete dual vector field** X on a primal mesh K is a map from the vertices of $\star K$ to $\mathbb{R}^N$ such that for every $\star\sigma^n$, $X(\star\sigma^n)$ is in the same minimal affine subspace as σ^n. The space of such vector fields is denoted by $\mathfrak{X}_d(\star K)$. $\diamondsuit$

For example, on a primal mesh K approximating a surface, X is valued at the circumcenter of each triangle in K. The vector value of X at a circumcenter must lie in the plane containing the triangle as this is an approximation of the tangent space. Note that this definition seems canonical enough as the tangent plane at a circumcenter is well-defined. Trying to define a vector field at vertices of a primal mesh, however, is more problematic unless the mesh is flat (meaning it is a complex of n-simplices embedded in $\mathbb{R}^n$). For more on this, see Hirani [25] Section 5.1.

2.12 Flat Operators: From Vector Fields to Forms

Vector fields and forms are closely related since both deal with vectors in the tangent space at a point. To convert a vector field into a form, we use what is known as a flat operator, denoted $\flat$. The smooth version of this operator is as follows.

Definition 2.30. Let Ω be a a Riemannian manifold with metric $(\cdot,\cdot)$ and X a vector field on Ω. The **flat** map takes X to the 1-form $X^\flat$ defined by

$$X^\flat(v) = (X, v)$$

for every point $x \in M$ and vector $v \in T_xM$. $\diamondsuit$

The definition of a discrete analogue of the flat operator depends on the answers to the following questions:

- Is the input a primal or dual discrete vector field?
- Is the interpolation of the discrete vector field primal-based or dual-based?

- Is the desired output a primal or dual discrete differential form?

These questions can be answered independently, meaning there are a total of 8 discrete flat operators [25]. For now, we only define the discrete flat operator for dual vector fields, primal-based interpolation, and primal discrete differential forms. This operator is denoted $\flat_{dpp}$ and defined as follows.

Definition 2.31. Let K be a primal mesh of dimension n and $X \in \mathfrak{X}_d(\star K)$ a dual discrete vector field on K. The **discrete DPP-flat** is a map $\flat_{dpp} : \mathfrak{X}_d(\star K) \to \mathcal{C}^1(K)$ defined by its evaluation of a primal 1-simplex σ^1 as

$$< X^{\flat_{dpp}}, \sigma^1 >= \sum_{\sigma^n \succ \sigma^1} \frac{|\star \sigma^1 \cap \sigma^n|}{|\star \sigma^1|} X(\star\sigma^n) \cdot \vec{\sigma}^1$$

where $\cdot$ is the usual dot product and $\vec{\sigma}^1$ indicates the vector with the same direction, length, and orientation as σ^1. $\diamondsuit$

Thus, the flat operator $\flat_{dpp}$ assigns a value at σ^1 based on the projection of X values at the circumcenters of adjacent n-simplices, weighted by geometrical relevance. These weights may seem somewhat arbitrary at the moment, however, they turn out to be the exact weights needed to create a discrete divergence theorem.

Definition 2.32. The **discrete divergence** div$X$ of a discrete vector field X is defined to be

$$\mathrm{div}(X) := -\delta_1 X^\flat = -\mathbb{M}_0^{-1}\mathbb{D}_0^T\mathbb{M}_1 X^\flat$$

where $\flat$ is $\flat_{dpp}$ if X is a dual discrete vector field and $\flat_{pdd}$ if X is a primal discrete vector field. $\diamondsuit$

Lemma 2.33. Discrete Divergence Theorem on a Dual n-cell. *(Hirani [25]) Let K be a primal mesh of dimension n and σ^0 a vertex in K. Let $X \in \mathfrak{X}_d(\star K)$ be a dual vector field. Then*

$$|\star \sigma^0| < \mathrm{div}(X), \sigma^0 >= \sum_{\sigma^1 \succ \sigma^0} \sum_{\sigma^n \succ \sigma^1} |\star \sigma^1 \cap \sigma^n| \left(X(\star\sigma^n) \cdot \frac{\vec{\sigma}^1}{|\sigma^1|} \right) \tag{8}$$

where the edges σ^1 are oriented so that they all point outward.

Equation (8) says the divergence of X at σ^0 is given by the flux of X through the boundary of the dual cell $\star\sigma^0$. This suggests that the formal definition of discrete divergence (which depended on our seemingly ad hoc choices for a discrete Hodge star and discrete flat operator) is in fact the exact definition required to capture the intuitive notion of divergence as a measurement of flux. This is emphasized further by the following Theorem and Corollary.

Theorem 2.34. Discrete Divergence Theorem on a Dual n-chain. *(Hirani [25]) Let c be a dual n-chain which, as a set, is a simply connected subset of $|K|$. Then the discrete divergence theorem is true over this set.*

Corollary 2.35. Uniqueness of DPP-flat *(Hirani [25]) The discrete divergence theorem on a dual n-cell is true if and only if the coefficients in the DPP-flat definition, Definition 2.31, are*

$$\frac{|\star \sigma^1 \cap \sigma^n|}{|\star \sigma^1|}.$$

Similar results hold for primal complexes with the PDD-flat.

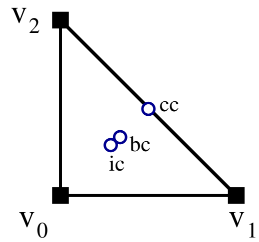

Figure 2: Reference for triangle notation.

2.13 Sample Calculation

To help illustrate how these operators are computed, we now explicitly state the discrete operators acting on a simple triangle in $\mathbb{R}^2$. Consider the triangle T in the xy plane with vertices v_0, v_1, and v_2 at (0,0), (1,0), and (0,1), respectively, as shown for reference in Figure 2. We choose edges to be oriented so that they point toward the vertex index of greater value and we assign the face a counterclockwise orientation.

First we compute the discrete exterior derivative operators as these are not geometry-dependent.

$$\mathbb{D}_0 = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix}, \qquad \mathbb{D}_1 = \begin{pmatrix} 1 & -1 & 1 \end{pmatrix}.$$

Now we turn to the Hodge star operator and begin first with a Hodge star defined directly via a dual mesh. We run into an immediate problem as T is not well-centered (see Definition 2.10). Therefore, the dual mesh, as defined in this document, cannot be constructed. In an attempt to overcome this, we consider alternative centers for the triangle: the bartycenter (the average of the three vertices) and the incenter (the center of the largest inscribed circle). These centers are:

$$\text{circumcenter (cc)} = \left(\frac{1}{2}, \frac{1}{2}\right), \quad \text{barycenter (bc)} = \left(\frac{1}{3}, \frac{1}{3}\right), \quad \text{incenter (ic)} = \left(\frac{1}{2+\sqrt{2}}, \frac{1}{2+\sqrt{2}}\right).$$

For each center, we use the definition provided in Example 2.26 to compute the Hodge star matrices $\mathbb{M}_0$ and $\mathbb{M}_1$ which act on discrete 0-forms and discrete 1-forms, respectively.

$$\mathbb{M}_0^{cc} = \begin{pmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{8} & 0 \\ 0 & 0 & \frac{1}{8} \end{pmatrix} \quad \mathbb{M}_0^{bc} \approx \begin{pmatrix} 0.167 & 0 & 0 \\ 0 & 0.167 & 0 \\ 0 & 0 & 0.167 \end{pmatrix} \quad \mathbb{M}_0^{ic} \approx \begin{pmatrix} 0.146 & 0 & 0 \\ 0 & 0.177 & 0 \\ 0 & 0 & 0.177 \end{pmatrix}$$

$$\mathbb{M}_1^{cc} = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \mathbb{M}_1^{bc} \approx \begin{pmatrix} 0.373 & 0 & 0 \\ 0 & 0.373 & 0 \\ 0 & 0 & 0.167 \end{pmatrix} \quad \mathbb{M}_1^{ic} \approx \begin{pmatrix} 0.359 & 0 & 0 \\ 0 & 0.359 & 0 \\ 0 & 0 & 0.207 \end{pmatrix}$$

The circumcentric dual gives a non-invertible $\mathbb{M}_1$ matrix since the circumcenter lies on the edge from v_1 to v_2. The barycentric and incentric duals lie interior so they give diagonal matrices with positive entries as desired.

To compute the coderivative, we use Definition 2.28 with $n = 2$ and $k = 1$. Hence $\delta_1 = -\mathbb{M}_0^{-1}\mathbb{D}_0^T\mathbb{M}_1$ yielding

$$\delta_1^{cc} = \begin{pmatrix} 2 & 2 & 0 \\ -4 & 0 & 0 \\ 0 & -4 & 0 \end{pmatrix} \quad \delta_1^{bc} \approx \begin{pmatrix} 2.236 & 2.236 & 0 \\ -2.236 & 0 & 1 \\ 0 & -2.236 & -1 \end{pmatrix} \quad \delta_1^{ic} \approx \begin{pmatrix} 2.449 & 2.449 & 0 \\ -2.029 & 0 & 1.172 \\ 0 & -2.029 & -1.172 \end{pmatrix}$$

It is evident from this example that the choice of "center" of a simplex has a significant effect on the geometry-dependent operators computed to act on that simplex.

For comparison, we now consider the approach of computing a discrete Hodge star via Whitney interpolatory forms. This is the approach employed in the thesis of Nathan Bell [7]. The Whitney 0-forms are the barycentric basis functions associated to the vertices of the triangle:

$$\begin{aligned} w_0 &= -x - y + 1 \\ w_1 &= x \\ w_2 &= y \end{aligned}$$

The three Whitney 1-forms for this example correspond to the edges (v_0, v_1), (v_0, v_2) and (v_1, v_2):

$$\begin{aligned} w_{01} &= w_0 \nabla w_1 - w_1 \nabla w_0 =< 1 - y, x > \\ w_{02} &= w_0 \nabla w_2 - w_2 \nabla w_0 =< y, 1 - x > \\ w_{12} &= w_1 \nabla w_2 - w_2 \nabla w_1 =< -y, x > \end{aligned}$$

We check two basic properties of Whitney forms for w_{01}. First, it should be identically 0 on vertices not on edge (v_0, v_1) and indeed $w_{01}(v_2) =< 0, 0 >$. Second, it should have value 1 on the edge (v_0, v_1), meaning its dot product with a unit tangent vector in the direction of the edge should equal 1. A simple calculation confirms this. The analagous properties hold for the other 1-forms. For more on Whitney form calucation, see, for instance, Chapter 5 in Bossavit [12].

Let i and j index the set $\{01, 02, 12\}$. The Hodge star is taken to be the mass matrix for the w_i, namely:

$$\mathbb{M}_1^{Whit} := (< w_i, w_j >)_{ij} = \left(\int_T w_i \cdot w_j dA \right)_{ij} = \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0 \\ \frac{1}{6} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{6} \end{pmatrix}$$

The downside to this Hodge star is that it is not diagonal meaning it is more computatinally expensive to use, especially for problems involving very large meshes. The upshot is that there is no need to choose or compute a dual mesh, thereby avoiding some potential numerical issues. Research on efficient and accurate Hodge stars is an ongoing challenge.

3 Darcy flow example

Recent work by Hirani et al. [26] uses a DEC method to model Darcy flow, a description of the flow of a viscous fluid in a permeable medium. We break down the problem using the three steps outlined in Section 1.2.

3.1 Step 1: Governing Equations

The first step is to fix the equations governing the phenomena in question and hence describe the PDE to be solved. Let $\Omega \subset \mathbb{R}^n$ be a bounded open domain with piecewise smooth boundary $\partial\Omega$ and $n = 2$ or 3. The goal is to solve for the Darcy velocity $v : \Omega \to \mathbb{R}^n$ [30] and for the pressure $p : \Omega \to \mathbb{R}$. The governing equations under the assumption of no external body force are given by

$$v + \frac{k}{\mu} \nabla p = 0 \quad \text{in } \Omega, \tag{9}$$

$$\text{div} v = \phi \quad \text{in } \Omega, \tag{10}$$

$$v \cdot \hat{n} = \psi \quad \text{on } \partial\Omega, \tag{11}$$

where $k > 0$ is the coefficient of permeability, $\mu > 0$ is the coefficient of viscosity, $\phi : \Omega \to \mathbb{R}$ is the prescribed divergence of velocity, and $\psi : \partial\Omega \to \mathbb{R}$ is the prescribed normal component of the velocity across the boundary. The functions ϕ and ψ are given as input (sometimes called the **load data**) and it is assumed that $\int_\Omega \phi d\Omega = \int_{\partial\Omega} \psi d\Gamma$.

3.2 Step 2: Domain, Variable, and Operator Replacement

The goal of this step is to write all the equations in terminology common to both smooth and discrete exterior calculus. First consider Equation (9), known as Darcy's law. The pressure p is a scalar valued function so it is immediately a 0-form. The gradient operator ∇ becomes the 0th exterior derivative operator d_0 in differential form language, meaning $\nabla p \to \mathrm{d}_0 p \in \Lambda^1$. Since v is being added to a 1-form, we must convert v from its vector field form to a 1-form, implying $v \to v^\flat$. The $\flat$ operator here is the smooth $\flat$ operator as defined in [1]. Our revised equation is then

$$v^\flat + \frac{k}{\mu}(\mathrm{d}_0 p) = 0.$$

Next, we turn to Equation (10), the continuity condition. We already know $v \to v^\flat$ and that the div operator corresponds to d_{n-1}. Since d_{n-1} must act on a $(n-1)$-form, we take the Hodge star of $v^\flat$, i.e. $\mathrm{div} v \to \mathrm{d}_{n-1}(*v^\flat)$. This implies the right side of the equation must be made into an n-form also which is accomplished by multiplying ω, the volume n-form on Ω, by the scalar data ϕ. The result is

$$\mathrm{d}_{n-1}(*v^\flat) = \phi\omega.$$

Finally, consider the boundary condition of Equation (11). The equation relates data on the boundary, i.e. information encoded in $(n-1)$-forms. Let γ be the natural volume $(n-1)$-form on the boundary, defined by the condition

$$\gamma(X_1, \ldots, X_{n-1}) = \omega(\hat{n}, X_1, \ldots, X_{n-1}),$$

for all vector fields $X_1, \ldots, X_{n-1}$ on $\partial\Omega$. Therefore, we will multiply ψ by γ for the right side of the equation. On the left side, $v \cdot \hat{n}$ becomes $*v^\flat$ by a converting from one notation to the other (for more on this see Abraham et al. [1] page 506). Thus, all three equations have now been re-written as

$$v^\flat + \frac{k}{\mu}(\mathrm{d}_0 p) = 0 \quad \text{in } \Omega, \tag{12}$$

$$\mathrm{d}_{n-1}(*v^\flat) = \phi\omega \quad \text{in } \Omega, \tag{13}$$

$$*v^\flat = \psi\gamma \quad \text{on } \partial\Omega. \tag{14}$$

For convenience, we define the volumetric flux (if $n = 3$) or area flux (if $n = 2$) as

$$f := *(v^\flat).$$

Taking $*$ of both sides of (12), we re-write the equations as

$$f + \frac{k}{\mu}(*\mathrm{d}_0 p) = 0 \quad \text{in } \Omega, \tag{15}$$

$$\mathrm{d}_{n-1} f = \phi\omega \quad \text{in } \Omega, \tag{16}$$

$$f = \psi\gamma \quad \text{on } \partial\Omega. \tag{17}$$

Having written the governing equations in the language of smooth exterior calculus, we are now ready to discretize. Unlike finite element methods, we do not explicitly define a solution space for f or p. Instead, we simply reinterpret equations (15), (16), and (17) in terms of their meanings in discrete theory.

Domain In the discrete setting, Ω is now taken to be a primal mesh K (see Definition 2.9) with ∂K defined by the usual boundary operator on simplicial complexes.

Variables The variables to be solved for are f and p. Since f measures flux through an $(n-1)$-face, it should be treated as a discrete primal $(n-1)$-form. Therefore, f becomes a column vector with $|\mathcal{C}^{n-1}|$ entries where the ith entry indicates the value of f on the ith $(n-1)$ simplex in K.[4]

Since f is a discrete primal $(n-1)$-form, equation (15) implies that $\frac{k}{\mu}(*\mathrm{d}_0 p)$ must be as well. Therefore $\mathrm{d}_0 p$ is a discrete dual 1-form and p is a discrete dual 0-form, meaning p is valued at the centers of n-simplices. Thus p is a column vector with $|\mathcal{C}_n|$ entries where the ith entry indicates the value of p at the center of the ith n simplex in K.

Operators The operator d_{n-1} becomes $\mathbb{D}_{n-1}$. The operator d_0 becomes $\mathbb{D}_0^{Dual}$ since it acts on the discrete *dual* 0-form p. Recall that

$$\mathbb{D}_0^{Dual} = (-1)^n \mathbb{D}_{n-1}^T$$

by Remark 2.19. The star operator here is acting on a discrete dual 1-form, hence, according to Definition 2.27, it is given by $(-1)^{n-1}\mathbb{M}_{n-1}^{-1}$. The appropriate choice of entries for $\mathbb{M}$ for this problem is discussed in Section 3.4.

Putting this all together, equation (15) becomes

$$f + \frac{k}{\mu}(-1)^{n-1}\mathbb{M}_{n-1}^{-1}(-1)^n \mathbb{D}_{n-1}^T p = 0. \tag{18}$$

We multiply (18) through by $-(\mu/k)\mathbb{M}_{n-1}$ to arrive at the discrete equations

$$-\frac{\mu}{k}\mathbb{M}_{n-1} f + \mathbb{D}_{n-1}^T p = 0 \quad \text{in } K, \tag{19}$$

$$\mathbb{D}_{n-1} f = \phi\omega \quad \text{in } K, \tag{20}$$

$$f = \psi\gamma \quad \text{on } \partial K. \tag{21}$$

We are now ready to write the linear system to be solved.

3.3 Step 3: Linear System

Equations (19) and (20) define the linear system

$$\begin{bmatrix} -(\mu/k)\mathbb{M}_{n-1} & \mathbb{D}_{n-1}^T \\ \mathbb{D}_{n-1} & 0 \end{bmatrix} \begin{bmatrix} f \\ p \end{bmatrix} = \begin{bmatrix} 0 \\ \phi\omega \end{bmatrix}. \tag{22}$$

Observe that the boundary conditions from (21) can be written as a list of statements of the form $f(\sigma_i^{n-1}) = a_i \in \mathbb{R}$ where σ_i^{n-1} are the $(n-1)$-simplices making up the boundary ∂K. These are incorporated into the linear system using a standard technique we now describe. Let $\mathbb{S}$ denote the four component matrix on the left side of (22) and let $\vec{z}_i$ denote the ith column in $\mathbb{S}$. Subtract $a_i\,[\vec{z}_i]$ from the right side of (22). Now remove the ith row from the entire system and remove

[4] Simplices are ordered by some fixed rule, for example, in dictionary order based on the indices of vertices. This indexing is usually fixed by the mesh data structure.

$\vec{z}_i$ from $\mathbb{S}$. Repeating this process for each boundary constraint, we reduce the dimension of the system by exactly the number of boundary elements, as desired.

We now echo the authors' observation that this matrix equation cleanly distinguishes the portions of the problem that are dependent on mesh connectivity (i.e. the blocks containing $\mathbb{D}$ matrices) and those that are dependent on the physical variable relations (i.e. the block containing the $\mathbb{M}$ matrix). Therefore, errors in physical measurements corrupt only a known part of the calculations. This is a useful property shared by some mixed finite element methods.

To implement this method, ϕ and ψ must be provided. Often ϕ is set to 0 to indicate that $\text{div} v = 0$ in Ω. Otherwise, ϕ may be set based on the solution to a known problem to test if the method captures the correct solution. Specification of ψ is an assignment of values to boundary $(n-1)$-simplices. The solver will then produce values of p at the center of each n-simplex and values of f at each edge.

For visualization and interpretation of the results, f is interpolated back to a smooth 1-form using the Whitney interpolant. Values of the 1-form are computed at specified domain points (the authors use barycenters for convenience) and the corresponding vector field is deduced. In particular, if $n = 2$ and the 1-form value at a point is $f = adx + bdy$ with a and b constant, then

$$v^\flat = -(*f) = -*(adx + bdy) = bdx - ady.$$

For the standard metric in $\mathbb{R}^2$, this means v is the vector $(b, -a)$. If $n = 3$ and the 1-form value is $f = ady \wedge dz + bdz \wedge dx + cdx \wedge dy$, then

$$v^\flat = *f = *(ady \wedge dz + bdz \wedge dx + cdx \wedge dy) = adx + bdy + cdz.$$

For the standard metric in $\mathbb{R}^3$, this means v is the vector (a, b, c). The results of a number of tests of this system are shown in the paper [26].

3.4 Hodge Star for Darcy Flow

Darcy flow modeling allows for the medium to be non-homogeneous meaning there may be different permeability constants in each n-dimensional simplex. Hence, the diagonal entry of $\mathbb{M}_{n-1}$ corresponding to an $(n-1)$-simplex σ^{n-1} ought to be weighted with respect to the permeability coefficients on either side of σ^{n-1}.

Here, the appropriate weights are determined by DEC theory in order to yield a discrete divergence theorem. Rather than take an arithmetic or geometric average, the weights are defined as follows. Let σ_+^n and σ_-^n be the n-simplices containing σ^{n-1} with permeabilities k_+ and k_-, respectively. Recall that $\star\sigma^{n-1}$ is the dual simplex to σ^{n-1}, i.e. an edge in the dual mesh. The weight is then given by

$$\frac{|\star\sigma^{n-1}|}{|\sigma^{n-1}|}\frac{|\star\sigma^{n-1}|}{k_+|\star\sigma^{n-1}\cap\sigma_+^n| + k_-|\star\sigma^{n-1}\cap\sigma_-^n|}, \tag{23}$$

where $|\cdot|$ represents the appropriate dimensional geometric measure. That this weighting scheme provides for a discrete divergence theorem is shown in [25], Figure 5.4, Section 5.5, and Section 6.1. Note that whenever $k_+ = k_-$, (23) reduces to the general purpose Hodge star defined in Equation (7).

3.5 The importance of well-centerdness

The DEC analysis used to derive this method requires that the solution $[f\ \ p]^T$ provide values of the flux f on $(n-1)$-simplices (i.e. edges in triangle meshes and triangles in tetrahedral meshes) and values of the pressure p at the circumcenters of n-simplices. For the pressure values to have any meaning, the mesh must be well-centered meaning the circumcenter of each simplex must lie in the interior of the simplex (recall Definition 2.10). Since this criterion is often violated by meshing schemes (e.g. an obtuse triangle is not well-centered), pressure is assigned instead to the barycenters of n-simplices. The authors point out that the error introduced by this modification prevents the exact representation of linear variation of pressure over the domain (see Figure 3 in the paper). If the mesh is well-centered, however, the DEC method gives excellent results (see Figures 10 and 11 in the paper, for example).

3.6 Conclusion and Future Work

At the heart of the Darcy Flow example presented above as well as many other numerical methods lies a need for a "good" discrete Hodge star. Here, "good" means both faithfully representing the properties of the smooth Hodge star at the discrete level and allowing for efficient computation via a diagonal or sparse matrix formulation.

Currently, there are two main camps on how this could be accomplished. One approach is to use Whitney forms to construct the operator, possibly allowing for lumping of elements [7] or higher order approximations [32]. The other approach is to try to construct well-centered dual meshes [33] and use barycentric duals when this is not possible. Auchmann and Kurz [4] attempt to bridge the two options by evaluating Whitney forms at the barycenters of elements to construct a Hodge star. Nonetheless, it is unlikely that there is a silver bullet solution to the problem as the needs of an individual application dictate the relative importance of the various properties a discrete Hodge Star might have. Hiptmair provides a useful albeit theoretical overview to the problem in [24].

In addition to research on discrete Hodge star operators, much work remains to be done in Discrete Exterior Calculus. On the theoretical side, other notions from smooth exterior calculus still need to be transfered to the discrete setting such as Lie derivatives (as discussed in Hirani's thesis [25]). On the computational side, few DEC-based solvers have been implemented and plenty remains to be studied regarding convergence and error analysis estimates. As a greater number of PDE problems are considered in a DEC framework, further inquiries will undoubtedly arise.

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