Discrete Exterior Calculus

Thesis by

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For

my parents Nirmal and Sati Hirani

my wife Bhavna and daughter Sankhya.

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Abstract

The language of modern mechanics is calculus on manifolds, and exterior calculus is an important part of that. It consists of objects like differential forms, general tensors and vector fields on manifolds, and operators that act on these. While the smooth exterior calculus has a long history going back to Cartan, Lie, Grassmann, Hodge, de Rham and many others, the need for a discrete calculus has been spurred on recently by the need to do computations.

This thesis presents the beginnings of a theory of *discrete exterior calculus* (DEC). This is motivated by potential applications in computational methods for field theories (elasticity, fluids, electromagnetism) and in areas of computer vision and computer graphics. One approach to approximating a smooth exterior calculus is to consider the given mesh as approximating some smooth manifold at least locally, and then defining the discrete operators by truncating the smooth ones. Another approach is to consider the discrete mesh as the only given thing and developing an entire calculus using only discrete combinatorial and geometric operations. The derivations may require that the objects on the discrete mesh, but not the mesh itself, are interpolated. It is this latter route that we have taken and this leads to a discrete exterior calculus.

Our theory includes not only discrete equivalents of differential forms, but also discrete vector fields and the operators acting on these objects. General tensors are not developed, though we suggest a possible way to do that towards the end. The presence of forms and vector fields allows us to address the various interactions between forms and vector fields which are important in applications. With a few exceptions, most previous attempts at discrete exterior calculus have addressed only differential forms, or vector fields as proxies for forms. We also show that the circumcentric dual of a simplicial complex plays a useful role in the metric dependent part of this theory. The importance of dual complexes in this field has been well understood, but with a few exceptions previous researchers have used barycentric duals.

The use of duals is reminiscent of the use of staggered meshes in computational mechanics. The appearance of dual complexes leads to a proliferation of the operators in the discrete theory. For example there are primal-primal, primal-dual etc. versions of many operators. This is of course unique to the discrete side. In many examples we find that the formulas derived from our discrete exterior calculus are identitical to the existing formulas in literature.

We define discrete differential forms in the usual way, as cochains on a simplicial complex. The discrete vector fields are defined as vector valued 0-forms, and they live either on the primal, or on the dual vertices.

We then define the operators that act on these objects, starting with discrete versions of the exterior derivative, codifferential and Hodge star for operating on forms. A discrete wedge product is defined for combining forms; discrete flat and sharp operators for going between vector fields and one forms; and discrete interior product operator and Lie derivatives for combining forms and vector fields. The sharp and flat allow us to define various vector calculus operators on simplicial meshes including a discrete Laplace-Beltrami operator.

Our development of the theory is formal in that we do not prove convergence to a smooth theory. We have tried instead to build a discrete calculus that is *self*-consistent and parallels the smooth theory. The discrete operator should be natural under pullbacks, when the smooth one is, important theorems like the discrete Stokes' theorem must be satisfied, and the operators should be local. We then use these operators to derive explicit formulas for discrete differential operators in specific cases. These cases include 2-surfaces in $\mathbb{R}^3$ built with irregular triangles, regular rectangular and hexagonal meshes in the plane, and tetrahedralization of domains in $\mathbb{R}^3$. At least in these simple but important examples we find that the formula derived from our discrete exterior calculus is identitical to the existing formula in the literature.

Numerical methods similar to those based on a discrete exterior calculus have been used in many physical problems, for example, in areas like electromagnetism, fluid mechanics and elasticity. This is due to the geometric content of many physical theories. In this thesis we give a glimpse into three fields of discrete, geometric computations, which we have developed without an exterior calculus framework. These are examples of areas which are likely to benefit from a working DEC. They include discrete shells, a Hodge type decomposition of discrete 3D vector fields on an irregular, simplicial mesh, and template matching.

One potential application of DEC is to variational problems. Such problems come equipped with a rich exterior calculus structure and so on the discrete level, such structures will be enhanced by the availability of a discrete exterior calculus. One of the objectives of this thesis is to fill this gap. An area for future work, is the relationship between multisymplectic geometry and DEC. There are many constraints in numerical algorithms that naturally involve differential forms, such as the divergence constraint for incompressibility of fluids. Another example is in electromagnetism since differential forms are naturally the fields in that subject, and some of Maxwell's equations are expressed in terms of the divergence and curl operations on these fields. Preserving, as in the mimetic differencing literature, such features directly on the discrete level is another one of the goals, overlapping with our goals for variational problems.

In future work we want to make a cleaner separation of metric independent and metric dependent parts of DEC. For example, the wedge product, pairing of forms and vector fields, interior product and Lie derivative, should all be metric independent. Divergence should depend on the metric, only through the appearance of volume form. The metric should play a role only in the definition of sharp and flat operators. In this thesis, we don't always make this distinction and sometimes use identities from smooth theory, where the metric dependence cancels. It is not clear that the same cancellation happens on the discrete side. In these cases we have also tried to give at least a partial development of a metric independent definition.

In this thesis we have tried to push a purely discrete point of view as far as possible. In fact, in various parts of the thesis we argue that this can only be pushed so far, and that interpolation is a useful device for developing DEC. For example, we found that interpolation of functions and vector fields is a very convenient device for understanding and deriving a discrete theory involving functions and vector fields. This naturally leads to the next step, that of interpolation of higher degree forms, for example using Whitney map. This is the methodology that is quite common in this field. In future work we intend to continue this interpolation point of view, especially in the context of the sharp, Lie derivative and interior product operators. Some preliminary ideas on this point of view are spread throughout the thesis.

Contents

Chapter 1

Introduction

This thesis presents the beginnings of a theory of *discrete exterior calculus* (DEC), motivated by potential applications in computational methods for field theories (elasticity, fluids, electromagnetism), and in areas of computer vision and computer graphics. This theory has a long history that we shall outline below in Section 1.3, but we aim at a comprehensive, systematic, as well as useful, treatment. Many previous works, as we shall review, are incomplete in terms of the objects and operators that they treat.

One approach to approximating a smooth exterior calculus is to consider the given mesh as approximating some smooth manifold at least locally, and then defining the discrete operators by truncating the smooth ones. Another approach is to consider the discrete mesh as the only given thing and developing an entire calculus using only discrete combinatorial and geometric operations. The derivations of the operators may require that the objects on the discrete mesh, but not the mesh itself, are interpolated. It is this latter route that we have taken and this leads to a discrete exterior calculus. General views of the subject area of DEC are common in the literature (see, for instance, Mattiussi [2000]), but they usually stress the process of discretizing a continuous theory and the overall approach is tied to this goal. However we take the point of view that the discrete theory can stand in its own right.

Applications to Variational Problems. One application is to variational problems. These arise naturally in mechanics and optimal control. In addition many problems in computer vision, image processing and computer graphics can also be posed naturally as variational problems. Some examples are template matching, image restoration, image segmentation and computation of minimal distortion maps. See, for example, Hirani et al. [2001]; Paragios [2002]; Gu [2002]; Desbrun et al. [2002]. Key ingredients for computations involving variational principles, at least in mechanics, are variational integrators designed for the numerical integration of mechanical systems, as in Lew et al. [2003]. These algorithms respect some of the key features of the continuous theory, such as their (multi)symplectic nature and exact conservation laws. They do so by discretizing the underlying variational principles of mechanics rather than discretizing the equations. It is well known (see the reference just mentioned for some of the literature) that variational problems come equipped with a rich exterior calculus structure and so on the discrete level, such structures will be enhanced by the availability of a discrete exterior calculus. One of the objectives of this thesis is to fill this gap.

Structured Constraints. There are many constraints in numerical algorithms that naturally involve differential forms, such as the divergence constraint for incompressibility of fluids. Another example is in electromagnetism, since differential forms are naturally the fields in that subject, and some of Maxwell's equations are expressed in terms of the divergence and curl operations on these fields. See Hehl and Obukhov [2000] for electromagnetism using differential forms. Preserving, as in the mimetic differencing literature, such features directly on the discrete level is another one of the goals, overlapping with our goals for variational problems.

Methodology. We believe that one way to proceed with this program is to develop a calculus on discrete manifolds which parallels the calculus on smooth manifolds. Indeed one advantage of developing a calculus on discrete manifolds is pedagogical. By using concrete examples of discrete two- and three-dimensional spaces one can explain most of discrete calculus at least formally. The machinery of Riemannian manifolds and general manifold theory from the smooth case is, strictly speaking, not required in the discrete world. The technical terms that will be used in the rest of this introduction will be defined in subsequent sections, but they should be already familiar to someone who knows the usual exterior calculus on smooth manifolds. Chapters 6 and 7 of Abraham et al. [1988] are a good standard reference.

Our development in this thesis is formal, in the sense that we choose appropriate geometric definitions of the various objects and quantities involved. We do not prove that these definitions converge to the smooth counterparts. The definitions are chosen so as to make some important theorems like the generalized Stokes' theorem true by definition, to preserve naturality with respect to pullbacks, and to ensure that operators are local. Often, an interpolation of objects is involved in reaching the discrete definition. In the cases where previous results are available, we have checked that the operators we obtain match the ones obtained by other means such as variational or other derivations. A proper study of convergence is clearly needed in the future after we have had some numerical experience with DEC.

1.1 Results of This Thesis

Our development of discrete exterior calculus includes discrete differential forms as well as vector fields, the Hodge star operator, the wedge product, the exterior derivative, as well as interior product and the Lie derivative. Our theory can be thought of as calculus on simplicial complexes of arbitrary finite dimension. We point out that the embedding of the complex can be local. We also hint at how it might generalize formulas from finite-difference theory on regular meshes. The inclusion of discrete differential forms and discrete vector fields allows us to address the various interactions between forms and vector fields which are important in applications. With a few exceptions, such as Bossavit [2003], previous attempts at discrete exterior calculus have addressed only differential forms, or have used vector fields as proxies for forms.

We use circumcentric duals of simplicial complexes in the metric parts of our theory. The importance of dual complexes in this field has been well understood, but most previous researchers have used barycentric duals. We show that circumcentric duals play a role in arriving at the metric dependent parts of a DEC theory. This includes the sharp and flat operators for going between vector fields and forms, and the Hodge star for operating on forms. The usefulness of circumcentric duality in these cases stems from the fact that the property of being normal to boundary comes automatically with circumcentric duality. This makes the expressions for fluxes very easy in terms of geometric objects like the dual cells. Indeed the importance of circumcentric duals in this context has also been known in some communities such as the mimetic differencing. But that has usually been for flat two- or three-dimensional logically rectangular meshes and only scalar and vector fields appear in that literature.

While most of the thesis is about discrete exterior calculus on a single discrete manifold we define discrete pullback between two complexes. Multiple meshes are important in applications where the mesh is changing, but the discrete pullback is important even for picking the right definition on a single complex in some cases. This is because it provides the criterion of naturality for discrete operators, i.e., commuting with pullback, which is important for a full calculus on manifold. This was pointed out to us very recently by Marco Castrillon and Jerry Marsden.

We argue in this thesis, that interpolation of objects is important for developing DEC. We use interpolation of 0-forms and vector fields viewed as vector valued 0-forms and argue that the proper development of sharp operator, and consequently of gradient and curl, requires the interpolation of 1-forms. In the Chapter on interior product and Lie derivative we argue that the interpolation of forms plays a crucial role in the derivation of discrete version of these operators. But we do not carry out this program of interpolation of higher degree forms in this thesis, leaving it for future work.

1.2 The Objects in DEC

To develop a discrete theory, one must define discrete differential forms along with vector fields and operators involving these. Once discrete forms and vector fields are defined, a calculus can be developed by defining the discrete exterior derivative ($\mathbf{d}$), codifferential ($\boldsymbol{\delta}$) and Hodge star ($*$) for operating on forms, discrete wedge product ($\wedge$) for combining forms, discrete flat ($\flat$) and sharp ($\sharp$) operators for going between vector fields and one forms and discrete interior product operator ($\mathbf{i}_X$) for combining forms and vector fields. Once these are done one can then define other useful operators. For example, a discrete Lie derivative ($\pounds_X$) can be *defined* by requiring that the Cartan magic (or homotopy) formula hold. A discrete divergence in any dimension and curl in $\mathbb{R}^3$ can also be defined. A discrete Laplace-Beltrami operator (Δ) can be defined using the usual definition of $\mathbf{d}\boldsymbol{\delta} + \boldsymbol{\delta}\mathbf{d}$. When applied to functions this is the same as the discrete Laplace-Beltrami operator (∇^2) which is the defined as $\operatorname{div} \circ \operatorname{grad}$. We define all these objects and operators in this thesis. In some cases we define the operators in multiple ways.

The discrete manifolds we work with are manifold-like oriented simplicial complexes (however we also show how DEC generalizes some finite-difference formulas on regular non-simplicial meshes). We will recall the standard formal definitions in Section 2.1 but familiar examples of simplicial complexes are meshes of triangles embedded in $\mathbb{R}^3$ and meshes made up of tetrahedra occupying a portion of $\mathbb{R}^3$. We will assume that the angles and lengths on such discrete manifolds are computed in the embedding space $\mathbb{R}^N$ using the standard metric of that space. In other words in this thesis we do not address the issue of how to discretize a given smooth Riemannian manifold and how to embed it in $\mathbb{R}^N$ since there may be many ways to do this. For example, $\mathrm{SO}(3)$ can be embedded in $\mathbb{R}^9$ with a constraint or in $\mathbb{R}^4$ using quaternions. For the purposes of exterior calculus, only local metric information is required, and we will comment in Section 2.8 on how to address the issue of embedding in a local fashion. We emphasize that we do *not* need a global embedding of the discretized manifold, since the operators of DEC are local, and intrinsic. For simplicity of presentation we don't always stress this point and often write as if a global embedding has been given.

1.3 History and Previous Work

The use of simplicial chains and cochains (defined in Chapter 3) as the basic building blocks for a discrete exterior calculus has appeared in several papers. See, for instance, Sen et al. [2000], Adams [1996], Bossavit [2002b] and references therein. These authors view forms as linearly interpolated versions of smooth differential forms, a viewpoint originating from Whitney [1957], who introduced the Whitney and de Rham maps that establish an isomorphism between simplicial cochains and Lipschitz differential forms. Similar ideas on non-simplicial meshes and from a finite-difference point of view are referred to in the papers of Hyman, Shashkov and their collaborators. See for instance Hyman and Shashkov [1997a] and the references therein. These papers however use vector fields as proxies for forms.

Discrete forms for logically rectangular meshes are defined in Chard and Shapiro [2000]. They however define only the $\mathbf{d}$ operator from exterior calculus. However it is interesting to see that the implementation of even a subset of DEC-like ideas can be interesting for computational mechanics. Cochains are discrete objects that can be paired with chains of oriented simplices or their geometric duals by the bilinear pairing of evaluation. Intuitively, the natural pairing of evaluation can be thought of as integration of the discrete form over the chain.

There is much interest in a discrete exterior calculus in the computational electromagnetics community, as represented by Bossavit [2001, 2002b,a, 2003], Gross and Kotiuga [2001], Hiptmair [1999, 2001a,b, 2002b], Mattiussi [1997, 2000], Teixeira [2001] and Tonti [2002]. This is the community that seems to have gone the furthest in terms of incorporating DEC-like ideas into their computational methods. This is perhaps because Maxwell's equations can be written purely in terms of differential forms. With the exception of some recent work of Bossavit on interior products (Bossavit [2003]) the computational electromagnetism community has used either a forms only theory or with vector fields as proxies for forms.

Many of the authors cited above, for example, Bossavit [2002b], Sen et al. [2000], Hiptmair [2002b,a], also introduce the notions of dual complexes in order to introduce the Hodge star operator. With the exception of Hiptmair, they mostly use barycentric duals. This works fine if one develops a theory of discrete forms and does not introduce discrete vector fields. We show later that to introduce discrete vector fields into the theory the notion of circumcentric duals seems to be convenient.

Other authors, such as Moritz [2000]; Moritz and Schwalm [2001]; Schwalm et al. [1999, 2001] have incorporated vector fields into the cochain based approach to exterior calculus by identifying vector fields with cochains, and having them supported on the same mesh. This may make it harder to encode physically relevant phenomena such as fluxes across boundaries that are important in some applications.

Another approach to a discrete exterior calculus is in Dezin [1995]. He defines a one-dimensional discretization of the real line in much the same way we would. However to generalize to higher dimensions he introduces a tensor product of this space. This results in logically rectangular meshes. Our calculus however is over simplicial meshes. A further difference is that like other authors in this field, Dezin [1995] does not introduce vector fields into his theory. A related effort for three-dimensional domains with logically rectangular meshes is that of Mansfield and Hydon [2001], who established a variational complex for difference equations by constructing a discrete homotopy operator. In Harrison [1993, 1999] one finds the development of a discrete calculus by extending the permitted domains of integration to include nonsmooth and fractal spaces. These papers not only develop a part of discrete calculus but also discuss convergence issues. Besides the exterior derivative, a Hodge star and Laplace-Beltrami are also defined in Harrison [1999] for very general spaces.

In computer graphics Meyer et al. [2002] define, for simplicial meshes, discrete differential geometry operators and vector calculus operators like Laplace-Beltrami. Recently Gu [2002] has done some very interesting work in applying homology and cohomology theory for some applications in graphics, such as, finding global conformal maps for arbitrary genus surfaces. However, they do not develop a discrete exterior calculus. For instance, their wedge product is the standard one (cross product) in $\mathbb{R}^3$.

Mimetic discretization (Hyman and Shashkov [1997a]) is a successful development of finite-difference and finite-volume type methods that satisfy various theorems like Stokes' theorem. It has been applied to a variety of physical problems. Once again, it is a theory that has been developed for forms only or vector fields as proxies for forms. Also, most of those methods seem to be for flat meshes. Moreover, we conjecture that a generalization of DEC for non-simplicial meshes will bring DEC and mimetic discretization closer, except that in addition one will have a theory of forms and fields with all the attendant operators, and have it for non-flat meshes as well. With the current version of DEC we have already made a start towards this, for simplicial meshes.

1.4 How This Thesis is Organized

In chapters 2-8 the preamble of each chapter, i.e. the part before the numbered sections of the chapter begin, summarizes what the chapter is about, the main new results in the chapter, the context in which the chapter fits into DEC. This is typically the content of the first or first few paragraph of each chapter's preamble. The second part of each preamble is generally a summary of what remains to be done and what is not well-understood etc. Chapter 9 is about other work and speculative work. The former consists of applications that we have done which would benefit from a DEC like framework for their future development. The latter, consists of some preliminary ideas about lattices and regular nonsimplicial complexes and general discrete tensors. In some chapters the last section is a summary and discussion section. Due to this organization of the thesis, we have not included a conclusions Chapter. The preambles and summary sections of the following chapters, and the next section of this Chapter can be read instead, to understand the scope, limitations and conclusions of this thesis.

1.5 Increasing Role of Interpolation

In this section we document our changing viewpoint about interpolation. Interpolation has been playing an increasing role as we have gained more experience with DEC. When we started work on DEC, we held the viewpoint of treating forms strictly as cochains, not only in the definition of forms, but also in the definition of operators on forms. That is, we wanted to define all the operators of exterior calculus as cochains, using only the values of the operands on chains. This was in contrast with another popular approach, such as that of Sen et al. [2000] and others, in which forms are interpolated using Whitney maps, and operators defined on the interpolated forms. An early consequence of our strictly discrete approach, was, for example the lack of associativity of wedge product, except for closed forms (Remark 7.1.4). But the straightforward interpolation approach mentioned above also suffers from not having an associative wedge product Sen et al. [2000]. Thus while this lack of associativity has consequences for the theory, we pressed ahead.

But slowly there were other signs that a strict discrete approach was inconvenient. For example, we had found a formula for a discrete flat operator without interpolating vector fields or forms. But it was found by guesswork, by requiring a discrete divergence theorem to be true. Later, we realized that if we interpolated vector fields, as interpolated vector valued 0-forms, we were able to give a derivation for the formula we had found, *and* find other types of discrete flats that we had missed. Thus the interpolation point of view seemed to be good not just for explaining existing formulas, but for finding new ones. Similarly, we found that for defining a discrete gradient, the point of view of interpolation of 0-forms inside simplices, was a useful one. Similar advantages held for other vector calculus operators as we saw in our vector field decomposition work in Tong et al. [2003].

Naturally, the question was, why stop at 0-forms ? Why not interpolate higher degree forms as well ? This was obvious when we considered sharp operator on 1-forms and interior product and Lie derivative. With the strictly discrete point of view, one can get quite far, but not all the way, it seems. We argue in this thesis that the development of a sharp, gradient, interior product and Lie derivative requires the interpolation of one and higher degree forms. The full development of this interpolation point of view is for future work.

One track for our future work, is the usual Whitney interpolation idea, studied by so many other authors. This is to interpolate forms using Whitney forms and then use the smooth operators. But we intend to use it to define operators like Lie derivative, that others have not explored. Another track we intend to explore, is if we can build higher degree forms, defined everywhere on the complex, from 1-forms. This is along the same lines as our preliminary suggestion to build general tensors by using tensor products of 1-forms as mentioned in Section 9.5.

Even while knowing the limitations of a purely discrete approach, in this thesis, we try to push the purely discrete point of view as far as possible. This is done, in part to expose the parts of DEC where interpolation is clearly the way to go. We have tried to include the basic ideas about interpolation at various places in the thesis, in preparation for our future work along this direction. This approach can be called a finite element approach to DEC. Here, the discretization of forms via the de Rham map of Section 3.3 takes a back seat and the interpolation of forms via Whitney maps or other means becomes more prominent. The operators are defined on interpolated forms, by using the smooth definitions where possible.

Various interpolation schemes can then be studied, including higher order ones. Building a higher order DEC requires that one find a closed way to construct higher degree forms from discrete 1-forms that are quadratic or higher order accurate. In any case, even in the lowest order case, with this interpolation, or finite element approach, there is no longer any need to define operators using metric information when the smooth operators do not depend on the metric. This simplifies the presentation of DEC which can then be organized into the metric-independent part like exterior derivative, wedge, interior product and Lie derivative, and the metric dependent part like sharp and flat. It is quite possible, as happened in the case of flat, that the interpolation based definition of some operators will eventually result in a purely discrete definition. This is because the operators are all local and many involve derivatives. The identities from smooth theory that we were forced to adopt as definitions in some cases, then become theorems in such a discrete theory.

The detailed exploration of such an interpolation based DEC, in which interpolation of higher degree forms, and not just of 0-forms, plays a prominent role, is left for our immediate future work.

Chapter 2

Primal and Dual Complexes

Results: In our formulation of discrete exterior calculus, K, an oriented manifold-like simplicial complex (defined below) discretizes a portion of M, the triangulable Riemannian n-manifold of interest. The starting point for our calculus *is* the given complex K. In this chapter we give basic definitions related to simplicial complexes and their dual cell complexes and orientations of these. We have found a simple geometric interpretation of orientation of duals which we give in this chapter. In contrast, in algebraic topology the definition of dual orientation usually requires some knowledge of homology and relative homology theory. The requirement of orientability may not be a problem in practice. This is because the operators in DEC are local and any point of an n-manifold is in an open set that is homeomorphic to an open set in $\mathbb{R}^n$ or in a half space, in the case of boundary points.

Shortcomings: A complete treatment of DEC should discuss how well K approximates M, and indeed how K is obtained from M in the first place. It should also include a discussion of how well the discrete operators approximate the smooth counterparts. But for this one needs to define a topology on the discrete side so that continuity and convergence can be discussed. This discussion, of discretization and approximation quality, is something we do not do in this thesis, although it is an important topic for future work. Nevertheless in Section 2.2 we discuss the idea of discretization at least roughly.

2.1 Simplicial Complex

We now recall some basic definitions of simplices and simplicial complexes. For more details see Munkres [1984] and Hatcher [2002]. Let $\{v_0, \ldots, v_p\}$ be a set of geometrically independent points in $\mathbb{R}^N$, i.e., the vectors $\{v_1 - v_0, \ldots, v_p - v_0\}$ or equivalently $\{v_1 - v_0, v_2 - v_1, \ldots, v_p - v_{p-1}\}$ are linearly independent.

Definition 2.1.1. A p-**simplex** σ^p is the convex hull of $p+1$ geometrically independent points $v_0, \ldots, v_p$. That is

$$\sigma^p = \left\{ x \in \mathbb{R}^N \middle|\ x = \sum_{i=0}^{p} \mu^i v_i \text{ where } \mu^i \geq 0 \text{ and } \sum_{i=0}^{n} \mu^i = 1 \right\} .$$

We'll write $\sigma^p = v_0 \dots v_p$. The points $v_0, \dots, v_p$ are in $\mathbb{R}^N$ and are called the **vertices** of the simplex, and the number p is called the **dimension** of the simplex. Any simplex spanned by a (proper) subset of $\{v_0, \dots, v_p\}$ is called a **(proper) face** of σ^p ; their union is called the **boundary** of σ^p and denoted $\mathrm{Bd}(\sigma^p)$. The **interior** of σ^p is $\mathrm{Int}(\sigma^p) = \sigma^p \setminus \mathrm{Bd}(\sigma^p)$ and is also called an **open simplex**. If σ^q is a proper ~~face~~ of σ^p, then we write $\sigma^q \prec \sigma^p$. Sometimes we will write σ^p as σ when the dimension is understood. By $|\sigma^p|$ we will mean the p-**volume** of σ^p in $\mathbb{R}^N$. For $p = 0$ this is defined to be 1. The smallest affine subspace of $\mathbb{R}^N$ containing σ is called the **plane** of σ and denoted $\mathrm{P}(\sigma)$. This can be obtained for example, by letting the coefficients μ above be negative. $\diamondsuit$

Definition 2.1.2. 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 dimension n of the largest dimensional simplex in K will be called the dimension of K. The union of simplices of K is a subset of $\mathbb{R}^N$ and will be called the **underlying space** of K or the **polytope** of K and denoted $|K|$. We will be only concerned with **finite** simplicial complexes (a complex with a finite number of simplices). In a **cell complex** (also known as **CW complex**) open simplices are replaced by **cells**, which are objects homeomorphic to open balls. See page 5 of Hatcher [2002] for another way to define cell complexes. $\diamondsuit$

Remark 2.1.3. Topology on underlying space: For a finite complex (the only kind we will consider in this work) the topology on $|K|$ will be the natural one (subspace topology) induced from $\mathbb{R}^N$. For a simplex σ^p of dimension $p \geq 1$ the meaning of $\mathrm{Int}(\sigma^p)$ and $\mathrm{Bd}(\sigma^p)$ coincides with the usual topological meanings of interior and boundary in the topology of $|K|$. However for $p = 0$, i.e., for points σ^0, $\mathrm{Int}(\sigma^0) = \sigma^0$ and $\mathrm{Bd}(\sigma^0) = \emptyset$, since a point has no proper faces (see Def. 2.1.1). However in the topology of $|K|$ a point has empty topological interior and is its own topological boundary. This special status of a 0-simplex is actually useful in defining duals as we will do in Def. 2.4.5. Another thing to keep in mind is that the $\mathrm{Int}(\sigma^p)$ for *any* dimension p is called an *open* simplex even though (for example) $\mathrm{Int}(\sigma^1)$ in a dimension 2 complex is not an open set in the subspace topology. For $p = n$ the open simplex $\mathrm{Int}(\sigma^p)$ is indeed an open set. $\diamondsuit$

Definition 2.1.4. A **flat** (or **linear**) **simplicial complex** K of dimension n in $\mathbb{R}^N$ is one of which all simplices are in the same affine n-subspace of $\mathbb{R}^N$. This coincides with our usual intuition of a flat 2-surface embedded in $\mathbb{R}^3$. $\diamondsuit$

Definition 2.1.5. A **simplicial triangulation** of the polytope $|K|$ is any simplicial complex L such that the union of the simplices of L (i.e., polytope $|L|$) is the polytope $|K|$. $\diamondsuit$

Definition 2.1.6. If L is a sub-collection of K that contains all faces of its elements, then L is a simplicial complex in its own right, and it is called a **subcomplex** of K. One subcomplex of K is the collection of all simplices of K of dimension at most p, which is called the p**-skeleton** of K and is denoted $K^{(p)}$. The **closed star** (or **one-ring**) of a simplex s in K is denoted $\overline{\mathrm{St}}\, s$ and is the union of all simplices of K having s as a face. Two p-simplices will be called **adjacent** of they share a $(p-1)$-face. $\Diamond$

2.2 Discretizing the Manifold

Let M be a smooth triangulable Riemannian n-manifold and define an abstract simplicial complex on M. See pages 15–19 of Munkres [1984] for the definition of and information on abstract simplicial complexes, but for our purpose it is enough to think of it as simplices "glued" to or "drawn on" M in such way that they form a "curved" simplicial complex. It is a cell complex in which the cells are simplices on the manifold.

Let K be a concrete geometric simplicial complex that is isomorphic to a part of the complex on M. It may be convenient to embed K in $\mathbb{R}^N$ where $N \geq n$. For example, this is often done in computational mechanics and graphics when a surface is approximated by a triangle mesh embedded in $\mathbb{R}^3$. We stress that the idea of discretization is *not* to put charts on the manifold and then triangulate the codomain of the chart into a simplicial complex. If we did this, then the idea of discrete approximation would be lost, because we would have to store the analytical information about the chart exactly. Sometimes this is not even possible. An example of this situation is when the smooth manifold can only be sampled by some physical measurement such as when the shape of an object is acquired by scanning. So the simplices of K approximate a portion of M for which we may only know a set of points. These then become the vertices of K. Nevertheless we will define the following map.

Definition 2.2.1. Let σ_M^p be an abstract simplex on M and a simplex σ_K^p be a simplex in K that approximates it. In order to transfer information (like forms and vector fields) from M to K we will need the exact or approximate map between the two. We will call such a map $\pi_\sigma : \sigma_M^p \to \sigma_K^p$ a **pasting map** and assume it is a smooth map. $\Diamond$

Remark 2.2.2. Pasting map as a formal device: We have mentioned above that in applications we may not even know M exactly. Thus the pasting maps will not be known in these cases. Even if they were, storing the pasting maps would defeat the idea of discretization. But there is no harm in using them during discretization. In general they are a formal device allowing one to talk about the transfer of information from M to K. In practice they may be a procedural scheme or a measurement device allowing one to discretize smooth information on M. If M is a domain in $\mathbb{R}^N$, then it may even be an identity map. $\Diamond$

Approximating a portion of M by K means that the metric on K induced from $\mathbb{R}^N$ approximates the metric on M in the portion being approximated. The embedding of the simplicial complex into an ambient space is a computational convenience. For the purposes of the theory, it is only necessary to specify the connectivity of the mesh in the form of an abstract simplicial complex, along with a local metric on the space of vertices. This is addressed in Section 2.8. Discretization of forms via de Rham map and interpolation of forms via Whitney maps is addressed in Section 3.3.

2.3 Oriented Primal Complex

For DEC we need a notion of orientation for the simplices and for simplicial complexes. We start with simplices.

Definition 2.3.1. Define two orderings of the vertices of a simplex σ^p to be equivalent if they differ from one another by an even permutation. If $p > 0$, then the orderings fall into two equivalence classes. Each of these classes is called an **orientation** of σ^p. An **oriented simplex** (also written σ^p) is a simplex together with an orientation. If $v_0, \ldots, v_p$ are the vertices of σ^p, then we'll use $[v_0, \ldots, v_p]$ for the oriented simplex σ^p with the equivalence class of the ordering $(v_0, \ldots, v_p)$. A 0-simplex has only one possible ordering so has no orientation (although it can have an **induced** orientation defined below). $\diamondsuit$

Definition 2.3.2. Given a simplex σ^p with vertices $\{v_0, \ldots, v_p\}$, the ordered collection of vectors $(v_1 - v_0, v_2 - v_0, \ldots, v_p - v_0)$, which is a basis for the plane $\mathrm{P}(\sigma)$, will be called a **corner basis at** v_0 of the simplex. The ordered collection $(v_1 - v_0, v_2 - v_1, \ldots, v_p - v_{p-1})$, which is also another basis, will be called **polyline basis from** v_0 of the simplex. $\diamondsuit$

Remark 2.3.3. Simplex orientation using a basis: A simplex σ is a closed connected subset of its plane $\mathrm{P}(\sigma)$ and of the same dimension as the plane. The plane $\mathrm{P}(\sigma)$ being an affine subspace of $\mathbb{R}^N$ is oriented in the usual sense of orientation by an ordered basis or equivalently a volume form. In particular the ordered corner basis and the polyline basis of the simplex orient the plane and hence the simplex itself. These notions of orientation via corner and polyline basis coincide with the orientation via permutations defined above. This means that the partition of the set of simplices into two orientation classes is the same in each case. See, for example, Lemma 5a on page 360 of Whitney [1957]. Thus orienting a simplex is equivalent to orienting its plane. From now we will use the word orientation to mean any of these equivalent notions of corner, polyline or permutation based orientation. $\diamondsuit$

Example 2.3.4. Oriented simplices: Consider 3 non-collinear points v_0, v_1 and v_2 in $\mathbb{R}^2$ labeling the vertices of a triangle in a counterclockwise fashion. Then these three points individually are examples of 0-simplices (hence these have no orientation). Examples of oriented 1-simplices are the oriented line segments $[v_0, v_1]$, $[v_1, v_2]$ and $[v_0, v_2]$. By writing the vertices in that order we have given orientations to these 1-simplices, i.e., $[v_0, v_1]$ is oriented from v_0 to v_1. The triangle $[v_0, v_1, v_2]$ is a counterclockwise oriented 2-simplex. $\blacklozenge$

Consider a simplex σ^p with vertices $\{v_0, \ldots, v_p\}$ with $p \geq 1$. By deleting one vertex at a time from this set we can enumerate the simplices that have dimension $(p - 1)$ and are faces of σ^p. There are $p + 1$

such faces and face i is spanned by $\{v_0, \ldots, \widehat{v_i}, \ldots, v_p\}$ for $i = 0, \ldots, p$. The hat means omit that vertex. An oriented simplex σ^p induces an orientation on each of these faces. The notion of induced orientation is related to the boundary operator to be defined in Chapter 3 in Def. 3.6.1. But induced orientation can be defined independently as follows.

Definition 2.3.5. Let $\sigma^p = [v_0, \ldots, v_p]$ be an oriented simplex, with $p \geq 1$. This orientation of σ gives each of the $(p-1)$-dimensional faces an **induced orientation**. For $p > 1$, if i is even the induced orientation of the face $v_0 \ldots \widehat{v_i} \ldots v_p$ is the same as the orientation of the oriented simplex $[v_0, \ldots, \widehat{v_i}, \ldots, v_p]$. Otherwise it is the opposite one. $\diamondsuit$

Example 2.3.6. Induced orientation: Given the counterclockwise oriented triangle $\sigma = [v_0, v_1, v_2]$ its unoriented 1-faces are v_1v_2, v_0v_2 and v_0v_1. The induced orientation on v_1v_2 is the same as the orientation of $[v_1, v_2]$. The induced orientation on v_0v_2 is the opposite of the orientation of $[v_0, v_2]$ and the induced orientation on v_0v_1 is the same as the orientation of $[v_0, v_1]$. As another example consider an oriented tetrahedron $[v_0, v_1, v_2, v_3]$ with v_0 at the top and v_1, v_2, v_3 labeling the bottom triangle in counterclockwise fashion when looked from outside. This has the same orientation class as the ordered collection of 3 vectors emanating from v_0 and pointing to the 3 vertices v_1, v_2 and v_3 in order, i.e., the corner basis at v_0. This corresponds to a right-hand rule orientation for the plane of the tetrahedron, i.e., for $\mathbb{R}^3$. By the definition of induced orientation the triangular faces of the tetrahedron get oriented counterclockwise when looking from outside. $\blacklozenge$

Remark 2.3.7. Comparing orientations: Consider two oriented simplices σ and τ embedded in $\mathbb{R}^N$. If their dimensions differ, then their orientations cannot be compared. So assume that they have the same dimension p and so $1 \leq p \leq n$ (0-simplices have no orientation). Then their orientations can be compared in the following cases:

1. Their planes coincide, i.e., $\mathrm{P}(\sigma) = \mathrm{P}(\tau)$

2. They share a face of dimension $p - 1$

In case 1 the two simplices σ and τ will have the same orientation iff their corner or polyline basis orients their plane the same way. In case 2 the two will have the same orientation if the induced orientation of the shared $p - 1$ face induced by the σ is opposite to that induced by τ. Fig. 2.1 clarifies this remark. $\diamondsuit$

Definition 2.3.8. Let σ^p and τ^p, with $1 \leq p \leq n$, be two simplices whose orientations can be compared, that is, they fall into one of the two cases of Rem. 2.3.7. If their orientations are in the same class we will say that the two simplices have a **relative orientation** of $+1$ otherwise -1. We will write this as $\mathrm{sgn}(\sigma^p, \tau^p) = +1$ or -1 respectively. $\diamondsuit$

The notion of a simplicial complex defined in this section is too general for our purpose. For example, in $\mathbb{R}^2$ a triangle with a line segment sticking out of one vertex is a simplicial complex. While such things may

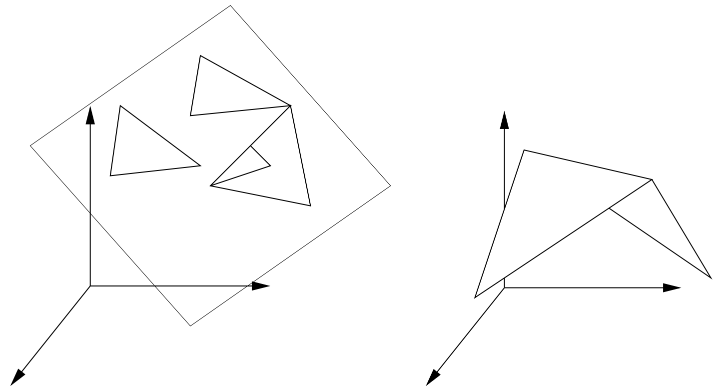


Figure 2.1: Situations where orientations of simplices can be compared: (a) All the triangles are in $\mathbb{R}^3$ but since their plane is identical (shown in the figure) the orientations can be compared using any of their corner basis or polyline basis. See Rem. 2.3.3 and 2.3.7 ; (b) Two triangles in $\mathbb{R}^3$ not in the same plane. But since they share an edge their orientations can be compared. Orienting them so that they induce opposite orientations on the shared edge gives the two triangles identical orientations.

be useful say, in modeling domains connected by wires in electromagnetism, in this thesis we exclude such cases by using the definition to be given below. Another type of complex to be excluded is, for example, two triangles touching only at a common vertex. Excluding such complexes is in line with this being a theory of exterior calculus. For example, in smooth exterior calculus the starting point is the notion of a smooth manifold. The examples just mentioned can be considered to be discretizations of smooth spaces that are not manifolds (not even manifolds with boundary) since they are not locally homeomorphic to $\mathbb{R}^n$ or to half space. This is captured in the following definition.

Definition 2.3.9. A simplicial complex K of dimension n is called a **manifold-like simplicial complex** if the underlying space $|K|$ is a C^0 manifold (possibly with boundary). In such a complex all simplices of dimension k with $0 \leq k \leq n-1$ must be a face of some simplex of dimension n in the complex. Also, by definition of C^0 manifolds each point on $|K|$ will have a neighborhood homeomorphic to $\mathbb{R}^n$ or n-dimensional half-space. See pages 143 and 478 of Abraham et al. [1988] for definitions of manifolds and manifolds with boundary. $\Diamond$

From now on we will work only with manifold-like simplicial complexes. Allowing only such complexes has the added advantage that we can now define orientability for simplicial complexes. In algebraic topology the definition of an orientable simplicial complex requires some technical machinery (such as homology n-manifolds and homology groups). In the following definition we can bypass such machinery.

Definition 2.3.10. A manifold-like simplicial complex K of dimension n is called an **oriented manifold-like simplicial complex** if adjacent n-simplices (i.e., those that share a common $(n-1)$-face) have the same orientation (orient the shared $(n-1)$-face oppositely) and simplices of dimensions $n-1$ and lower are oriented individually. From now on the name **primal mesh** will be used to mean a manifold-like oriented simplicial complex. $\Diamond$

2.4 Dual Complex

An important ingredient of DEC is the dual complex (defined below) of a manifold-like simplicial complex. The dual complex will usually not be a simplicial complex. However if the primal mesh satisfies some conditions, then the dual *can* be built from a simplicial refinement of the primal mesh. The notion of duality we use is circumcentric (or Voronoi) duality. The other popular choice in this subject is barycentric duality and we compare the two types in Section 2.6.

Remark 2.4.1. Metric-dependence and duality: The metric-dependent and metric-independent parts of DEC can be developed separately. Operators, that in the smooth theory do not use metric information, should have that property in the discrete theory as well. For example, the exterior derivative, wedge product, natural pairing of forms and vector fields, interior product and Lie derivative are all example of such operators. On the other hand Hodge star, sharp and flat depend on the metric. Divergence is an operator in which metric enters only through its dependence on the volume form of the metric. Dual meshes seem to be required only in the metric-dependent parts of DEC. However, in applications these might be all mixed up and thus one is forced to invent versions of metric-independent operators for the dual mesh as well. An example is say, the Lagrangian for harmonic maps, $\mathbf{d}\, f \wedge * \mathbf{d}\, f$. Since the wedge and Hodge are both present, one may expect the dual mesh to play a role.

In this thesis, we have not always followed a strict separation of discrete operators into metric-independent and metric-dependent types. But in those cases where we give a metric-dependent definition, we generally accompany it with a metric-independent one as well. Also, the metric-dependent definitions used are such that at least in the smooth theory, the metric dependence cancels, although in the discrete case we don't know if this is the case.

In our future work, we intend to maintain a more strict distinction between metric-independent and metric-dependent operators. The computational implication of this distinction is that the computation of discrete operators that are metric-independent may not require a dual complex, as it occasionally seems to, in this thesis. $\Diamond$

Definition 2.4.2. The **circumcenter** of a p-simplex σ^p is given by the center of the p-circumsphere, where the p-circumsphere is the unique p-sphere that has all $p+1$ vertices of σ^p on its surface. Equivalently, the circumcenter is the unique point in $\mathrm{P}(\sigma)$ that is equidistant from all the $p+1$ vertices of the simplex. We will denote the circumcenter of a simplex σ^p by $c\,(\sigma^p)$. If the circumcenter of a simplex lies in its interior we call it a **well-centered simplex**. In $\mathbb{R}^2$ a triangle with all acute angles is an example. A simplicial complex all of whose simplices (of all dimensions) are well-centered will be called a **well-centered simplicial complex**. $\Diamond$

The circumcenter of a simplex σ^p can be obtained by taking the intersection of the normals to the $(p-1)$ -

dimensional faces of the simplex, where the normals are emanating from the circumcenter of the face. This allows us to recursively compute the circumcenter. We use the names Voronoi dual and circumcentric dual synonymously since the dual of a simplex is its circumcenter (equidistant from all vertices of the simplex).

To build a circumcentric dual complex of a simplicial complex we have to first subdivide the original complex to yield one with smaller simplices. Then some of the simplices will be combined to give the dual complex. This general procedure of building a dual complex by subdivision and aggregation is described in detail in Munkres [1984] on pages 83–88 (for subdivision) and pages 377–381 (for aggregation). While he specializes the general construction to barycentric subdivision, under some conditions the same procedure with the barycenters replaced by circumcenters produces a circumcentric subdivision.

This requires that K be well-centered in the sense defined above because otherwise circumcentric subdivision may not produce a simplicial complex. See Section 2.6 for implications of this restriction. However if K is well-centered, then the subdivision operator sd of Munkres [1984] can be replaced by a circumcentric subdivision operator csd as defined below.

Given a simplicial complex K then $\mathrm{csd}\ K$ will be a simplicial complex from which to build the dual complex. The underlying spaces $|K|$ and $|\mathrm{csd}\ K|$ are the same. In Lemma 15.3 Munkres [1984] gives the form of the simplices in $\mathrm{sd}\ K$. Instead we will use this as the definition of subdivision.

Definition 2.4.3. The **circumcentric subdivision** of a well-centered simplicial complex K of dimension n is denoted $\mathrm{csd}\ K$, and it is a simplicial complex with the same underlying space as K and consisting of all simplices (each of which is called a **subdivision simplex**) of the form $[c(\sigma_1), \dots, c(\sigma_k)]$ for $1 \leq k \leq n$ (note that the index here is *not* dimension since it is a subscript). Here $\sigma_1 \prec \sigma_2 \prec \dots \prec \sigma_k$ (i.e., σ_i is a proper face of σ_j for all $i < j$) and the σ_i are in K. That this is a simplicial complex follows from the properties given on pages 83–88 of Munkres [1984]. This is because in a well-centered simplicial complex all circumcenters lie inside their simplices and this is sufficient for the subdivision construction of Munkres [1984] to produce a simplicial complex.

Each subdivision simplex in a given simplex σ^p will be called a **subdivision simplex of** σ^p. Of these, a q simplex ($q \leq p$) will be called a **subdivision** q**-simplex of** σ^p. $\Diamond$

Example 2.4.4. Circumcentric subdivision: Consider a simplicial complex K with vertices v_0, v_1 and v_2, i.e., the complex consists of a triangle $v_0v_1v_2$, its edges and its vertices. Then $L = \mathrm{csd}\ K$ consists of the following elements:

- $L^{(0)}$ (the 0-simplices of $\mathrm{csd}\, K$): consists of the circumcenters $c(v_0) = v_0$, $c(v_1) = v_1$ and $c(v_2) = v_2$, the midpoints of the edges $c(v_0v_1)$, $c(v_1v_2)$ and $c(v_0v_2)$ and the circumcenter of the triangle, i.e., $c(v_0v_1v_2)$,

- $L^{(1)}$ (the 1-simplices of $\mathrm{csd}\, K$): consists of 12 edges – the two halves of each edge and edges joining the circumcenter of the triangle to the vertices and midpoints of the edges,

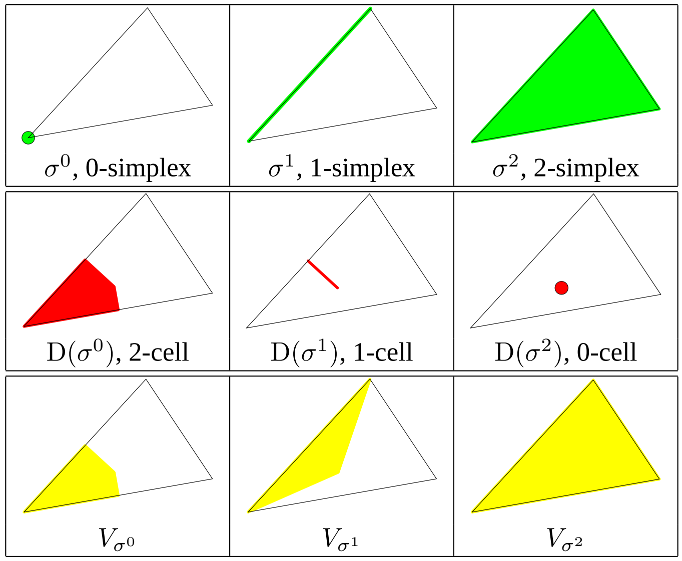


Figure 2.2: Primal and dual mesh elements in 2D. Top row shows primal mesh (Def. 2.3.10) with one simplex of dimensions 0, 1 and 2 highlighted in the 3 figures; Middle row shows the corresponding dual cells (Def. 2.4.5), shown here restricted to the original primal triangle ; Bottom row shows the support volumes (Def. 2.4.9). See Fig. 2.3 for 3D example.

- $L^{(2)}$ (the 2-simplices of $\operatorname{csd} K$): consists of 6 triangles of the form $v_0 c(v_0 v_1) c(v_0 v_1 v_2)$.

See pages 87 and 378 of Munkres [1984] for more examples. Fig. 2.4 shows many triangles that have been subdivided. ♦

If K is a manifold-like simplicial complex, then the underlying space $|K|$ can be partitioned into subsets that are cells (see Def. 2.1.2) (in Munkres [1984] Section 64 such dual cells are called blocks because he is working with homology manifolds where spheres are homological spheres). This partitioning gives the dual cell decomposition of $|K|$. Each dual cell is made by aggregating together certain simplices from $\operatorname{sd} K$. Instead we will use $\operatorname{csd} K$ and end up with a circumcentric version of the dual block decomposition of K. We summarize this procedure below. For details see pages 377-381 of Munkres [1984].

Definition 2.4.5. Let K be a well-centered manifold-like simplicial complex of dimension n and let σ^p be one of its simplices. The **circumcentric dual cell** of σ^p will be denoted $\mathrm{D}(\sigma^p)$ and defined as

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

For $r = 0$, interpret $\sigma^p \prec \sigma_1 \prec \ldots \prec \sigma_r$ simply as σ^p. The closure of the dual cell of σ^p is written $\overline{\mathrm{D}}(\sigma^p)$ and called the **closed dual cell**. We will call each $(n-p)$-simplex $c\left(\sigma^p\right) c\left(\sigma^{p+1}\right) \ldots c\left(\sigma^n\right))$ an **elementary dual simplex** of σ^p. This is an $(n-p)$-simplex in $\operatorname{csd} K$. The collection of dual cells is called the **dual cell decomposition** of K. This is a cell complex and will be denoted $\mathrm{D}(K)$. The union of the cells of dimension at most p will be denoted $K_{(p)}$ and called the **dual p-skeleton** of K. For a closed dual cell $\overline{\mathrm{D}}(\sigma^p)$ and

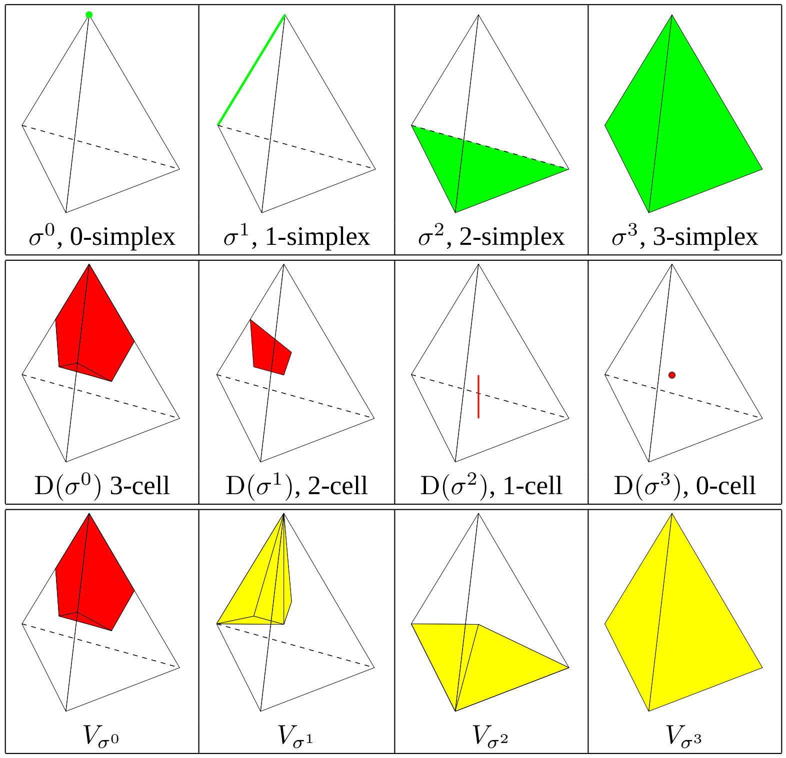


Figure 2.3: Primal, dual cells and support volumes in 3D. Top row shows primal mesh (Def. 2.3.10) with one simplex of dimensions 0, 1, 2 and 3 highlighted in the 4 figures; Middle row shows the corresponding dual cells (Def. 2.4.5), shown here restricted to the original primal triangle ; Bottom row shows the support volumes (Def. 2.4.9). See Fig. 2.3 for 2D example.

$q < (n-p)$, any element of $K_{(q)}$ that is a subset of $\overline{\mathrm{D}}(\sigma^p)$ will be called a **proper face**. For $0 \le p \le n-1$, the $(n-p-1)$-faces of $\overline{\mathrm{D}}(\sigma^p)$ are $\overline{\mathrm{D}}(\sigma^{p+1})$ for all $\sigma^{p+1} \succ \sigma^p$. $\Diamond$

Remark 2.4.6. Unions and sums using proper faces: The above definition is the first time in this thesis that we have used the notation $\sigma^1 \prec \ldots \prec \sigma^r$ etc. for indexing a union. This is a very convenient notation for writing unions (or in the case of chains in next chapter, sums) without having to index the individual simplices of all dimensions. A union like

$$\bigcup_{\sigma^{p_1} \prec \ldots \prec \sigma^{p_k}} \quad \text{or} \quad \bigcup_{\sigma_{j_1} \prec \ldots \prec \sigma_{j_k}} \quad \text{or} \quad \bigcup_{\sigma^{p} \prec \ldots \prec \sigma_{j_k}}$$

is a union over all simplices of a given simplicial complex that satisfy the proper face relationships under the operator. Notice in particular the third union above. The first simplex is of dimension p but the rest of the simplices in the proper face relations have been indexed by numbers, not dimension. Such mixing of indexing is allowed. $\Diamond$.

The dual cell decomposition gives a CW complex (see Def. 2.1.2 above or pages 214–221 of Munkres [1984] or page 5 of Hatcher [2002] for more details on cell (or CW) complexes). Fig. 2.2 and 2.3 show

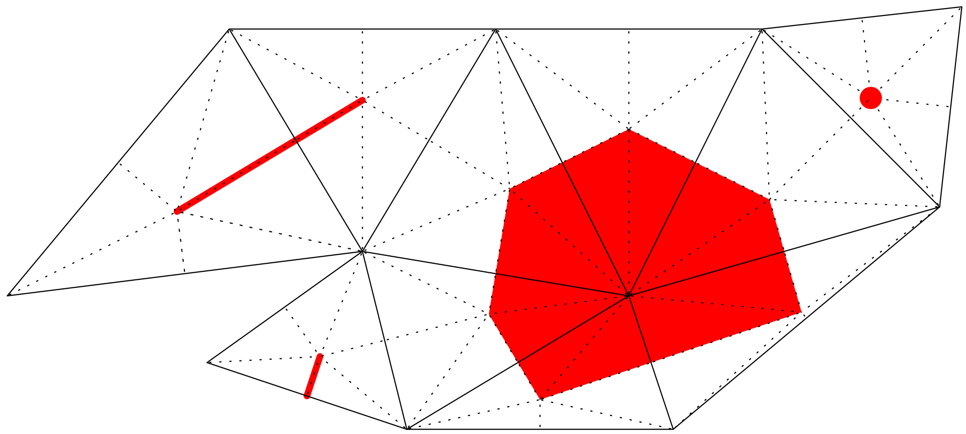


Figure 2.4: A simplicial complex K is subdivided into the simplicial complex $\operatorname{csd} K$ and some dual cells of dimension 0,1 and 2 are marked. See Example 2.4.4 and 2.4.7. The new edges introduced by the subdivision are shown dotted. The dual cells shown are colored red. Some elementary dual simplices and subdivision simplices appearing in this figure are pointed out in Example 2.4.7.

examples of dual cells as does Example 2.4.7 and associated Fig. 2.4. See pages 378–379 of Munkres [1984] for more examples.

Example 2.4.7. Dual cells and elementary dual simplices: By definition of dual cell the dual of a vertex σ^0 is

$$\mathrm{D}(\sigma^0) = \left\{\mathrm{Int}(c\left(\sigma^0\right))\right\} \cup \bigcup_{\sigma^0 \prec \sigma_1} \mathrm{Int}\left(c\left(\sigma^0\right) c\left(\sigma_1\right)\right) \cup \ldots \cup \bigcup_{\sigma^0 \prec \sigma_1 \ldots \prec \sigma_n} \mathrm{Int}\left(c\left(\sigma^0\right) c\left(\sigma_1\right) \ldots c\left(\sigma_n\right)\right) .$$

Now recall from Rem. 2.1.3 that the first term above is the 0-simplex $c\left(\sigma^0\right)$ since the interior of a 0-simplex is the 0-simplex itself. The second term is all the open edges starting at σ^0 and going to the circumcenters of: the edges containing σ^0, the triangles containing σ^0, and so on. The last term is the union of all the open simplices of dimension n containing σ^0. Thus we get the open Voronoi region around σ^0.

Refer to Fig. 2.4 for this part of the example. Consider the simplicial complex of dimension 2 shown in the figure. The dual cell of a vertex is the topological interior of the Voronoi region around it as shown shaded in the figure. This dual cell is made up of the t~~he~~ vertex whose dual it is, interiors of the open edges emanating from that vertex, and interiors of the elementary dual simplices (Def. 2.4.5) of the vertex. An example of an elementary dual simplex of is a triangle starting with vertices consisting of a vertex of the complex, the circumcenter of an edge incident on the vertex and the circumcenter of a triangle containing that edge. The dual cell of an edge in the simplex consists of the circumcenter of that edge and the two open edges emanating from it and going to the circumcenters of the triangles adjacent to it. This is shown by shading the dual cell of an internal edge and a boundary edge in Fig. 2.4. Note that for the boundary edge the dual has only one piece since there is only one triangle adjacent to that boundary edge. Note that if the complex is not flat, then the dual edge will not be straight line. An elementary dual simplex of an edge starts at the circumcenter of the edge and ends at the circumcenter of an adjacent triangle. In the figure the dual of a triangle is shown as the circumcenter.

Now consider a dimension 3 complex in $\mathbb{R}^3$ and an edge σ^1 in it. We want to find $\mathrm{D}(\sigma^1)$. The vertices of one of the elementary dual simplex of σ^1 are the circumcenters: $c\left(\sigma^1\right)$, $c\left(\sigma^2\right)$, $c\left(\sigma^3\right)$ which form a triangle. Here σ^1 is a proper face of σ^2 which is a proper face of a tetrahedron σ^3. These circumcenters are 3 vertices and so the elementary dual simplex is a triangle as expected. Here $p = 1$ and $n = 3$ and so the elementary dual simplices are simplices of dimension $3 - 1 = 2$. Now let σ^0 be a vertex contained in σ^1. Then the tetrahedron $c\left(\sigma^0\right) c\left(\sigma^1\right) c\left(\sigma^2\right) c\left(\sigma^3\right)$ lies inside the tetrahedron σ^3 and has the same plane as σ^3. ♦

Remark 2.4.8. Properties of dual cells and related simplices: Let K be a well-centered manifold-like simplicial complex of dimension n. Let σ^0, σ^1, …, σ^n be simplices in K of dimensions 0,1, …, n such that

$$\sigma^0 \prec \sigma^1 \prec \ldots \sigma^n$$

that is, σ^0 is a proper face of σ^1 which is a proper face of σ^2 and so on. Then the following are true:

1. The dual cell $\mathrm{D}(\sigma^p)$ is homeomorphic to an open ball of dimension $n - p$ and so it can be oriented (as we shall do in Section 2.5),

2. The dual cells are disjoint and their union is $|K|$. Also, $\overline{\mathrm{D}}(\sigma^p)$ is a polytope of $\operatorname{csd} K$ of dimension $n - p$ (Theorem 64.1 pages 378–379 of Munkres [1984]),

3. A p-simplex ν^p like $c\left(\sigma^0\right) \ldots c\left(\sigma^p\right)$ is a subdivision p-simplex (Def. 2.4.3) of σ^p and its plane is identical to that of σ^p, i.e., $\mathrm{P}(\nu^p) = \mathrm{P}(\sigma^p)$,

4. An $(n - p)$-simplex $\delta^{(n-p)}$ like $c\left(\sigma^p\right) \ldots c\left(\sigma^n\right)$ is an elementary dual simplex (Def. 2.4.5) of σ^p,

5. An n-simplex τ^n like $c\left(\sigma^0\right) \ldots c\left(\sigma^n\right)$ is inside σ^n and has the same plane as σ^n, i.e., $\mathrm{P}(\tau^n) = \mathrm{P}(\sigma^n) = \mathbb{R}^n$,

6. The subdivision p-simplex ν^p and the elementary dual $(n - p)$-simplex $\delta^{(n-p)}$ are transverse, i.e.,

$$\mathrm{P}(\nu^p) \oplus \mathrm{P}\left(\delta^{(n-p)}\right) = \mathrm{P}(\sigma^n) = \mathbb{R}^n \,.$$

   This equality is vacuously true for $p = 0$ or n.

These properties will be useful for orienting the dual cells in Section 2.5. ♢

Now we define something called a support volume of a simplex. For a p-skeleton of the primal mesh the support volumes tile the primal mesh for any $0 \le p \le n$. That is, the union of the support volumes of all the p-simplices in the primal mesh is the mesh and the intersections are along some $(p - 1)$ simplices of $\operatorname{csd} K$. This concept will be useful in Chapter 5 in defining discrete flat operator.

Definition 2.4.9. Let K be an n-dimensional manifold-like well-centered simplicial complex and σ^p one of its simplices. The union of convex hulls of σ^p and its dual cells in each n-simplex of which σ^p is a face, forms an n-volume that we call **support volume** of σ^p and we denote it by V_{σ^p}. That is

$$V_{\sigma^p} := \bigcup_{\sigma^n \succ \sigma^p} \operatorname{convexhull}\left(\{\mathrm{D}(\sigma^p) \cap \sigma^n, \sigma^p\}\right)$$

The support volumes of all the p-simplices of K (for any p) tile $|K|$. Some examples of support volumes in two- and three-dimensional complexes are given in Fig. 2.2 and 2.3. $\Diamond$

2.5 Oriented Dual Complex

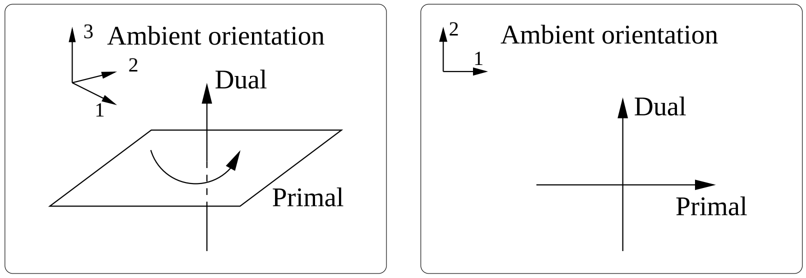
The dual cells introduced above are unoriented subsets of $|K|$. We next discuss how to give them an orientation. The properties listed in Rem. 2.4.8 will now prove useful. First of all, according to that remark each dual cell is homeomorphic to an open ball of that dimension. For example, the $\mathrm{D}(\sigma^0)$ for a vertex σ^0 in a primal mesh of dimension 2 is homeomorphic to a two-dimensional open ball. So is the dual cell of an edge in a dimension 3 complex. Thus dual cells are orientable subcomplexes of $\operatorname{csd} K$. They can be oriented by orienting just one of the elementary dual simplices. The orientations for the other elementary dual simplices follow from Rem. 2.3.7, case 2.

Let σ^0, $\sigma^1, \ldots, \sigma^n$ be simplices in an n-dimensional primal mesh K such that $\sigma^0 \prec \sigma^1 \prec \ldots \sigma^n$ and let σ^p be one of these simplices, with $1 \leq p \leq n-1$. The task is to orient the elementary dual simplex $\delta^{(n-p)} = c\left(\sigma^p\right) \ldots c\left(\sigma^n\right)$. According to Rem. 2.4.8, σ^p and $\delta^{(n-p)}$ are transverse. Furthermore they are both subsets of σ^n and the direct sum of their planes equals the plane of σ^n. Thus σ^p and $\delta^{(n-p)}$ are transverse orientable objects both living in the same oriented ambient space. So out of these 3 orientations (ambient space σ^n, primal σ^p and elementary dual $\delta^{(n-p)}$) if 2 are given then there is a well defined way to define the third one. This corresponds to the situation explained in Fig. 2.5. The following algorithmic procedure orients $\delta^{(n-p)}$ unambiguously, even for $p = 0$ or n.

Remark 2.5.1. Algorithm to orient elementary duals: Consider first the case of $1 \leq p \leq n-1$. Let the correctly oriented elementary dual simplex be $s\left[c\left(\sigma^p\right), \ldots, c\left(\sigma^n\right)\right]$, where $s = \pm 1$, and the correct value of s has to be determined. The primal mesh is oriented. Recall that this means that the n-simplices are all oriented the same way and the $n-1$ and lower dimensional simplices have been individually oriented. We will use σ^p and σ^n to denote the *oriented* simplices of the primal mesh.

By the properties in Rem 2.4.8 the orientations of σ^p and $\left[c\left(\sigma^0\right), \ldots, c\left(\sigma^p\right)\right]$ can be compared since they have the same planes. Similarly the orientations of σ^n and $\left[c\left(\sigma^0\right), \ldots, c\left(\sigma^n\right)\right]$ can be compared for the same reason. Then we define

$$s := \operatorname{sgn}\left(\left[c\left(\sigma^0\right), \ldots, c\left(\sigma^p\right)\right], \sigma^p\right) \times \operatorname{sgn}\left(\left[c\left(\sigma^0\right), \ldots, c\left(\sigma^n\right)\right], \sigma^n\right) \tag{2.5.1}$$



(a) (b)

Figure 2.5: Relationship between orientations of embedding space, embedded “primal” manifold and an embedded “dual” manifold transverse to the primal (meaning that at the intersection point of the primal and dual the direct sum of their tangent spaces is the tangent space of the embedding manifold). Given any two of the three orientations the third one is determined. See Section 2.5. This can also be thought of in terms of internal and external orientations of the primal as in Bossavit [2002b]. The roles of primal and dual can be switched and so can the order of putting primal tangent space before the that of the dual. This is a matter of convention. The point is that there is a consistent way to define the third orientation given any two of the orientations ; (a) If the primal 2-manifold is oriented as shown, then the dual 1-manifold has only one orientation such that the orienting basis for the primal followed by the one for the dual together gives the orientation of the embedding space that has been given as right hand rule. (b) Similar situation in 2D.

where sgn is the relative orientation defined in Def. 2.3.8. This method implements the idea embodied in Fig. 2.5. Example 2.5.2 clarifies this idea. For $p = n$ the dual is of dimension 0 and so has no orientation. For $p = 0$, we define $s := \operatorname{sgn}(\left[c\left(\sigma^0\right), \dots, c\left(\sigma^n\right)\right], \sigma^n)$. $\Diamond$

Example 2.5.2. Orienting elementary duals: Consider the well-centered manifold-like simplicial complex of dimensions 2 shown in Fig. 2.6. The orientations of the simplices are as shown in the figure. Let $p = 1$ and we list below the simplices appearing in Rem. 2.5.1.

$$\begin{aligned}
&\text{primal simplex: } \sigma^p = \sigma^1 = [v_1, v_0]\\
&\sigma^0 \prec \sigma^1 \prec \sigma^2 \text{ instance: } v_0 \prec [v_1, v_0] \prec [v_0, v_1, v_2]\\
&\left[c\left(\sigma^0\right), c\left(\sigma^1\right)\right] = [v_0, c_{01}]\\
&\text{elementary dual: } s\left[c\left(\sigma^1\right), c\left(\sigma^2\right)\right] = s[c_{01}, c_{012}]\\
&\text{subdivision simplex: } \left[c\left(\sigma^0\right), c\left(\sigma^1\right)\right] = [v_0, c_{01}]\ .
\end{aligned}$$

The task is to determine if $s = +1$ or -1. By the algorithm above

$$\begin{aligned}
s &= \operatorname{sgn}\left(\left[c\left(\sigma^0\right), c\left(\sigma^1\right)\right], \sigma^1\right) \times \operatorname{sgn}\left(\left[c\left(\sigma^0\right), c\left(\sigma^1\right), c\left(\sigma^2\right)\right], \sigma^2\right)\\
&= \operatorname{sgn}\left([v_0, c_{01}], [v_1, v_0]\right) \times \operatorname{sgn}\left([v_0, c_{01}, c_{012}], [v_0, v_1, v_2]\right) = (-1)(+1) = -1\,.
\end{aligned}$$

This means that the elementary dual simplex $c_{01}c_{012}$ should be oriented as $-[c_{01}, c_{012}] = [c_{012}, c_{01}]$. Note that $\left[c\left(\sigma^0\right), c\left(\sigma^1\right)\right]$ has the same plane as σ^1 and so their orientations can be compared (“plane” here is the line containing both). Similarly for $\left[c\left(\sigma^0\right), c\left(\sigma^1\right), c\left(\sigma^2\right)\right]$ and σ^2. We would have obtained the same

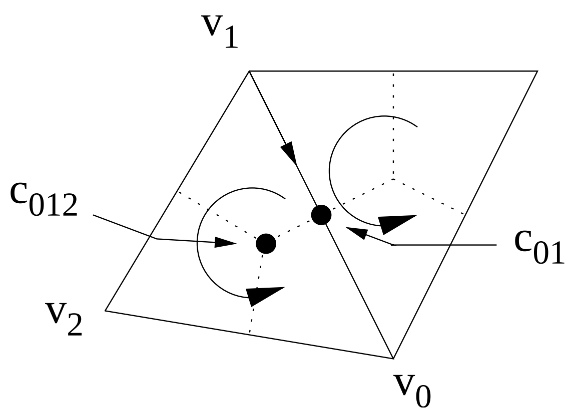


Figure 2.6: Orienting an elementary dual simplex. See Example 2.5.2. Here we have written c_{012} for the circumcenter $c([v_0, v_1, v_2])$ etc.

answer even if we had chosen some other subdivision simplex. ♦

Definition 2.5.3. Let $0 \leq p \leq n-1$ and consider the closed dual $\overline{\mathrm{D}}(\sigma^p)$. This is an $(n-p)$-dimensional oriented dual object. It has $(n-p-1)$-dimensional faces that inherit an orientation from $\overline{\mathrm{D}}(\sigma^p)$. This is called the **dual induced orientation** of an $(n-p-1)$-face. It is defined as the orientation induced (Def. 2.3.5) from the closure of the n-simplex that is an elementary dual simplex making up $\mathrm{D}(\sigma^p)$ whose boundary includes part of the $(n-p-1)$-face. Here we assume that the elementary dual simplex has been oriented correctly according to the algorithm in Rem. 2.5.1. ♢

Example 2.5.4. Dual induced orientation: Consider a 1-ring of triangles with each triangle oriented counterclockwise. The dual of the central vertex is its Voronoi region on the complex. By the above definition the dual induced orientation of the boundary will make each dual edge oriented so that the boundary goes around counterclockwise. Each dual edge in the boundary of the Vornoi region is dual to a primal edge. The dual edge induces an orientation on the circumcenters that lie at its end. ♦

2.6 Circumcentric and Barycentric Duality

As we pointed out earlier, the importance of using a dual mesh is well known in many computational fields and in physics. For example, barycentric dual meshes are used in Sen et al. [2000] for the discretization of an abelian Chern-Simons theory. In computational electromagnetism they have been used by Bossavit [2002b] and many others as a space on which dual forms are defined, just as we will use circumcentric duals in Chapter 3. In computational electromagnetism circumcentric duals also appear in the work of Hiptmair. See for instance Hiptmair [2002a]. In mimetic differencing one often sees the appearance of circumcentric duality to define differential operators for logically rectangular meshes. See for instance Hyman and Shashkov [1997a,b]. Circumcentric duality for defining differential operators on simplicial meshes is used in Nicolaides

[1992]. In none of the above works however is a circumcentric dual mesh used to develop a full discrete exterior calculus. Most deal with either forms only or vector fields as proxies for forms.

Both types of dual meshes have good and bad properties. For example, barycentric duals have a very nice property that barycentric subdivision (which is the first step for building a barycentric dual) always produces a simplicial complex. This is unlike the situation in circumcentric subdivision which requires that the complex be a well-centered simplicial complex because otherwise $\operatorname{csd} K$ may not be a simplicial complex. Thus if in a computation a mesh is changing, the barycentric dual will remain well-defined whereas a circumcentric dual may soon become invalid due to some circumcenters leaking out of their simplices. Maybe this problem can be ameliorated by mixed Eulerian-Lagrangian methods where the mesh is moved for a few time steps and then interpolation brings one back to a nice reference mesh. This has to be investigated further in future work.

On the other hand it appears as if circumcentric duals are useful in building that part of the theory of DEC that involves metric operations like Hodge star, flat and sharp. The dual of an $(n-1)$-face is an edge perpendicular to it. Similarly the dual of an edge is an $(n-1)$-cell. Thus circumcentric duals seem to give simple expressions for fluxes in the coordinate systems of faces and their dual normals. We don't claim that circumcentric duality is the only way to make the operators that relate forms and vector field (such as discrete flat) work. But at least its use in the metric parts of the theory seems to produce simple formulas that are self-consistent and satisfy theorems like Gauss' divergence theorem for vector fields. We should point out that the generalized Stokes' theorem is a non-metric theorem when expressed via forms and so it has nothing to do with the dual.

Even the construction of circumcentric dual meshes may be computationally challenging in high dimensions. Suppose we are given the vertices from which a primal mesh is to be built. Delaunay triangulation will produce a simplicial complex in which the interiors of circumspheres do not contain other vertices. But our requirement of well-centeredness is stronger and may require the introduction of new vertices. Even Delaunay triangulation for dimension higher than 2 is a computationally challenging task. See, for example, Bern et al. [1995]. Delaunay triangulation is equivalent in complexity to complexity of finding convex hulls in one higher dimension. See, for example, Boissonnat and Yvinec [1998].

For some computations the Delaunay triangulation is desirable in that it reduces the maximum aspect ratio of the mesh, which is a factor in determining the rate at which the corresponding numerical scheme converges. But in practice there are problems (for example those involving anisotropy) for which even Delaunay triangulations are a bad idea and so well-centered simplices might not be very useful. See, for example, Shewchuck [2002]; Bern et al. [1995].

In the generalization of DEC to some simple regular meshes as done in Section 9.4, the absence of well-centeredness seems to cause no problem in computing quantities like Laplacian which do not involve a flux across a boundary and are quantities to be evaluated at nodes. This is probably because the closed dual cells of primal nodes are Voronoi cells and by definition these tile the underlying space even when the mesh is not well-centered. So vertex related quantities can be computed at least for regular non-simplicial meshes even for non-well-centered complexes.

In this thesis we will ignore all these computational difficulties and assume that we are given a primal mesh satisfying the required conditions and that the mesh is not changing with time. We will proceed to build exterior calculus objects and operators on such a mesh.

2.7 Interpolation Functions

Later in the thesis we will need to interpolate values that are defined at either primal or dual vertices. For this we will need some basis functions that we now discuss.

Definition 2.7.1. Let K be a well-centered manifold-like simplicial complex. Consider a 1-ring of a vertex σ^0 and $\sigma^n \succ \sigma^0$, i.e., an n-simplex in the 1-ring. Then the following functions, all maps from $\mathbb{R}^N$ to $\mathbb{R}$ are called **interpolation functions**.

(i) ϕ_{σ^0,σ^n} is the **primal-primal** interpolation function supported on σ^n and it is the unique affine function that has the value 0 at all vertices of σ^n other than σ^0 and the value 1 at σ^0,

(ii) $\phi_{\sigma^0,\mathrm{D}(\sigma^0)}$ is the **primal-dual** interpolation function supported on $\mathrm{D}(\sigma^0)$ with value 1 there and 0 elsewhere,

(iii) $\phi_{D(\sigma^n),\sigma^n}$ is the **dual-primal** interpolation function supported on $\mathrm{Int}(\sigma^n)$ with value 1 there and 0 elsewhere,

(iv) $\phi_{D(\sigma^n),D(\sigma^0)}$ is the **dual-dual** interpolation function supported on $\overline{\mathrm{D}}(\sigma^0)$ and defined as the barycentric basis for convex non-simplicial polyhedra as defined in Warren et al. [2003]. This requires that K be a flat complex. $\diamondsuit$

See Fig. 2.7 for a cartoon representation of the interpolation functions.

The primal-primal interpolation function is Whitney 0-form (or element). Whitney forms of higher degress are used by many authors working in DEC. We don't make use of any higher degree Whitney forms in this thesis, but that is likely to change in our future work. Whitney forms are defined in Section 3.3.

Remark 2.7.2. Sum and gradient of primal-primal interpolation functions: Note that $\nabla\phi_{\sigma^0,\sigma^n}$ is constant in $\mathrm{int}(\sigma^n)$ and normal to the face opposite to vertex σ^0. Its length (in the standard inner product induced from $\mathbb{R}^N$) is $1/h$ where h is the height of vertex σ^0 above the face opposite to σ^0. Furthermore,

$$\sum_{\sigma^0 \prec \sigma^n} \phi_{\sigma^0,\sigma^n}(x) = 1 \tag{2.7.1}$$

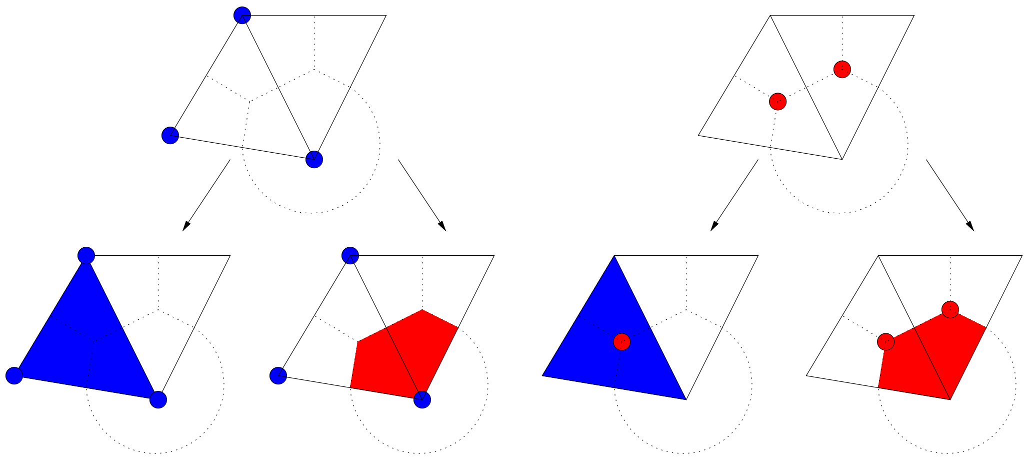


Figure 2.7: Cartoon representation of the four types of interpolation functions defined in Def. 2.7.1. The dotted arc represents a one-ring of triangles of which only 2 triangles are being shown here. *Top row:* primal (left) and dual (right) scalar data; *Bottom row:* (left to right) primal-primal, primal-dual, dual-primal and dual-dual interpolation functions. In primal-primal, data is barycentric interpolated (affinely) in each simplex; in primal-dual it is made constant in each dual of primal vertex; in dual-primal it is made constant in each primal simplex; and in dual-dual it is barycentric interpolated (rational polynomial) using the generalized barycentric coordinates of Warren et al. [2003]. The simplicial complex can be non-flat in the first three cases.

for all $x \in \sigma^n$ and so

$$\sum_{\sigma^0 \prec \sigma^n} \nabla \phi_{\sigma^0, \sigma^n} = 0 \tag{2.7.2}$$

in the interior of σ^n. Here the sum is over all simplices σ^n containing the vertex v. $\Diamond$

2.8 Local and Global Embeddings

The operators of DEC are local and operate in local regions like a 1-ring, the support volume etc. Furthermore, the quantities used in the formulas turn out to be intrinsic quantities, in the plane of each simplex, and they are independent of how the 1-ring etc. is embedded in $\mathbb{R}^N$. As in the smooth case, a quantity like mean curvature which depends on the embedding is not part of an exterior calculus with real valued forms. In the general case the proper development of such quantities requires Lie algebra valued forms and a theory of connections, which is something we do not address in this thesis. As a result it is not essential to embed the entire discretized manifold K and one can work instead with local embedding. It is also not important how the local piece is embedded, as long as the metric in each simplex is respected and the metric on each shared face between simplices agrees.

To achieve this one can define a local metric on the vertices of the simplicial complex which is now an abstract simplicial complex, i.e. a collection of vertices and connectivity information. This was pointed out to us by Alan Weinstein. Distances between two vertices are only defined if they are part of a common n-

simplex in the simplicial complex. Then the local metric is a map $d : \{(v_0, v_1) \mid v_0, v_1 \in K^{(0)}, [v_0, v_1] \prec \sigma^n \in K\} \to \mathbb{R}$. The axioms for a local metric are as follows,

(i) **Positive** $d(v_0, v_1) \geq 0$, and $d(v_0, v_0) = 0$, $\forall [v_0, v_1] \prec \sigma^n \in K$.

(ii) **Strictly Positive** If $d(v_0, v_1) = 0$, then $v_0 = v_1$, $\forall [v_0, v_1] \prec \sigma^n \in K$.

(iii) **Symmetry** $d(v_0, v_1) = d(v_1, v_0)$, $\forall [v_0, v_1] \prec \sigma^n \in K$.

(iv) **Triangle Inequality** $d(v_0, v_2) \leq d(v_0, v_1) + d(v_1, v_2)$, $\forall [v_0, v_1, v_2] \prec \sigma^n \in K$.

Now each n-simplex can be locally embedded into $\mathbb{R}^n$, and all the necessary metric dependent quantities can be computed within the plane of the simplex. For example, the volume of a k-dual cell will be computed as the sum of the k-volumes of the dual cell restricted to each n-simplex in its local embedding into $\mathbb{R}^n$.

Example 2.8.1. Local discretization of a Riemannian manifold: Suppose we are given a Riemannian manifold and some points on it. To discretize this information we would first define an abstract simplicial complex on it, i.e., “glue”, or “draw” a simplicial complex on the manifold, with the given points as the vertices. The measurement of lengths of the edges of this complex gives the data needed for a local embedding. For example for a surface we would embed each triangle individually in $\mathbb{R}^2$ using the edge lengths from the abstract complex as the lengths of the edges of the triangle. Now the metric is implicitly defined inside the embedded triangle. Since adjacent triangles share an edge, the metric of the two matches on the edge which is a useful feature. This is all that is needed for a local theory like DEC. Of course the information about quantities like mean curvature, which depends on the embedding, is lost. These quantities are not a part of the basic exterior calculus with real valued forms, even in the smooth case. ♦

2.9 Summary and Discussion

This chapter is not a repeat of what is found in algebraic topology textbooks although such books are the starting point for it. We have given details about primal and dual complexes that should allow one to implement the required concepts in a program. This is in contrast with most available treatments in algebraic topology, where, for instance, orientation of dual complexes requires much more background than our geometric, algorithmic interpretation. We have also discussed the primal orientation in more detail than is usual in DEC literature where the concepts like comparing orientations, or the requirement of the complex being manifold-like, are rarely mentioned. We have spelled out the restrictions that we place on our meshes in detail, such as requiring well-centered, manifold-like oriented simplicial complexes. Ample examples have been given to clarify all the technical terms and concepts that are introduced. The discussion on local embeddings is to suggest that one does not need to be given the entire manifold of interest discretized and embedded globally as a simplicial complex in $\mathbb{R}^N$.

We have compared barycentric and circumcentric duality. Some reasons were conjectured as to why circumcentric duality might be preferable in those parts of DEC that involve metric. However, a full understanding of which duality is better when, remains yet to be achieved. This is in part due to the fact that metric seems to play a role in the current version of DEC in operators where it should not. Even if the metric information seems to cancel out overall, a much cleaner DEC will likely limit the use of metric to only Hodge star, flat and sharp. We have started to address this and we will point out some preliminary results as we go along.

Chapter 3

Discrete Forms and Exterior Derivative

Results: Now we will define discrete forms, which are objects that discretize differential forms of smooth theory. The objects that are important in this chapter are chains and dual chains, which are made up of simplices and other cells. We take the standard view of discrete forms as cochains, that is, as certain types of functions on chains. For discrete exterior derivative also, we use its standard definition, as a dual of the boundary operator. As is well-known and as we point out later in this chapter, this makes a discrete Stokes' theorem true by definition. The only thing new in this chapter is discrete pullback. We define it and show that discrete exterior derivative and pullback commute as in smooth theory.

Shortcomings: We place no continuity requirements on discrete forms as cochains. But many authors do and rightly so. To prove convergence of discrete objects and operators to their smooth counterparts, one needs a topology on the space of all chains possible from discretization (and not just on the chains of a given complex). Next one needs to assume that cochains are continuous in this topology and discrete operators continuous in cochain topology. As stated previously, we have done no convergence analysis yet and it is an important topic for future work. Therefore, in this thesis we will not require continuity in the definition of cochains as functions on chains. However Section 3.7 we speculate on such topology issues.

3.1 Differential Forms and Discrete Forms

We will define the discrete analogue of differential forms. Some terms from algebraic topology will be defined and used but it will become clear by looking at the examples that one can gain a clear and working notion of what a discrete form is without any knowledge of algebraic topology.

In smooth theory 0-forms are functions, 1-forms are differentials and 2 or higher degree forms (and vacuously even 0- and 1-forms) are antisymmetric tensors. See Chapter 6 of Abraham et al. [1988]. One of the uses for forms is that a p-form can be integrated on a p-manifold as described in Chapter 7 of Abraham et al. [1988]. Forms play a crucial role in modern geometric mechanics. For example, the symplectic form of Hamiltonian mechanics is a 2-form and many differential equations of mechanics can be framed in terms of forms and vector fields. See, for instance, Marsden and Ratiu [1999], Abraham and Marsden [1978], Arnol′d [1989]. Thus it is worthwhile to try and discretize forms. There is a huge amount of literature on this which we summarize and then add to in this chapter.

In the discrete theory the role of p-manifold is played by a p-chain (a formal sum of simplices). We will find that the integration has been done at discretization and from then on the role of integration is replaced by an evaluation operation – evaluation of a discrete form on a chain. Discrete forms will be defined as objects that can be evaluated on chains and hence will be called cochains. This is one kind of duality. We have already seen another, geometric duality in the previous chapter where under some conditions every simplicial complex was found to have an associated circumcentric dual complex. Since there are primal and dual complexes naturally there are primal and dual chains and so there are primal and dual discrete forms.

3.2 Primal Chains and Cochains

We start with a few definitions for which more details can be found on pages 27, 28 and 251 of Munkres [1984].

Definition 3.2.1. Let K be a simplicial complex. We denote the free abelian group generated by a basis consisting of oriented p-simplices by, $C_p(K;\mathbb{Z})$. This is the space of finite formal sums of the oriented p-simplices, with coefficients in $\mathbb{Z}$. Elements of $C_p(K;\mathbb{Z})$ are called **primal p-chains**. Some examples are shown in Fig. 3.1. $\Diamond$

Remark 3.2.2. Chains as arrays: Since p-chains are formal sums with integer coefficients or elements of a free abelian group one way of thinking about chains is that a p-chain is simply an array or table of the oriented p-simplices of the given complex K. An integer is entered corresponding to each simplex. Two such tables can be added by adding the corresponding entries etc. This set of tables is clearly an abelian group. $\Diamond$

We view discrete p-forms as maps from the space of p-chains to $\mathbb{R}$. Recalling that the space of p-chains is a group we require these maps that define the forms to be homomorphisms into the additive group $\mathbb{R}$. Thus discrete forms are what are called cochains in algebraic topology. We will define cochains below in the definition of forms but for more context and more details readers can refer to any algebraic topology text, for example, page 251 of Munkres [1984].

This point of view of discrete forms as cochains is not new. Hassler Whitney did a lot of work in this subject as detailed in Whitney [1957]. In applications the idea appears for example in the works of Bossavit [2002b], Adams [1996], Dezin [1995], Hiptmair [1999], Sen et al. [2000]. Our point of departure is that the other authors go on to develop a theory of discrete exterior calculus of forms only. We have both forms and vector fields and in the current version of DEC we only interpolate 0-forms and vector fields. It is possible that in future work we will use Whitney forms for interpolating discrete forms. The formal definition of discrete forms follows.

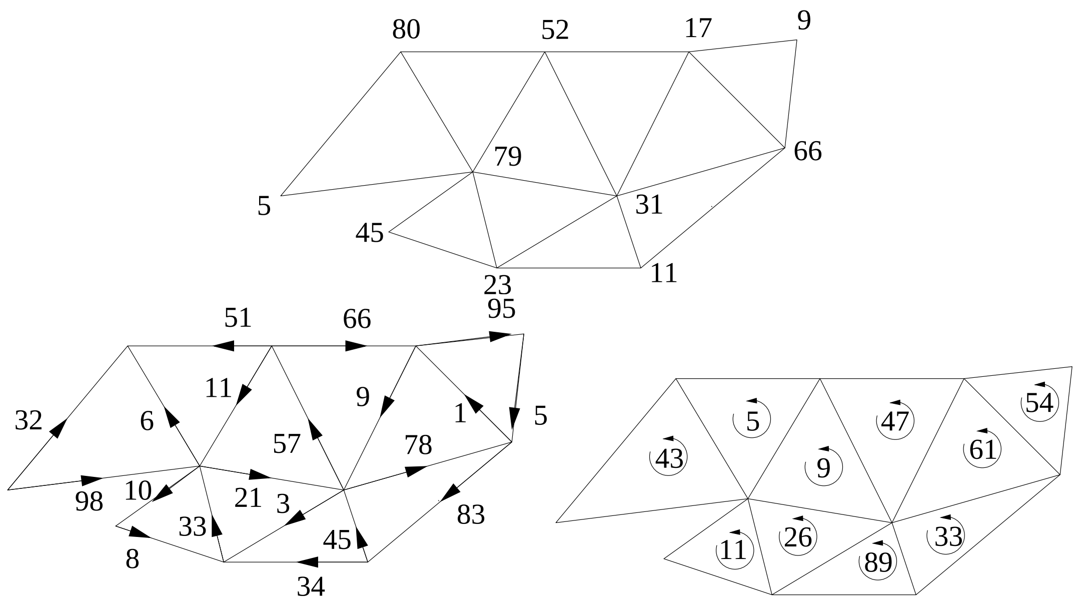


Figure 3.1: Examples of a discrete 0-form, 1-form and 2-forms. In all of these mesh is assumed to be oriented by orienting say, each triangle counterclockwise. The 0-form shown in top row is just numbers assigned to vertices. The 1-form in bottom left is numbers attached to oriented edges. The edges have to be oriented independently of the oriented triangles. On bottom right is a 2-form, here just numbers assigned to oriented triangles. In each of these examples one could also have a multiplicity associated with each vertex, edge or triangle, here assumed to be 1.

Definition 3.2.3. A **primal discrete** p**-form** α is a homomorphism from the chain group $C_p(K;\mathbb{Z})$ to the additive group $\mathbb{R}$. Thus a discrete p-form is an element of $\mathrm{Hom}(C_p(K),\mathbb{R})$ the space of **cochains**. This space becomes an abelian group if we add two homomorphisms by adding their values in $\mathbb{R}$. The standard notation for $\mathrm{Hom}(C_p(K),\mathbb{R})$ in algebraic topology is $C^p(K;\mathbb{R})$. But we will often use the notation $\Omega^p_d(K)$ for this space as a reminder that this is the space of discrete (hence the d subscript) p-forms on the simplicial complex K. Thus $\Omega^p_d(K) := C^p(K;\mathbb{R}) = \mathrm{Hom}(C_p(K),\mathbb{R})$. $\Diamond$

Note that by the above definition for p-chain $\sum_i a_i c^p_i$ (where $a_i \in \mathbb{Z}$) and a discrete p-form α, $\alpha\,(\sum_i a_i c^p_i)$ $= \sum_i a_i \alpha(c^p_i)$ and for two discrete p-forms $\alpha, \beta \in \Omega^p_d(K)$ and p-chain $c \in C_p(K;\mathbb{Z})$ we have $(\alpha+\beta)(c)$ $= \alpha(c) + \beta(c)$.

Remark 3.2.4. Real coefficients in chains: We could just as well have defined the chain group as the set of formal sums with real coefficients instead of integers so we get $C_p(K;\mathbb{R})$ instead of $C_p(K;\mathbb{Z})$. This has the advantage that this is a vector space with the p-simplices of K as the basis. This is useful when doing analysis on chains and cochains. It is also useful in the definitions of Whitney maps in the next section. $\Diamond$

3.3 Whitney and de Rham Maps

In this section we will discuss discretization of smooth forms by using the de Rham map, and interpolation of cochains using the Whitney map. In the usual exterior calculus on smooth manifolds integration of p-forms on an orientable p-dimensional manifold is defined in terms of the familiar integration in $\mathbb{R}^p$. This is done roughly speaking by doing the integration in local coordinates and showing that the value is independent of the choice of coordinates due to the change of variables theorem in $\mathbb{R}^p$. For details on this see the first few pages of Chapter 7 of Abraham et al. [1988].

In the discrete theory the above integration of smooth forms is used during discretization via the de Rham map to be defined below. This map, in association with the pasting map, produces discrete forms from smooth ones. Recall that a discrete form is a cochain hence a function on chains. The value of a discrete form on a chain is defined as the value assigned during discretization via the de Rham and pasting maps. This is made more clear in the following definitions and discussion.

Conversely Whitney maps allow us to define smooth forms corresponding to cochains. The definitions we use are from Whitney [1957]. On pages 138–140 he introduces "elementary forms" which are now called Whitney forms (Bossavit [1998]; Sen et al. [2000]). Whitney uses the notation ψ for de Rham map and ϕ for what is now called the Whitney map and we will continue to use his notation. Amongst our interpolation functions defined in Section 2.7, were the primal-primal interpolation functions written as ϕ_{σ^0,σ^n} and these were the Whitney 0-forms.

Let M be a smooth triangulable n-manifold and let K be a simplicial complex in $\mathbb{R}^N$ and π a homeomorphism of K onto M. Due to the local nature of DEC, as discussed in Section 2.8 we don't need the entire M to be discretized as K and embedded. It is enough to do the embedding locally as discussed in that section. Here π restricted to a simplex of K is what we called the pasting map in Def. 2.2.1. Whitney [1957] requires some conditions on this map, but we will use it only formally in this thesis and so we skip those technicalities.

For an abstract simplex σ^p in M let the corresponding approximating simplex be $\tau^p = \pi^{-1}(\sigma^p)$ in K. Such simplices in M form a complex L. We can define chains $c \in C_p(L;\mathbb{R})$ on this complex as formal linear combination of simplices in L and integrate p-forms on M over such p-chains. This leads to the definition of the de Rham map. The space of p-chains now is a vector space with the p-simplices as the basis elements. The space of cochains will still be denoted as $C^p(L;\mathbb{R})$ but it now stands for the vector space dual of $C_p(L;\mathbb{R})$.

Definition 3.3.1. Given a smooth p-form $\alpha \in \Omega^p(M)$, the function $\int_c \alpha$ is linear in c and hence defines a p-cochain $\psi^p\alpha$ of L. The space of cochains of chains in L will be denoted $C^p(L;\mathbb{R})$. The map $\psi^p : \Omega^p(M) \to C^p(L;\mathbb{R})$ is called the **de Rham map** and is defined by its value on simplices $\sigma^p \in L$:

$$\psi^p(\alpha)(\sigma^p) = \langle \psi^p(\alpha), \sigma^p \rangle := \int_{\sigma^p} \alpha \,.$$

To discretize a smooth form α on M we define a cochain α_d on K by defining its value on a simplex

$\pi^{-1}(\sigma^p) = \tau^p \in K$ as

$$\alpha_d(\tau^p) := \langle \psi^p(\alpha), \sigma^p \rangle \ .$$

Thus the cochain α_d on K is a discrete form produced from a smooth form on M by using a de Rham map and a pasting map. $\diamondsuit$

Definition 3.3.2. The **natural pairing** of a discrete p-form $\alpha_d = \psi^p(\alpha)$ and a p-chain c in K is the value of the discrete form on the chain, defined as the bilinear pairing $\langle \alpha_d, c \rangle = \alpha_d(c) := \langle \psi^p(\alpha), \pi(c) \rangle$. $\diamondsuit$

Remark 3.3.3. Discrete form-chain pairing in the limit: We can consider the limiting value of the evaluation of a discrete 1-form on a 1-simplex in a simplicial complex K. This limit is taken in the topology of the underlying space $|K|$. In the limit the average value of the pairing of 1-simplex and cochain becomes the natural pairing of a form and tangent vector in the direction of the simplex. This can probably be generalized to higher degree forms, but we have not done that yet. For 1-forms, the following informal calculation on a smooth manifold makes the above statement more specific.

Let M be a smooth Riemannian manifold with inner product $\langle\!\langle \ , \rangle\!\rangle$ and $c_\epsilon : (-\epsilon, +\epsilon) \to M$ be a curve on M such that $c_\epsilon(0) = x_0 \in M$. Let $v \in T_{x_0}M$ and $v = c'_\epsilon(0)$ and α a 1-form on M. Then

$$\int_{c_\epsilon} \alpha = \int_{-\epsilon}^{+\epsilon} \langle\!\langle \alpha, c'_\epsilon(t) \rangle\!\rangle \ dt \approx 2\epsilon \, \langle\!\langle \alpha(x_0), v \rangle\!\rangle$$

Thus

$$\langle\!\langle \alpha(x_0), v \rangle\!\rangle = \lim_{\epsilon \to 0} \frac{1}{l(c_\epsilon)} \int_{c_\epsilon} \alpha$$

where $l(c_\epsilon)$ is the length of the curve c_ϵ. $\diamondsuit$

Let M be a smooth manifold and L its abstract simplicial complex as before. The Whitney maps are defined by lifting the barycentric coordinates from the approximating complex K to the abstract simplicial complex L on M and defining a partition of unity on M. For technical details see page 139 of Whitney [1957]. We give the explicit expression for the maps below. The Whitney maps defined below allow us to define smooth forms $\phi\alpha_d$ corresponding to cochains α_d of L. The space of cochains is the space $C^p(L;\mathbb{R})$ and in this section we will let σ_i^p denote not only an oriented simplex or a chain, but also the cochain defined by $\sigma_i^p(\sigma_j^p) = \delta_i^j$. Then the σ_i^p form a basis for the p-cochains on L.

Definition 3.3.4. Given a simplex $\sigma^p = [v_{\lambda_0}, \ldots, v_{\lambda_p}]$ in L define the **Whitney map** $\phi^p : C^p(L;\mathbb{R}) \to \Omega^p(M)$ as a map from cochains on L to smooth forms on M by:

$$\phi^p([v_{\lambda_0}, \ldots, v_{\lambda_p}]) = p! \sum_{i=0}^{p} \phi_{\lambda_i} \, \mathbf{d}\, \phi_{\lambda_0} \wedge \ldots \widehat{\mathbf{d}\, \phi_{\lambda_i}} \wedge \ldots \wedge \mathbf{d}\, \phi_{\lambda_p} \, .$$

As mentioned above, we have abused notation and written $[v_{\lambda_0}, \ldots, v_{\lambda_p}]$ for the cochain on L that takes value 1 on that simplex and 0 elsewhere. An example of a Whitney map is $\phi(v_i) = \phi_i$ and $\phi(v_i v_j) =$

$\phi_i \, \mathbf{d} \, \phi_j - \phi_j \, \mathbf{d} \, \phi_i$. This map can be formally extended to be from discrete forms on K to smooth forms on M by using the pasting map to transfer values from the simplices of K to the simplices of L. $\diamondsuit$

The de Rham and Whitney maps satisfy the following important properties. Let $\alpha \in \Omega^p(M)$ be a smooth p-form on M, and let $\alpha_d \in C^p(L; \mathbb{R})$ be a cochain on L. Then

$$\begin{aligned} \psi \, \mathbf{d} \, \alpha &= \mathbf{d} \, \psi \alpha \\ \phi \, \mathbf{d} \, \alpha_d &= \mathbf{d} \, \phi \alpha_d \\ \psi \phi \alpha_d &= \alpha_d \\ \phi I^0 &= 1 \end{aligned}$$

where I^0 is the unit 0-cochain of L and on the RHS, 1 is the constant function on M with value 1 everywhere. There are other important properties that are given in Whitney [1957], page 139. For example for any $p \in M$, $\sum \phi_i(p) = 1$ and $\sum \mathbf{d} \, \phi_i(p) = 0$ which are like the properties of the usual barycentric coordinates on ordinary simplices. The Whitney map, of a cochain dual to a simplex σ, is supported in $\mathrm{St}(\sigma)$. The exterior derivative of each Whitney map has the nice formula:

$$\mathbf{d} \, \phi([v_{\lambda_0} \ldots v_{\lambda_p}]) = (p+1)! \, \mathbf{d} \, \phi_{\lambda_0} \wedge \ldots \wedge \mathbf{d} \, \phi_{\lambda_p} \, .$$

This expression, along with induction, is used in Whitney [1957] to show the very useful property that

$$\int_{\sigma_i^p} \phi \sigma_j^p = \delta_i^j \, .$$

Thus for example, the Whitney 1-form corresponding to an edge when integrated on that edge gives the value 1. Because of the barycentric coordinate like properties of summing to 1 and having a sum of differentials equal to 0 allows the Whitney forms to be used as the basis for defining forms from discrete forms. We do not use this interpolation of any forms higher than degree 0, but expect to do so in future work.

3.4 Dual Chains and Cochains

In Chapter 2 we defined the dual cell complex $\mathrm{D}(K)$. There is an associated cellular chain group which Munkres [1984] calls $\mathrm{D}_p(K)$. This is just the group of formal sums of cells with integer coefficients. In the cells in $\mathrm{D}(K)$ the information about the constituent elementary dual simplices is lost. In computations we often want to retain that information. For example, we are often interested in the value of some quantity on each elementary dual simplex making up the dual cell. To retain this bookkeeping information we define a duality operator which takes values in the chain group $C_p(\mathrm{csd}\, K; \mathbb{Z})$. This is done below.

Definition 3.4.1. Let K be a well-centered manifold-like simplicial complex of dimension n. The **star duality operator** $\star : C_p(K,\mathbb{Z}) \to C_{n-p}(\operatorname{csd} K;\mathbb{Z})$ is defined by

$$\star(\sigma^p) = \sum_{\sigma^p \prec \sigma^{p+1} \prec \ldots \prec \sigma^n} s_{\sigma^p,\ldots,\sigma^n} \left[c(\sigma^p), c(\sigma^{p+1}), \ldots, c(\sigma^n)\right]$$

where the sign coefficient $s_{\sigma^p,\ldots,\sigma^n}$ is chosen as ± 1 using algorithm in Rem. 2.5.1. $\Diamond$

This definition is similar to, but simpler than Def. 2.4.5. Here, only $(n-p)$-simplices are used in the union. As sets, the set $\overline{\mathrm{D}}(\sigma^p)$, and $\star(\sigma^p)$, are equal. The difference is in semantics and bookkeeping since in $\star\sigma^p$ one retains the information about the simplices it is made of.

Definition 3.4.2. The subset of chains of $C_p(\operatorname{csd} K;\mathbb{Z})$ that are equal to the cells of $\mathrm{D}(K)$ as sets, forms a subgroup of $C_p(\operatorname{csd} K;\mathbb{Z})$. This is the set of chains $\star K = \{\star\sigma | \sigma \in K\}$. As sets these form a cell complex identitical to $\mathrm{D}(K)$. We will denote this subgroup of $C_p(\operatorname{csd} K;\mathbb{Z})$ by $C_p(\star K;\mathbb{Z})$. Thus $\star K$ is a basis set for this. $\Diamond$

Definition 3.4.3. The star duality operator is a map from the primal simplicial complex to a subgroup $C_p(\star K;\mathbb{Z})$ of the chain complex of the subdivision complex. But we can formally extend the star operator to a map from $\star K$ to K by defining $\star\star\sigma^p = \pm\sigma^p$. Here the sign is defined by the following:

$$\star\star(\sigma^p) = (-1)^{p(n-p)}\sigma^p. \tag{3.4.1}$$

In other words dual of the dual of a simplex is defined to be the same simplex with orientation adjusted by ± 1. $\Diamond$

Definition 3.4.4. Cochains of cells in $C_p(\star K;\mathbb{Z})$ are the **dual discrete forms**. The space of dual p-forms will be denoted by $\Omega^p_d(\star K)$. $\Diamond$

3.5 Maps Between Complexes and Pullback of Forms

A very important aspect of calculus on manifolds is the notion of maps between manifolds. This is important for example in applications like elasticity where the object of interest is moving and changing shape with time. Indeed maps are crucial for defining the flow of a vector field since the flow, for a fixed time, is a map of a manifold to itself. Flow in turn is used in the smooth theory for defining Lie derivatives, a most important operator in applications. See, for example, Abraham et al. [1988].

Most of this thesis deals with the discretization of objects and operators defined on only one manifold. However, recently Marco Castrillon and Jerry Marsden pointed out the fact that even for defining operators on a single manifold, pullbacks are useful. This is because naturality under pullbacks can rule out definitions of operators that would not generalize to a full calculus on manifolds involving maps. We point out such an example in the definition of the wedge product in Chapter 7.

In a full calculus maps are used to pull back and push forward objects. For example vector fields can be pushed forward and forms can be pulled back naturally. A discrete map is the unique piecewise affine map obtained by extending a bijection between vertices of two complexes that are isomorphic in the category of simplicial complexes. In algebraic topology such a map is called a simplicial homeomorphism or an isomorphism. A more general concept is that of a simplicial map in which the simplex of one complex can be mapped to a different dimension. The definitions reproduced here are actually a couple of Lemmas on pages 12 and 13 of Munkres [1984].

Definition 3.5.1. Let K and L be two simplicial complexes, and $f : K^{(0)} \to L^{(0)}$ be a map. Suppose that whenever vertices $v_0 \ldots v_m$ of K span a simplex of K, the points $f(v_0), \ldots, f(v_m)$ are vertices of a simplex of L. Then f can be extended to a continuous map $g : |K| \to |L|$ such that

$$x = \sum_{i=0}^{m} \mu_i v_i \Rightarrow g(x) = \sum_{i=0}^{m} \mu_i f(v_i)$$

and g is called the (linear) **simplicial map** induced by the vertex map f. If f is a bijection and $v_0 \ldots v_m$ span a simplex of K iff $f(v_0), \ldots, f(v_m)$ span a simplex of L then the induced simplicial map g is a homeomorphism and called a **simplicial homeomorphism**, or an **isomorphism**, of K with L. $\Diamond$

Now we can define a discrete pullback. In the discrete theory, since forms are cochains, discrete pullback is defined by making the change of variables formula true by definition.

Definition 3.5.2. Let K and L be simplicial complexes and $\varphi : |K| \to |L|$ be a piecewise affine simplicial isomorphism between them. Then the **primal discrete pullback** by φ, of a p-form $\alpha \in \Omega_d^p(L)$, is written as $\varphi^* \alpha$ and defined by its evaluation on a p-simplex $\sigma^p \in K$ by:

$$\langle \varphi^*(\alpha), \sigma^p \rangle := \langle \alpha, \varphi(\sigma^p) \rangle \ .$$

Thus it makes a discrete version of the change of variable formula true by definition since the evaluation of a form on a simplex is a discrete version of integration. $\Diamond$

3.6 Exterior Derivative

Now we can define the discrete exterior derivative which we will call $\mathbf{d}$ as in the usual exterior calculus. The discrete exterior derivative will be defined as the dual with respect to the natural pairing defined above, of the boundary operator which is defined below. This operator will turn out to be local, natural with respect to pullbacks and its composition with itself will be 0, just as in smooth calculus.

Definition 3.6.1. The **boundary** operator $\partial_p : C_p(K;\mathbb{Z}) \to C_{p-1}(K;\mathbb{Z})$ is a homomorphism defined by defining it on a simplex $\sigma^p = [v_0, \ldots, v_p]$,

$$\partial_p \sigma^p = \partial_p \left([v_0, v_1, \ldots, v_p]\right) = \sum_{i=0}^{p} (-1)^i \, [v_0, \ldots, \hat{v}_i, \ldots, v_p]$$

where $[v_0, \ldots, \hat{v}_i, \ldots, v_p]$ is the $(p-1)$-simplex obtained by omitting the vertex v_i. Note that $\partial_p \circ \partial_{p+1} = 0$. $\diamondsuit$

Example 3.6.2. Boundary of a triangle: Given an oriented triangle $[v_0, v_1, v_2]$ the boundary by the above definition is the chain $[v_1, v_2] - [v_0, v_2] + [v_0, v_1]$ which are the 3 boundary edges of the triangle. ♦

Definition 3.6.3. On a simplicial complex of dimension n, a **chain complex** is a collection of chain groups and homomorphisms ∂_p such that

$$0 \longrightarrow C_n(K) \xrightarrow{\partial_n} \cdots \xrightarrow{\partial_{p+1}} C_p(K) \xrightarrow{\partial_p} \cdots \xrightarrow{\partial_1} C_0(K) \longrightarrow 0\,,$$

and $\partial_p \circ \partial_{p+1} = 0$. $\diamondsuit$

Definition 3.6.4. The **coboundary operator** $\delta^p : C^p\,(K) \to C^{p+1}\,(K)$ defined by duality to the boundary operator using the natural bilinear pairing between discrete forms and chains. Specifically, for a discrete form $\alpha^p \in \Omega_d^p(K)$ and a chain $c_{p+1} \in C_{p+1}(K; \mathbb{Z})$ we define δ^p by

$$\langle \delta^p \alpha^p, c_{p+1} \rangle = \langle \alpha^p, \partial_{p+1} c_{p+1} \rangle \tag{3.6.1}$$

that is

$$\delta^p(\alpha^p) = \alpha^p \circ \partial_{p+1}\,.$$

This definition of the coboundary operator induces the **cochain complex**,

$$0 \longleftarrow C^n(K) \xleftarrow{\delta^{n-1}} \cdots \xleftarrow{\delta^p} C^p(K) \xleftarrow{\delta^{p-1}} \cdots \xleftarrow{\delta^0} C^0(K) \longleftarrow 0\,,$$

where it is easy to see that $\delta^{p+1} \circ \delta^p = 0$. $\diamondsuit$

Definition 3.6.5. The **discrete exterior derivative** denoted by $\mathbf{d} : \Omega_d^p(K) \to \Omega_d^{p+1}(K)$ is defined to be the coboundary operator δ^p. An example is shown in Fig. 3.2. $\diamondsuit$

Remark 3.6.6. Stokes' Theorem: With the above definition of the exterior derivative $\mathbf{d} : \Omega_d^p(K) \to \Omega_d^{p+1}(K)$ and the relationship between the natural pairing and integration one can regard equation (3.6.1) as a discrete generalized Stokes' theorem. Thus given a p-chain c and a discrete p-form α the discrete Stokes' theorem, which is true by definition, states that $\langle \mathbf{d}\alpha, c \rangle = \langle \alpha, \partial c \rangle$. $\diamondsuit$

Remark 3.6.7. Properties of discrete exterior derivative: By definition discrete exterior derivative is a local operator. Furthermore, it also follows immediately from the definition that, $\mathbf{d}^{p+1}\mathbf{d}^p = 0$, since the

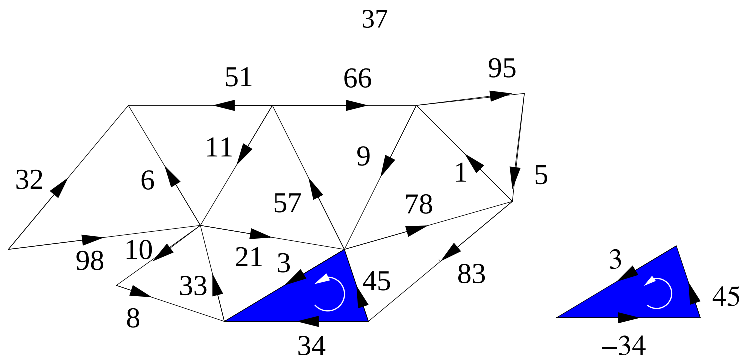


Figure 3.2: Computation of discrete exterior derivative. A 1-form is shown on the left, as numbers on oriented edges. The $\mathbf{d}$ of this will be a 2-form. The computation of this 2-form is shown on an oriented shaded triangle in the mesh. The same triangle is shown separately on the right. Its orientation induces an orientation on its boundary, shown here as going counterclockwise. This makes the numbers on the edges change sign if the induced orientation is opposite of that edge's original orientation shown on the left. The sum of these numbers is the $\mathbf{d}$ of the 1-form on the left evaluated on the shaded oriented triangle.

boundary of a boundary is empty. Finally, the discrete exterior derivative is natural with respect to discrete pullback, i.e., it commutes with discrete pullback. To see this, note that for $\alpha \in \Omega_d^p(L)$, $\varphi : |K| \to |L|$ a simplicial homeomorphism, and $\sigma^{p+1} \in K$ we have that :

$$\left\langle \varphi^*(\mathbf{d}\,\alpha), \sigma^{p+1} \right\rangle = \left\langle \mathbf{d}\,\alpha, \varphi(\sigma^{p+1}) \right\rangle = \left\langle \alpha, \partial\varphi(\sigma^{p+1}) \right\rangle = \left\langle \varphi^*\alpha, \partial\sigma^{p+1} \right\rangle = \left\langle \mathbf{d}(\varphi^*\alpha), \sigma^{p+1} \right\rangle$$

which shows the naturality of discrete pullback and exterior derivative. ◊

Definition 3.6.8. The **dual boundary** operator $\partial_p : C_p(\star K; \mathbb{Z}) \to C_{p-1}(\star K; \mathbb{Z})$ is a homomorphism defined by defining it on $\star\sigma^{n-p} = \star[v_0, \ldots, v_{n-p}]$,

$$\partial \star [v_0, ..., v_{n-p}] = \sum_{\sigma^{n-p+1} \succ \sigma^{n-p}} \star(s_{\sigma^{n-p+1}}\ \sigma^{n-p+1})\,.$$

For $0 \le p \le n-1$, the sign $s_{\sigma^{n-p+1}} = \pm 1$ is chosen so that the orientation induced on σ^{n-p} by each of the $s_{\sigma^{n-p+1}}\ \sigma^{n-p+1}$ is the same as the original orientation of σ^{n-p}.

For $p = n$ the sign s_{σ^1} is chosen so that the orientation of $\star(s_{\sigma^1}\ \sigma^1)$ is the same as that induced on $\overline{\mathrm{D}}(\sigma^1)$ by $\overline{\mathrm{D}}(\sigma^0)$. Thus for the $p = n$ case, i.e., when defining the boundary of the Voronoi dual of a primal vertex σ^0, one orients the edges incident on σ^0 so that they are all pointing inwards or outwards depending on the orientation of the complex. ◊

Remark 3.6.9. Dual boundary is not the geometric boundary: The reason that it is not enough to define the dual boundary as the geometric boundary is that near the boundary of a manifold that would be wrong. For example consider the complex in Fig. 3.3. The dual of the vertex shown is the Voronoi region shown shaded. Its geometric boundary has 5 sides (two half primal edges and 3 dual edges), whereas the dual boundary according to the definition above consists of just the dual edges as it should. ◊

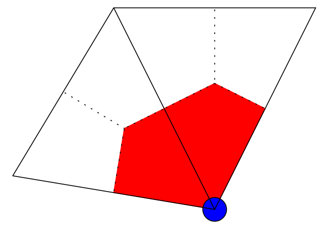


Figure 3.3: The dual boundary is not the same as the geometric boundary near the boundary of the manifold. See Rem. 3.6.9.

3.7 Speculations on Convergence

As mentioned earlier, in this thesis we do not address the issue of convergence. We don't answer questions like whether our operators converge to their smooth counterparts, and if yes, then how fast do they converge, and so on. The answers will depend on what topologies on the spaces of chains and cochains are chosen. In the case of chains we mean here the topology on the space of all chains obtained from discretization, not the point set topology on the given simplicial complex. The cochains will have to be continuous in that topology or satisfy even stronger requirements. It is not clear to us what topology to use or even how to pose the question of convergence.

In practice when one takes a sequence of meshes converging to a limit the mesh itself will move and change in its embedding space. Otherwise refining a coarse simplicial mesh would only give smaller simplices without changing the geometric shape of the complex. It is also well known that the quality of triangulation plays a subtle and important role in convergence questions. See for instance Shewchuck [2002].

Whitney [1957] defines three norms on chains and cochains – mass norm, sharp norm and flat norm. According to Harrison [2003] none of these seems enough to get convergence. With the sharp norm one can find Hodge star in the limit, but not the exterior derivative $\mathbf{d}$. The flat norm carries with it $\mathbf{d}$ but not Hodge star. Mass continuity of cochains is also not enough to retrieve the full calculus in the limit. For example Almgren [1965] has shown that mass continuous cochains are differential forms.

One possibility is to take the Hausdorff metric on the space of all chains obtainable from discretization of a manifold. This makes sense in physical problems. Discrete forms will come from the measurement by some physical device. These measurements should not change when the device is moved slightly. This is the view taken by Bossavit [2002b]. We leave these convergence questions for future work.

3.8 Summary and Discussion

In this chapter we have covered the background material needed for defining discrete forms and discrete exterior derivatives. This can be usually found in some form or other in most works in DEC and in algebraic topology. Perhaps the only unique aspect of this chapter (thanks to Castrillon Lopez [2003]) is the introduction of a discrete pullback and the proof that it commutes with exterior derivative.

One serious shortcoming of our work is that we have not done any convergence analysis. As a first step, in future work we plan to study convergence issues in flat meshes, before attempting the more difficult questions of convergence for non-flat meshes.

Chapter 4

Hodge Star and Codifferential

Results: We define a discrete Hodge star as an equality of averages between primal and their dual forms. Hodge star is an operator that involves the metric. Thus the use of metric information, in the form or circumcentric duals appears in line with the nature of the Hodge star operator. Once the Hodge star is defined, a codifferential can be defined which then immediately leads to a useful operator like the Laplace-Beltrami operator, the generalization of the usual Laplacian of Euclidean space to manifolds.

Shortcomings: In some applications there is more than one metric involved, leading to multiple Hodge star operators. An example is 3D electromagnetism in which two Hodge star operators appear. One way to handle this is to use two different embeddings of the simplices, corresponding to the two metrics. The other, is to use 4D spacetime electromagnetism, which has only 1 metric. The latter solution has the difficulty that no edge must be in the light direction. This problem is specific to relativistic applications. We have not studied these questions in detail yet.

4.1 Hodge Star

In the exterior calculus for smooth manifolds the Hodge star denoted $*$ is an isomorphism between the space of p-forms and $(n-p)$-forms. The Hodge star is useful in defining the adjoint of the exterior derivative and this adjoint is called the codifferential. For the definition of Hodge star in the smooth case see page 411 of Abraham et al. [1988].

The appearance of p and $n-p$ in the definition of Hodge star may be taken to be a hint that primal and dual meshes will play some role in the definition of a discrete Hodge star since the dual of a p-simplex is an $(n-p)$-cell. Indeed this is the case.

Definition 4.1.1. The **discrete Hodge Star** is a map $* : \Omega_d^p(K) \to \Omega_d^{n-p}(\star K)$ defined by its value over simplices and duals of simplices. Let $1 \leq p \leq n-1$. For a p-simplex σ^p and a discrete p-form α

$$\frac{1}{|\star\sigma^p|} \left\langle *\alpha, \star\sigma^p \right\rangle := \frac{1}{|\sigma^p|} \left\langle \alpha, \sigma^p \right\rangle \ . \tag{4.1.1}$$

Here recall that $|\sigma^p|$ is the unsigned p-volume of σ^p in the embedding space $\mathbb{R}^N$.

For $p = 0$ we define the Hodge star by

$$\frac{1}{s\,|\star\sigma^0|}\left\langle *\alpha, \star\sigma^0\right\rangle := \frac{1}{|\sigma^0|}\left\langle \alpha, \sigma^0\right\rangle \ .$$

Here s is ± 1. Its value depends on the orientation of K and the dimension n. The value of s decided by the following rule. Consider an edge $\sigma^1 \succ \sigma^0$ oriented so that it points away from σ^0. Give $\partial(\star\sigma^0)$ the orientation induced from $\star\sigma^0$. Then

$$s = (-1)^{n-1}\ \mathrm{sgn}(\partial(\star\sigma^0), \star\sigma^1)\ .$$

That is, if the dual of an outgoing edge is oriented the same as the orientation induced by $\star\sigma^0$ on its boundary, then the sign $s = (-1)^{n-1}$, otherwise it is the opposite of that.

For $p = n$ define the Hodge star by

$$\frac{1}{|\star\sigma^n|}\left\langle *\alpha, \star\sigma^n\right\rangle := \frac{1}{s\,|\sigma^n|}\left\langle \alpha, \sigma^n\right\rangle \ .$$

Again $s = \pm 1$ and the value of s decided by the following rule. Give σ^{n-1} the orientation induced from σ^n. If $\star\sigma^{n-1}$ points away from $\star\sigma^n$, then $s = (-1)^{n-1}$ otherwise it is the opposite sign. $\Diamond$

Remark 4.1.2. Special treatment for $p = 0$ and n: The reason for the special treatment of $p = 0$ and n is as follows. The 0-simplices have no inherent orientation. Thus for $p = 0$, in equation 4.1.1, the RHS is independent of orientation of K, but LHS is not. For $p = n$ the opposite is true. Thus the formula must be corrected by making the orientation-independent side depend on the orientation of K in some way. This amounts to using the signed volume for the n-volume in the formula. Thus for $p = 0$ we must use a signed volume $\pm|\star\sigma^0|$ on the LHS, and for $p = n$ we must use a signed volume $\pm|\sigma^n|$ on the RHS of formula (4.1.1).

Note that for other values of p, both sides of (4.1.1) depend on the orientation of K, since for $1 \leq p \leq n-1$, the orientation of the dual $\star\sigma^p$ changes when the orientation of K changes. The use of signed volume only in the case of n-volumes is consistent with the fact that even in the smooth theory, in an n-manifold, the n-volumes are signed, but lower dimensional volumes don't have any intrinsic sign. For example, in the plane we can assign a sign to an area, relative to the orientation of the manifold, in a well-define manner. But we cannot do this for lengths. Which specific sign convention is chosen for the n-volumes, is a matter of convention. We choose the one we do so that the boundary normals in the discrete divergence theorems of Chapter 6 will point outwards.

As an example of the sign used, in dimension $n = 2$, if the complex K is oriented by orienting all triangles counterclockwise, then for $p = 0$, the signed volume $s|\star\sigma^0|$ used will be $-|\star\sigma^0|$, since $(-1)^{n-1} = -1$. If K was oriented the other way, this would be $+|\sigma^0|$. In dimension $n = 3$, if the complex is oriented by orienting each tetrahedron by the right-hand rule, then the signed volume $s|\star\sigma^0|$ will be $+|\sigma^0|$, since $(-1)^{n-1} = +1$. $\Diamond$

The idea that the discrete Hodge star maps primal discrete forms to dual forms and vice versa is well known. See for example Sen et al. [2000]. However, notice we now make use of the volume of these primal and dual meshes. Similar ideas seem to appear in Hiptmair [2002a] and Harrison [1999]. The definition implies that the primal and dual *averages* must be equal. This idea has already been introduced, not in the context of exterior calculus, but in an attempt at defining discrete differential geometry operators in Meyer et al. [2002].

Lemma 4.1.3. *For a p-form α we have that $**\alpha = (-1)^{p(n-p)}\alpha$.*

Proof. The proof is a simple calculation using the property that for a simplex or a cell σ^p, $\star\star(\sigma^p) = (-1)^{p(n-p)}\sigma^p$ (equation 3.4.1). ■

4.2 Codifferential

Definition 4.2.1. Given a simplicial or a dual cell complex K the **discrete codifferential operator $\boldsymbol{\delta}$** : $\Omega_d^{p+1}(K) \to \Omega_d^p(K)$ is defined by $\boldsymbol{\delta}(\Omega_d^0(K)) = 0$ and on $p+1$ discrete forms to be $\boldsymbol{\delta}\beta = (-1)^{np+1} * \mathbf{d} * \beta$. $\diamondsuit$

With the discrete forms, Hodge star, $\mathbf{d}$ and $\boldsymbol{\delta}$ defined so far we already have enough to do an interesting calculation involving the Laplace-Beltrami operator. We will show this calculation in Section 6.1 after we have introduced discrete divergence and curl operators.

4.3 Summary and Discussion

We have defined a discrete Hodge star when there is only 1 metric involved. We will see later, that this Hodge star, yields definitions of discrete Laplace-Beltrami and various vector calculus operators that have been found by other researchers. In some applications, multiple metrics are involved and this leads to multiple Hodge star operators. What should be done when there are multiple metrics involved ?

An example, is 3D electromagnetism in a non-uniform medium. Here one has the constitutive relationships $d = *_\epsilon e$ and $b = *_\mu$, where e and h are 1-forms and d and b are two forms. Thus $*_epsilon$ and $*_mu$ are two different Hodge stars based on two different metrics. One obvious possibility for addressing this might be to embed the simplices of the complex in multiple ways, once for each metric. As mentioned in Section 2.8 each of these embeddings can be local. However we have not studied the implications of such a method.

Another solution, specific to the case of electromagnetism, might be to use spacetime formulation which involves only 1 metric. However, as pointed out to us by Castrillon Lopez and Fernandez Martinez [2003], other difficulties arise in such a formulation. Consider for example spacetime with 1 spatial dimension. If this is triangulated and a triangle has one edge in the light direction then the circumcenter will lie on this edge. One possibility for avoiding this may to use prisms with faces in spatial direction and straight lines in time direction. But this would require generalizing DEC to such cell-complexes. Thus work remains to be done in treating discrete Hodge star in problems in which multiple metrics are involved.

In the interpolation view of DEC that we will explore in future work, the codifferential, and hence the Hodge star will be determined by requiring the codifferential to be adjoint of the exterior derivative. In the end the use of a dual mesh may turned out to be a shortcut for that procedure. This needs to be explored further.

Chapter 5

Forms and Vector Fields

Results: One of the unique aspects of our work is the simultaneous presence of forms and vector fields in our theory, just as in smooth theory. This is in contrast with most previous works in this field which have had one or the other but rarely both. One exception is the work of Bossavit, such as Bossavit [2003].

In this chapter we define discrete vector fields, and discrete sharp and flat operators for going between 1-forms and vector fields. Due to the presence of primal and dual meshes, the discrete theory has many sharps and flats, unlike the smooth theory. The sharp and flat operators are used in Chapter 6 to define vector calculus operators. In the case of two of the discrete flats defined here, we prove uniqueness, dictated by requiring the discrete divergence theorem to be true.

Note that the flat and sharp are not *just* for translating vector calculus into exterior calculus. In mechanics, some quantities of interest are *defined* with these operators. An example is vorticity in fluid mechanics, which is $\mathbf{d}\, u^\flat$ where u is the fluid velocity field. Here u is not a proxy for a 1-form, it is a genuine vector field. Thus it is worthwhile to discretize sharps and flats.

Shortcomings: The discrete vector fields of this thesis are actually semi-discrete in that their domain of definition is a finite discrete set but the values are in vector spaces. It is not yet clear if this is the only or the best way to proceed with discretization of vector fields. Also, our study of discrete flats is more thorough than that of discrete sharps and it still remains to be seen if there is a flat and a sharp in DEC which are inverses of each other. This is required for some important vector calculus identities to be true. In this thesis, discrete flats are defined systematically via interpolation, but the definitions of sharps are ad hoc. For a proper definition of sharps, we believe that interpolation of 1-forms, say using Whitney maps, might be an important step that we do not take in this thesis. Furthermore, the pairing between forms and vector fields suggested here seems to be metric dependent unlike smooth theory. Interpolation of forms in future work may yield a metric independent definition.

5.1 Discrete Vector Fields

Just as discrete forms come in two flavors of primal and dual (being cochains of primal or dual chains) discrete vector fields also come in two flavors. They are defined either on the primal nodes or the dual nodes. Considered as vector valued 0-forms this data can then be interpolated in various ways using the 4 types of interpolation functions defined in Def. 2.7.1. For example, the dual vector fields can be made constant inside n-simplices or interpolated inside the Voronoi regions of primal vertices by using generalized barycentric coordinates of Warren et al. [2003]. The primal vector fields can be made constant inside the Voronoi region of a primal vertex, or linearly interpolated inside a primal n-simplex using the usual barycentric interpolation inside simplices. See Def. 2.7.1 for more on interpolation.

Thus this leads to four types of interpolated vector fields defined almost everywhere on the underlying space $|K|$. These are either constant over primal n-simplices or over dual n-cells or barycentric interpolated in these regions. These ideas are made more precise in the following definitions.

Definition 5.1.1. A **discrete dual vector field** X on a well-centered manifold-like simplicial complex K is a map from the 0-dimensional subcomplex $K_{(0)}$, the dual vertices of $\mathrm{D}(K)$, to $\mathbb{R}^N$ such that for every $\star\sigma^n$, $X(\star\sigma^n)$ is in the same plane as σ^n, that is $X(\star\sigma^n) \in \mathrm{P}(\sigma^n)$. We will denote the space of such vector fields by $\mathfrak{X}_d(\star K)$. See Fig. 5.1 for an example. The arrows drawn at the centers of triangles (dual vertices) together form an example of a dual vector field. $\Diamond$

Definition 5.1.2. Let K be a *flat* well-centered manifold-like simplicial complex of dimension n. A **discrete primal vector field** X is a map from the 0-dimensional subcomplex $K^{(0)}$, the primal vertices of K, to $\mathbb{R}^n$. We will denote the space of such vector fields by $\mathfrak{X}_d(K)$. See Fig. 5.1 for an example. The arrows drawn at the primal vertices together are an example of a primal vector field. $\Diamond$

Remark 5.1.3. Why we require flat complex for primal vector fields: In this thesis we have defined the primal vector fields only for flat meshes. This is because when the mesh is not flat (for instance a non-flat piecewise linear surface i.e., a triangle mesh in 3D) then it is not obvious what should play the role of tangent space at a vertex. It is important that at a fixed vertex the tangent space have dimension n and *not* depend on the number of n-simplices around the vertex. This is something for future work. But note that in many applications this is not a limitation since one can use dual vector fields which are perfectly well defined for non-flat meshes. Also in many important applications in computational mechanics flat mesh case is very common, for example in 3D elasticity (although not in thin shells). $\Diamond$

Definition 5.1.4. The following vector fields on the underlying space of a complex are defined by interpolating the discrete vector field data over various cells of the complex. We assume that K is a primal mesh.

(i) For a flat primal mesh K and $X \in \mathfrak{X}_d(K)$, the **primal-primal interpolated** vector field

$$\sum_{\sigma^n} \sum_{\sigma^0 \prec \sigma^n} X(\sigma^0) \phi_{\sigma^0, \sigma^n}$$

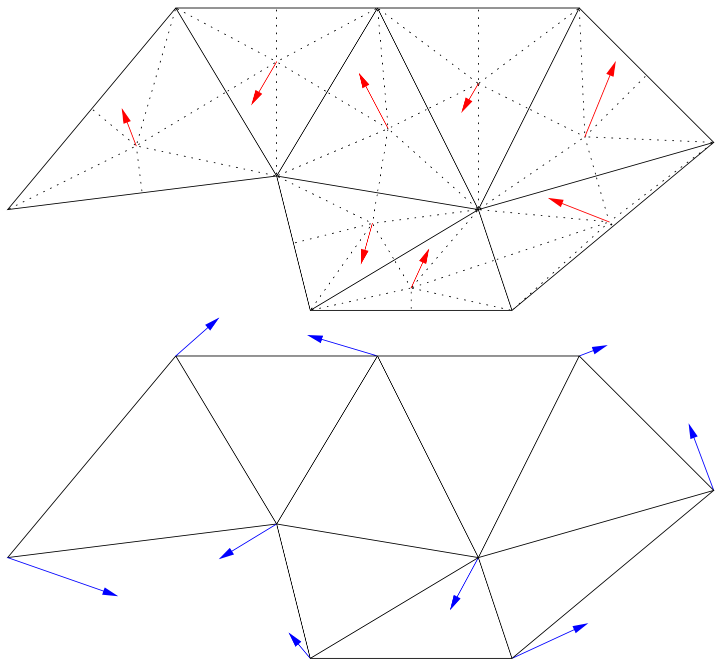


Figure 5.1: Examples of a dual (top) and a primal (bottom) discrete vector field in dimension 2. The primal mesh is in solid lines and the dotted lines are subdivision edges. For the dual field (arrows at the circumcenters of the triangles) the complex can be non-flat. Each vector should then be in the plane of its triangle. For the primal field to be defined (arrows on primal nodes) the complex has to be flat in the current version of our theory. See Def. 5.1.1, Def. 5.1.2 and Rem. 5.1.3.

is a continuous piecewise affine vector field on $|K|$, affine in each n-simplex and continuous on $|K|$,

(ii) For a flat primal mesh K and $X \in \mathfrak{X}_d(K)$, the **primal-dual interpolated** vector field

$$\sum_{\sigma^0} X(\sigma^0)\phi_{\sigma^0,\mathrm{D}(\sigma^0)}$$

is a piecewise constant vector field which is defined in each $\mathrm{D}(\sigma^0)$ (which is an open set in $|K|$) and constant there,

(iii) For a primal mesh (not necessarily flat) K and $X \in \mathfrak{X}_d(\star K)$, the **dual-primal interpolated** vector field

$$\sum_{\sigma^n} X(\star\sigma^n)\phi_{\mathrm{D}(\sigma^n),\sigma^n}$$

is a piecewise constant vector field which is defined in $\mathrm{Int}(\sigma^n)$ for each σ^n and is constant there,

(iv) For a flat primal mesh K and $X \in \mathfrak{X}_d(\star K)$, the **dual-dual interpolated** vector field

$$\sum_{\sigma^0} \sum_{\sigma^n \succ \sigma^0} X(\star\sigma^n)\phi_{\mathrm{D}(\sigma^n),\mathrm{D}(\sigma^0)}$$

is a piecewise smooth vector field continuous on $|K|$ and smooth in each $\mathrm{D}(\sigma^0)$.

See Def. 2.7.1 for more on interpolation. When we don't want to specify the type of interpolation we will use the notation $\sum X\phi$ to mean one of the above types of interpolated vector fields. $\Diamond$

5.2 Smooth Flat and Sharp

As in the smooth exterior calculus we want to define the discrete flat ($\flat$) and sharp ($\sharp$) operators to relate forms to vector fields. This allows one to write various vector calculus identities in terms of exterior calculus. Furthermore sharp and flat are important even for defining operators like divergence, gradient, curl and Laplacian. The use of sharps and flats for some common 3D vector calculus identities can be seen for the smooth case on page 426 of Abraham et al. [1988].

Now we recall the definitions of flat and sharp in the smooth case. Sharp and flat involve a metric so we assume we have a Riemannian manifold.

Definition 5.2.1. Let M be a Riemannian manifold with metric $\langle\!\langle\, , \rangle\!\rangle$ and $\alpha \in \Omega^1(M)$ a 1-form. Then the **sharp** ($\sharp$) map from 1-forms to vector fields is defined by $\left\langle\!\left\langle \alpha^\sharp, v \right\rangle\!\right\rangle = \alpha(v)$ for every point $x \in M$ and any tangent vector $v \in T_x M$. $\Diamond$

Recall that 1-forms are real valued linear functions on vector spaces so $\alpha(v)$ in the equation above is a number. For finite dimensional manifolds the existence and uniqueness of this map is guaranteed by the Riesz Representation Theorem. In coordinates the above definition can be written as follows. Let g be the Riemannian metric $\langle\!\langle\, , \rangle\!\rangle$ and let the matrix corresponding to it in some local coordinates be $[g_{ij}]$. In the same coordinate system let α_i be the coordinates of α. Then the above definition is equivalent to $(\alpha^\sharp)^i = g^{ij}\alpha_j$ where $[g^{ij}]$ is the inverse of the matrix corresponding to the metric g. The inverse of the sharp map is the flat ($\flat$) map which maps vector fields to 1-forms. Thus it can be defined as follows.

Definition 5.2.2. Let M be as above and $X \in \mathfrak{X}(M)$ a vector field on M. Then the **flat** ($\flat$) map from vector fields to 1-forms is defined by $\langle\!\langle X, v \rangle\!\rangle = X^\flat(v)$ for every point $x \in M$ and tangent vector $v \in T_x M$. $\Diamond$

To see that $\flat$ and $\sharp$ are inverses of each other note that for vector fields X and V on a Riemannian manifold M we have

$$\begin{aligned}\left\langle\!\!\left\langle (X^\flat)^\sharp, V \right\rangle\!\!\right\rangle &= X^\flat(V) = \langle\!\langle X, V \rangle\!\rangle \\ (\alpha^\sharp)^\flat(V) &= \left\langle\!\left\langle \alpha^\sharp, V \right\rangle\!\right\rangle = \alpha(V)\,.\end{aligned}$$

Example 5.2.3. Sharp and flat in gradient: The most common example of the use of sharps and flats is the gradient operator. See page 353 of Abraham et al. [1988] for details. Let f be a smooth real valued function on M. Then the gradient of f written ∇f is defined as $\nabla f = (\mathbf{d}f)^\sharp$ or equivalently $(\nabla f)^\flat = \mathbf{d}f$. $\blacklozenge$

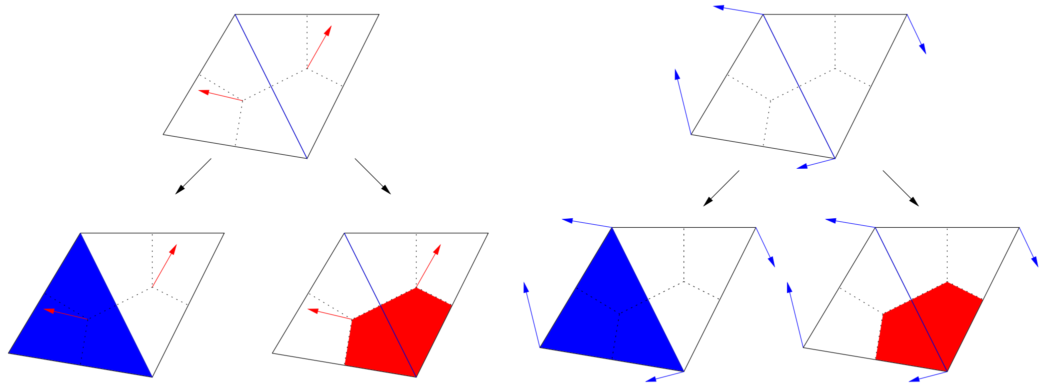


Figure 5.2: *Top row:* dual (left) and primal (right) vector fields X for which $X^\flat$ is desired on the shared edge ; *Bottom row:* (left to right) dual-primal, dual-dual, primal-primal and primal-dual interpolations. See Def. 2.7.1 for more on interpolation. The bottom row corresponds to the configuration for the discrete flats $\flat_{\mathrm{dpp}}$, $\flat_{\mathrm{ddp}}$, $\flat_{\mathrm{ppp}}$ and $\flat_{\mathrm{pdp}}$. A dual destination would yield 4 more flats for a total of 8 discrete flats.

5.3 Proliferation of Discrete Flats and Sharps

Unlike smooth exterior calculus the discrete theory has at least 8 flat operators. There are also multiple discrete sharp operators. Consider first, discrete flats. The reason for the proliferation is first of all the fact that we have primal and dual vector fields and 1-forms. In addition we can interpolate the data in the discrete vector fields to get vector fields on the underlying space $|K|$ defined (almost) everywhere on it. This interpolation can be done in 2 ways for each type of data. Thus with 2 types of data, 2 types of interpolations and 2 types of destinations we get 8 flat maps.

We decorate the 8 flats with 3 letter subscripts, using d for dual and p for primal and write $\flat_{\mathrm{ppp}}$, $\flat_{\mathrm{ppd}}$, $\flat_{\mathrm{pdp}}$, $\flat_{\mathrm{pdd}}$, $\flat_{\mathrm{dpp}}$, $\flat_{\mathrm{dpd}}$, $\flat_{\mathrm{ddp}}$ and $\flat_{\mathrm{ddd}}$, for the various flats. Thus, for example, $\flat_{\mathrm{dpp}}$ is a flat operator taking a (d)ual vector field, via a dual-(p)rimal interpolation, to a (p)rimal 1-form. See Fig. 5.2 for a pictorial depiction of 4 of these. In Section 5.5 we derive the DPP-flat ($\flat_{\mathrm{dpp}}$) and in Section 5.6 a few others.

For sharps we have to consider interpolation of data living on edges since the sharps are maps from 1-forms. In this thesis however we take a shortcut and give ad hoc definitions of some sharps without considering interpolation. In future work we will consider interpolation of 1-forms into the support volumes of primal or dual edges and interpolation of primal 1-forms into n-simplices using Whitney forms. In this thesis we will decorate the discrete sharp operators as $\sharp_{\mathrm{pp}}$, $\sharp_{\mathrm{pd}}$, $\sharp_{\mathrm{dp}}$, $\sharp_{\mathrm{dd}}$, indicating only the type of source and destination in the subscripts (and not the interpolation type). In Section 5.8 we define a PP-sharp ($\sharp_{\mathrm{pp}}$) and in Section 5.7 a PD-sharp for exact forms.

5.4 Discrete Flats

Now we describe the strategy for defining discrete flats. In the next two sections we specialize this to derive expressions for some discrete flats. Here we start with some basic facts about the smooth flat which will lead us to the discrete definitions.

Let M be a Riemannian manifold with inner product $\langle\!\langle\ ,\ \rangle\!\rangle$ and Y a smooth vector field on M. Let r be a smooth curve on M arbitrarily parameterized by $t \in [t_a, t_b] \subset \mathbb{R}$. Then by definition of smooth flat

$$\int_r Y^\flat = \int_{t_a}^{t_b} \langle\!\langle Y(r(t)), \dot{r}(t) \rangle\!\rangle \; dt \, . \tag{5.4.1}$$

Since the integral is parameterization independent we can choose arc-length parameterization s and we get

$$\int_r Y^\flat = \int_0^L \langle\!\langle Y(r(s)), \hat{r}(s) \rangle\!\rangle \; ds \tag{5.4.2}$$

where $\hat{r}(s)$ is the unit vector along r at the point $r(s)$ and L is the length of r in the metric of M.

Now, let X be a discrete primal or dual vector field on a simplicial complex K. It can be interpolated into almost all of the underlying space $|K|$ by using one of the four types of interpolations of Def. 5.1.4. Then we can define the discrete flat in terms of the flat of the piecewise interpolated vector field using equation (5.4.1). That is, define $X^\flat$, the discrete flat of discrete vector field X by its evaluation on any piecewise smooth curve r in $|K|$ by

$$\left\langle X^\flat, r \right\rangle := \int_r \left(\sum X\phi\right)^\flat \tag{5.4.3}$$

where $\sum X\phi$ is the notation for interpolated vector field. Then evaluate the RHS by using equation (5.4.1) over the various pieces of r. In a discrete theory we will generally be interested in the case when $r = c^1$ is a 1-chain (primal or dual).

By construction, the interpolated vector field $\sum X\phi$ is defined almost everywhere and hence the integral on the RHS is well defined almost everywhere in $|K|$. However, there are curves in $|K|$ where the interpolation is not defined. Specifically, primal-primal and primal-dual interpolation are defined everywhere on $|K|$. But primal-dual is not defined on the dual $(n-1)$-faces and dual-primal is not defined on primal $(n-1)$-faces. The interesting parts of the definition of a discrete flat operator are these very cases and we address this in the next two sections.

5.5 A Dual-Primal-Primal Flat

Let $X \in \mathfrak{X}_d(\star K)$ be a discrete dual vector field on K where K can be non-flat. In the case of a DPP-flat, we start with such an X, i.e., data defined on the dual vertices. The interpolation used is dual-primal interpolation (simplex-constant) and we are interested in evaluating the resulting discrete 1-form on a primal edge $\sigma^1 \in K$.

The interpolated vector field is

$$\bar{X} = \sum_{\sigma^n} X(\star\sigma^n)\phi_{D(\sigma^n),\sigma^n}$$

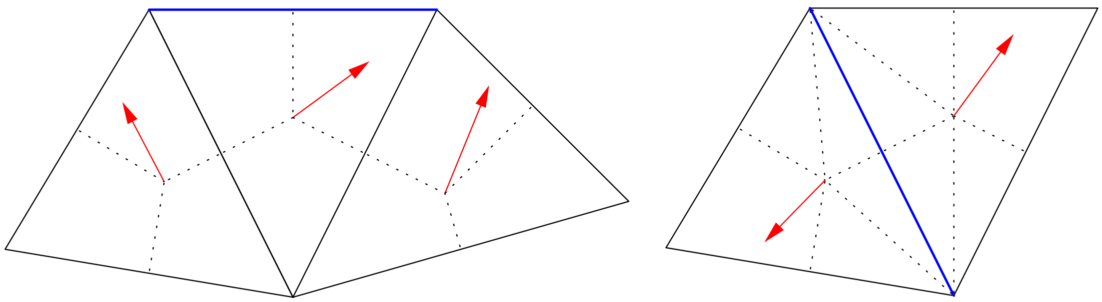


Figure 5.3: (a) For a boundary edge in 2D there is no ambiguity about the the dual vector field to use for defining a DPP-flat. The vector in the triangle containing the edge is used ; (b) On the shared edge the vector field is not well defined. In 2D the two values to choose from are in the triangles sharing the edge. See Fig. 5.4, Def. 5.5.2, and the explanation of that definition for a resolution of the ambiguity.

and this interpolated vector field is piecewise constant almost everywhere on $|K|$. Let r be a straight line segment on which $\bar{x}$ is defined. For example r can be a straight line in the interior of any face of a simplex. In this case equation (5.4.2) of previous section, with Y replaced by the interpolated field $\bar{X}$ becomes

$$\int_r \bar{X}^\flat = \langle\langle \bar{X}, \hat{r} \rangle\rangle \; L = \langle\langle \bar{X}, \vec{r}\, \rangle\rangle \tag{5.5.1}$$

where $\hat{r}$ is the unit vector along r and $\vec{r}$ is the vector along the segment r and of the same length as r. In fact the inner product is the standard inner product of the embedding space $\mathbb{R}^N$ and so we can write equation (5.5.1) as

$$\int_r \bar{X}^\flat = \langle\langle \bar{X}, \vec{r} \rangle\rangle = \bar{X} \cdot \vec{r}\,. \tag{5.5.2}$$

We can *define* this to be the value of $X^\flat$ on the straight line r on which the interpolated field $\bar{X}$ is defined.

However, as mentioned in the previous section, often the interesting cases are precisely the ones where the interpolated field $\bar{X}$ is *not* defined. In the DPP-flat we want to evaluate $X^\flat$ on primal edges and the dual-primal interpolated vector field is undefined precisely there. Fig. 5.3 explains the situation with a 2D examples.

In Fig. 5.3 (a) the primal edge σ^1 in question is a boundary edge, the top edge of the middle triangle in the figure. Even though the interpolation is not defined on σ^1, it is clear that using $\bar{X} = X(\sigma^2)$ in equation (5.5.2), where $\sigma^2 \succ \sigma^1$, will complete the definition of DPP-flat in this case. This won't work in higher dimension. For example in dimension 3, a boundary edge may be shared by many tetrahedra. The more interesting case is shown in Fig. 5.3 (b). Now the edge σ^1 in question is the edge shared by the two triangles. Since the dual-primal interpolation of X is not defined on σ^1, what should one use for $\bar{X}$ on the RHS of equation (5.5.2) ? The answer is in Def. 5.5.2 and the reasoning for it follows.

Let $\sigma^1 \in K$ be a shared edge. To give meaning to equation (5.5.2) for $r = \sigma^1$ we propose to use an average, constant value of $\bar{X}$ along σ^1. One should use a local average, using only the values of the interpolated vector field from near σ^1. For example one *could* extend $\bar{X}$ to σ^1 by defining it to be

$$\bar{X} = \sum_{\sigma^n \succ \sigma^1} \frac{|\sigma^n|}{\sum_{\sigma^n \succ \sigma^1} |\sigma^n|} X(\star\sigma^n) \,.$$

Or in general

$$\bar{X} = \sum_{\sigma^n \succ \sigma^1} \frac{a_{\sigma^n}}{\sum_{\sigma^n \succ \sigma^1} a_{\sigma^n}} X(\star\sigma^n)$$

where a_{σ^n} are constants equal to the volume of the portion of σ^n chosen in the weighting of $X(\star\sigma^n)$. We prove in Corollary 6.1.4 that discrete divergence theorem (Theorem 6.1.3) for a general dual discrete vector field is true if and only if the factors a_{σ^n} are the *unique* factors that appear Def. 5.5.2, i.e., if and only if

$$a_{\sigma^n} = |\star\sigma^1 \cap \sigma^n|$$

which is equivalent to

$$\frac{a_{\sigma^n}}{\sum_{\sigma^n \succ \sigma^1} a_{\sigma^n}} = \frac{|\star\sigma^1 \cap \sigma^n|}{|\star\sigma^1|}$$

The geometric meaning of these factors is the content of the following simple proposition.

Proposition 5.5.1. *For a primal mesh K of dimension n, a primal edge $\sigma^1 \in K$, and an n-simplex $\sigma^n \succ \sigma^1$, the following geometric identity is true :*

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

Proof. Consider an arbitrary, simply connected, compact subset of a hyperplane in $\mathbb{R}^n$, i.e, an object of dimension $n-1$. Let V be its $(n-1)$-volume. Now consider the object obtained by translating the shape in a transverse direction while scaling it uniformly and linearly in each of its $n-1$ dimensions until it reaches a size 0. That point will be called the apex and the original object the base. This pyramid like structure will be called a pyramid. If the transverse direction is orthogonal to the hyperplane containing the original object, we will call the resulting pyramid a right pyramid. For example, in dimension 3, if one starts with a triangle, one gets a tetrahedron. Starting with a square, one ends up with the usual pyramid. In dimension 2, if one starts with an edge one gets a triangle.

The volume of a pyramid, created from a base object of volume V is $(1/(n+1))Vh$ where h is the orthogonal distance of the apex from the base. For example the area of a triangle is $(1/2)$ base $\times$ height. The volume of a tetrahedron is $(1/3)$ base $\times$ height. The support volume of an edge in dimension n consists of $2k$ right pyramids, two in each of the k n-simplices containing the edge. For example the support volume of a shared edge of two triangles, consists of 4 right triangles. By construction, both the pyramids in each n-simplex will be congruent and hence of same volume. The base object of each of these is the dual of the

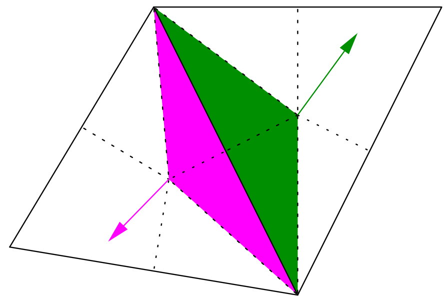


Figure 5.4: In DPP-flat the ambiguity about the vector field value at shared edge is resolved by defining a weighted average vector field on the support volume of the edge. The average vector field is defined as being constant there. The vectors are weighted by fraction of the support volume of the shared edge that falls in the corresponding n-simplex (in this case triangles). There is a simple expression for this fraction, as stated in Prop. 5.5.1. This leads to the definition of the DPP-flat in Def. 5.5.2. In Corollary 6.1.4 we show that these are the *unique* factors that make the discrete divergence theorem true.

edge lying inside the n-simplex. This is the quantity $|\star\sigma^1 \cap \sigma^n|$. Thus the volume of each of the two pyramids in each σ^n is

$$|\star\sigma^1 \cap \sigma^n| \, \frac{|\sigma^1|}{2} \, \frac{1}{n+1} \, .$$

Thus

$$\frac{|V_{\sigma^1} \cap \sigma^n|}{|V_{\sigma^1}|} = \frac{2 \, |\star\sigma^1 \cap \sigma^n| \, (|\sigma^1|/2) \, (1/(n+1))}{2 \, |\star\sigma^1| \, (|\sigma^1|/2) \, (1/(n+1))}$$

which proves the desired identity. ∎

Definition 5.5.2. Let K be a simplicial complex of dimension n, and $X \in \mathfrak{X}_d(K)$ a given dual vector field on K. The **discrete DPP-flat** is a map $\flat_{\rm dpp} : \mathfrak{X}_d(\star K) \to \Omega^1_d(K)$ and is defined by its evaluation on a primal 1-simplex σ^1 by

$$\left\langle X^{\flat_{\rm dpp}}, \sigma^1 \right\rangle = \sum_{\sigma^n \succ \sigma^1} \frac{|\star \sigma^1 \cap \sigma^n|}{|\star \sigma^1|} X(\sigma^n) \cdot \vec{\sigma}^1 \tag{5.5.3}$$

where $X(\sigma^n) \cdot \vec{\sigma}^1$ is the usual dot product of vectors in $\mathbb{R}^N$ and $\vec{\sigma}^1$ stands for the vector corresponding to σ^1 and with the same direction as the orientation of σ^1. The sum is over all σ^n containing the edge σ^1. The volume factors are in $n-1$ dimensions. We will sometimes write $X^\flat$ instead of $X^{\flat_{\rm dpp}}$. ◊

In the smooth theory the flat and sharp are inverses of each other. The next proposition shows that at least the DPP-flat does not have an inverse in the literal sense. We have not investigated yet, if an inverse exists in some other, for example, averaged sense.

Proposition 5.5.3. *The discrete flat $\flat_{\rm dpp}$ is neither surjective nor injective. Thus it does not even have a one-sided inverse.*

Proof. Fig. 5.5 shows an example of a vector field that is not zero but whose DPP-flat is 0. Since the discrete DPP-flat function is a linear function of the vector field data, this implies that it is not injective. It is also

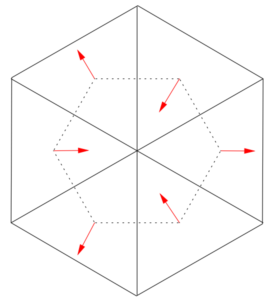


Figure 5.5: A dual vector field that shows that the $\flat_{\mathrm{dpp}}$ is not one-one. The arrows are based at circumcenters and are supposed to be of equal lengths and orthogonal to the corresponding outer boundary edge.

not surjective. Just consider an equilateral triangle and a 1-form that takes value 1 on each edge. There is no vector field whose DPP-flat will give this 1-form. ■

5.6 Other Discrete Flats

Now we will discuss the remaining 7 types of discrete flats. For some we give the explicit expression and for the more complicated ones we describe the construction in words.

PPP-flat: Barycentric interpolation inside an n-simplex reduces to barycentric interpolation along the edge, i.e., linear interpolation along the edge. Thus we have for $\sigma^1 = [v_0, v_1]$

$$\left\langle X^{\flat_{\mathrm{ppp}}}, \sigma^1 \right\rangle = \int_{\sigma^1} \bar{X} \cdot \vec{\sigma}^1$$

where $\bar{X}$ is the linear interpolation of the values $X(v_0)$ and $X(v_1)$ along σ^1.

PPD-flat: Here the vectors at the vertices of σ^n are linearly interpolated inside the simplex. If $\bar{X}$ is this interpolation then for $\sigma^{n-1} \prec \sigma^n$

$$\left\langle X^{\flat_{\mathrm{ppd}}}, \sigma^1 \right\rangle = \int_{\sigma^1} \bar{X} \cdot \star\sigma^{n-1} .$$

PDP-flat: The vector field in Voronoi region of each vertex is constant. Thus for $\sigma^1 = [v_0, v_1]$

$$\begin{aligned} \left\langle X^{\flat_{\mathrm{pdp}}}, \sigma^1 \right\rangle &= X(v_0) \cdot \frac{\vec{\sigma}^1}{2} + X(v_1) \cdot \frac{\vec{\sigma}^1}{2} \\ &= \frac{X(v_0) + X(v_1)}{2} \cdot \vec{\sigma}^1 \end{aligned}$$

and so the average value along the edge is used.

PDD-flat: Like the previous case, the interpolated vector field is constant in the Voronoi region of a vertex. Let $\sigma^{n-1} \prec \sigma^n$ and consider the dual edge $\star\sigma^{n-1}$ where the flat is to be evaluated. This dual edge intersects σ^{n-1} at the circumcenter $c(\sigma^{n-1})$. Thus *every point* on the dual edge is equidistant to every vertex $\sigma^0 \prec \sigma^{n-1}$. Thus clearly the values $X(\sigma^0)$ should be combined with the same factor 1. Indeed this is also the conclusion of Corollary 6.1.8 of the proof of primal discrete divergence theorem in Chapter 6. In other words, a primal discrete divergence theorem is true if and only if PDD-flat is defined as below:

$$\left\langle X^{\flat_{\mathrm{pdd}}}, \star\sigma^{n-1} \right\rangle := \sum_{\sigma^0 \prec \sigma^{n-1}} X(\sigma^0) \ \cdot \ (\star\sigma^{n-1})$$

where we have used $\star\sigma^{n-1}$ to mean both the dual edge and the dual edge considered as a vector.

DPP-flat: This has been derived in the previous section.

DPD-flat: Here X is made constant inside an n-simplex. Let $\star\sigma^{n-1}$ be the dual edge on which we want to evaluate the flat. We define

$$\left\langle X^{\flat_{\mathrm{dpd}}}, \star\sigma^1 \right\rangle = \sum_{\sigma^n \succ \sigma^{n-1}} X(\sigma^n) \cdot (\star\sigma^{n-1} \cap \sigma^n)$$

where by abuse of notation, $\star\sigma^{n-1} \cap \sigma^n$ stands for the vector corresponding to the dual edge in σ^n.

DDP-flat and **DDD-flat:** These two require the new barycentric interpolation of Warren et al. [2003] and we will not use them in this thesis.

5.7 A Primal-Dual Sharp for Exact Forms

As mentioned in Section 5.3 a proper development of the discrete flat operator should probably start with interpolating the discrete 1-form data. The two choices for interpolation might be into the support volume, and into the simplex by using Whitney forms of Section 3.3. We do not do that in this thesis, and instead, we shortcut the process of interpolation and define 4 types of sharps based on 2 types of sources and 2 types of destination. Of these we will only discuss PD-sharp for exact forms and PP-sharp.

To motivate the definition of primal-dual sharp for exact forms we do the following simple calculation of gradient. Let $\bar{f}$ be the function that is obtained by linearly interpolating in an n-simplex the discrete 0-form f . Thus for a point $x \in \sigma^n$, using the interpolation functions we have that

$$\bar{f}\big|_{\sigma^n}(x) = \sum_{\sigma^0 \prec \sigma^n} f(\sigma^0) \ \phi_{\sigma^0,\sigma^n}(x)\,.$$

Taking the usual gradient of this smooth function in $\operatorname{Int} \sigma^n$ we have

$$(\nabla \bar{f})\big|_{\operatorname{Int}(\sigma^n)} = \sum_{\sigma^0 \prec \sigma^n} f(\sigma^0) \nabla \phi_{\sigma^0, \sigma^n} \, . \tag{5.7.1}$$

Let $[v_0, \dots, v_n] = \sigma^n$. Then by equation (2.7.2) we have that

$$\nabla \phi_{v_0, \sigma^n} = - \sum_{1 \le i \le n} \nabla \phi_{v_i, \sigma^n} \, .$$

Substituting this into (5.7.1) we get

$$\begin{aligned} (\nabla \bar{f})\big|_{\operatorname{Int}(\sigma^n)} &= \sum_{0 \le i \le n} f(v_i) \nabla \phi_{v_i, \sigma^n} \\ &= \sum_{1 \le i \le n} f(v_i) \nabla \phi_{v_i, \sigma^n} - \sum_{1 \le i \le n} f(v_0) \nabla \phi_{v_i, \sigma^n} \\ &= \sum_{1 \le i \le n} (f(v_i) - f(v_0)) \nabla \phi_{v_i, \sigma^n} \, . \end{aligned}$$

Thus

$$(\nabla \bar{f})\big|_{\operatorname{Int}(\sigma^n)} = \sum_{1 \le i \le n} (f(v_i) - f(v_0)) \nabla \phi_{v_i, \sigma^n} \, .$$

Note that here the coefficients $f(v_i) - f(v_0)$ are nothing but $\mathbf{d} \, f$ evaluated on the edge $[v_0, v_i]$. Since $\nabla \bar{f} = \mathbf{d} \, \bar{f}$ in the simplex interior, the above equation suggests the following definition for a primal-dual sharp.

Definition 5.7.1. Let f be a discrete 0-form on a primal mesh, σ^n a simplex in this mesh and v a vertex of σ^n. Then the **discrete primal-dual sharp for exact forms** is defined by

$$\left\langle (\mathbf{d} \, f)^{\sharp_{\mathrm{pd}}}, \star \sigma^n \right\rangle := \sum_{\sigma^0 \prec \sigma^n} (f(\sigma^0) - f(v)) \nabla \phi_{\sigma^0, \sigma^n} \, . \tag{5.7.2}$$

We state without proof that the value is independent of which v is chosen as the distinguished vertex. This is clear from the calculation of gradient done above. A pictorial depiction of this formula is in Fig. 5.6. $\Diamond$

We did not define the primal-dual sharp for general forms because in that case the choice of the vertex v *will* in general, affect the answer. One could try to take all vertices of σ^n one by one, and use some sort of weighting, such as $|\star\sigma^0 \cap \sigma^n|/\sigma^n$. Then in equation (5.7.2) above, $f(\sigma^0) - f(v)$ would be replaced by $\left\langle \alpha, [\sigma^0, v] \right\rangle$ where α is the discrete 1-form whose sharp is desired. However, this is an ad hoc weighting and as we have been stressing, perhaps the right way to build discrete sharps is to first interpolate the discrete 1-forms, using, for example, Whitney maps.

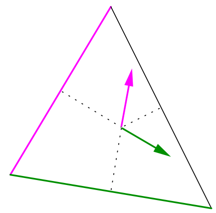


Figure 5.6: The geometry of PD-sharp for exact forms. The color coding shows the values that are related. The arrows are gradients of primal-primal interpolation functions. The sum is taken at a vertex, any vertex will do and will give the same result. The value of the exact form on each edges incident on that vertex is used.

5.8 A Primal-Primal Sharp

If we start with a primal 1-form and want to produce from it a primal vector field at a vertex, then one ad hoc definition is to compute the sharp in each simplex of a one-ring around the vertex. This can be done by using that vertex as the distinguished vertex v of equation (5.7.2) and using evaluations of the 1-form on edges instead of evaluation of $\mathbf{d}\, f$ in that equation. Then one can use some weighting for each simplex, say the portion of the Voronoi region that falls in each simplex. Or, the fraction of volume that the simplex represents, of the one-ring volume. The former choice would lead to the following definition. Unlike our uniqueness result in the discrete flat case, we have not attempted any uniqueness proofs in discrete sharps, since the future development will probably involve interpolation of 1-forms.

Definition 5.8.1. Let K be a flat simplicial complex of dimension n and let $\alpha \in \Omega^1_d(K)$ be a discrete primal 1-form. The **discrete primal-primal sharp** is $\sharp_{\mathrm{pp}} : \Omega^1_d(K) \to \mathfrak{X}_d(K)$ (but we'll just write $\sharp$) and is defined by its evaluation on a given vertex v as follows

$$\alpha^\sharp(v) = \sum_{[v,\sigma^0]} \left\langle \alpha, [v,\sigma^0] \right\rangle \sum_{\sigma^n \succ [v,\sigma^0]} \frac{|\star v \cap \sigma^n|}{|\sigma^n|} \nabla \phi_{\sigma^0,\sigma^n} \,. \tag{5.8.1}$$

The outer sum is over all 1-simplices $[v,\sigma^0]$ containing the given vertex v and the inner sum is over all σ^n containing the 1-simplex $[v,\sigma^0]$. The volume factors are in dimension n. The maps ϕ_{σ^0,σ^n} are the primal-primal interpolation functions. A pictorial depiction is in Fig. 5.7. $\diamondsuit$

5.9 Composing Sharps and Flats

Note that $\flat_{\mathrm{dpp}}$ goes from dual vector fields to primal 1-forms. But $\sharp_{\mathrm{pp}}$ goes from primal 1-forms to primal vector fields. Thus although sharp and flat in the smooth theory are inverses, here *these* particular the discrete sharp and flats cannot be inverses of each other. We have see also in Prop. 5.5.3 that the DPP-flat cannot have an inverse in the usual sense.

The incompatibility of domains and codomains for DPP-flat and PP-sharp seems similar to the incon-

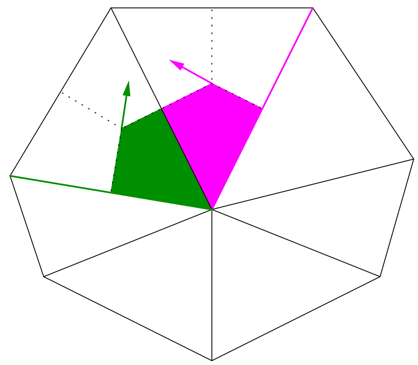


Figure 5.7: The geometry of PP-sharp definition. The color coding shows the quantities that are related. The arrows are the gradients of interpolation functions.

sistency of domains and ranges of mimetic div, grad, curl described on page 85 of Hyman and Shashkov [1997a]. It is possible that analogous to the discrete Hodge star case some flats and sharps are inverses in terms of averages but this is something we have not studied yet. Neither have we studied all possible combinations of discrete flats and sharps. We also note that we implicitly define a sharp and flat in Tong et al. [2003] so that $\mathrm{div} \circ \mathrm{curl} = 0$ and $\mathrm{curl} \circ \mathrm{grad} = 0$. Although we do not use DEC formalism there, the above result, which in exterior calculus is a consequence of sharp and flat being inverses of each other, is reproduced in Section 9.3. $\diamondsuit$

5.10 Natural Pairing of Forms and Vector Fields

In the smooth theory pairing of forms and vector fields is a metric independent operation. At a point on the smooth manifold, 1-forms are the usual linear algebraic duals of the vectors at that point. So the pairing is just evaluation of the real-valued linear functions (1-forms) on the vector at that point.

Here we define the natural pairing of discrete 1-forms and vector fields that seems to depend on a metric. After that we suggest how we may give a metric independent definition. We can use equation in Def. 5.2.1 which is the definition of $\sharp$ in the smooth case but now we use it as the definition of the natural pairing. This gives us the following definition for discrete natural pairing.

Definition 5.10.1. Let K be a flat simplicial complex of dimension n, $\alpha \in \Omega^1_d(K)$ a discrete primal 1-form and $X \in \mathfrak{X}_d(K)$ a discrete primal vector field. Then their **discrete natural pairing**, $\alpha(X)$ at a 0-simplex σ^0 is defined as

$$\alpha(X)(\sigma^0) = \alpha^\sharp(\sigma^0) \cdot (X(\sigma^0))$$

where $\cdot$ is the usual dot product in the embedding space $\mathbb{R}^n$. $\diamondsuit$

In future work we intend to consider interpolation of 1-forms using Whitney forms and also into the support volumes of edges. Once the form is interpolated, one can use the smooth definition of pairing between forms and vector fields to yield a discrete definition of pairing.

5.11 Summary and Discussion

The focus of this chapter has been the definition of sharps and flats. These are metric dependent operators that were defined in the smooth theory, so that vector calculus could be brought under the umbrella of exterior calculus. In this chapter we have made explicit the translation between discrete forms and discrete vector fields using the metric information in specific, geometric formulas. In works on DEC that use vector fields as proxies for forms, this is usually done implicitly by assuming flat space, and often even in $\mathbb{R}^3$. Our development is explicit and general and works for non-flat meshes, when the choice of vector field and interpolation scheme allows non-flatness. This allows one to define discrete vector calculus operators using DEC. This is not essential for equations of mechanics, but it does help in discretizing equations that are written in terms of div, grad and curl.

We have been able to define flats by using interpolation of vector fields which we treat as vector valued 0-forms. For a proper definition of sharps it may be necessary to first interpolate 1-forms. Instead, here we gave some ad hoc definitions. One drawback of these definitions is that the resulting definition of form-vector field pairing is metric dependent. We also did not demonstrate a discrete sharp-flat inverse pair. In addition, we showed that one of the discrete flats that we studied in detail cannot have an inverse in the usual sense. There may be an inverse pair, or the inverse may exist in some kind of average manner. That is for future study. Indirect evidence that such might be the case comes from our other work, on vector field decomposition in which we have found vector calculus operators that satisfy the usual identities which are, in smooth theory, a consequence of sharp and flat being inverses of each other and the fact that $\mathbf{d} \circ \mathbf{d} = 0$.

Chapter 6

Div, Grad, Curl and Laplace-Beltrami

Results: In smooth theory, divergence is defined in terms of the Lie derivative of a volume form. We will define it first via an identity of exterior calculus involving flat operator. We show that we get a primal and a dual discrete divergence theorem. Corollaries of the proofs of these also show that the factors in the definition of DPP-flat and PDD-flat are unique. Also, in the 2D case our formula for discrete divergence is the same as that appearing in other literature such as Polthier and Preuss [2002]. Then we briefly discuss the other definition of divergence, based on derivative of volume. We define Laplace-de Rham operator, of which, a special case is the Laplace-Beltrami of functions on manifolds. In a 2D calculation, our DEC definition reproduces a well-known Laplace-Beltrami formula found in computer graphics by Meyer et al. [2002]. The formula can also be derived variationally, using a DEC framework, as shown to us recently by Castrillon Lopez and Fernandez Martinez [2003]. Our discrete gradient is defined using the PD-sharp for exact forms from the previous chapter and another one using an averaging property of the PP-sharp. For curl we show a 2D definition and a 3D definition and show that the 2D formula in DEC agrees, modulo an area factor, with that found by Polthier and Preuss [2002].

Shortcomings: The definition of divergence involves two Hodge stars and a flat operator. It is an identity in smooth theory that the metric inherent in these, finally enters the divergence formula only via the volume form. We have not shown that the same is true in discrete theory. However we give some preliminary comments on the volume based definition of divergence in this chapter. We have derived a 3D curl in our other work in Tong et al. [2003] that satisfies all the usual vector calculus identities. But we have not yet reproduced that definition via a DEC derivation. We think that the proper definitions of a general gradient and 3D curl requires that the sharp operator be build from interpolation of 1-forms, like the flat was built from interpolation of 0-forms.

6.1 Divergence

In the smooth theory, divergence is defined via a Lie derivative by $(\operatorname{div} X)\mu = \pounds_X \mu$ where μ is the volume form associated with the given metric. In future work we plan to explore this definition in the discrete theory. Some preliminary comments about this are given at the end of this section, in the context of Def. 6.1.9 where a volume based definition is given. This volume based definition is the straightforward, intuitive interpretation of the Lie derivative definition.

The main content of this section however, is the definition of a discrete divergence using an identity from smooth theory. We don't know yet if Lie derivative based definition and the present definition will turn out to be identical. But we point out that the present flat based definition does result in a discrete divergence theorem, for both primal and dual vector fields. This is the content of Theorem 6.1.3 and 6.1.7. First we prove some lemmas that establish a discrete divergence theorem on a single dual n-cell and a single primal n-simplex. Later we combine many dual n-cells or primal n-simplices to produce the divergence theorems.

Definition 6.1.1. For a discrete vector field X the **discrete divergence**, $\operatorname{div}(X)$ is defined to be

$$\operatorname{div}(X) := -\boldsymbol{\delta} X^\flat = * \, \mathbf{d} * X^\flat \, .$$

The above definition is actually a theorem in smooth exterior calculus and a consequence of the Lie derivative based definition. See, for example, page 458 of Abraham et al. [1988]. If X is a dual vector field, the discrete flat used above is $\flat_{\mathrm{dpp}}$. For a primal vector field, $\flat_{\mathrm{pdd}}$ is used. In other words if $X \in \mathfrak{X}_d(\star K)$ then

$$\left\langle \operatorname{div}(X), \sigma^0 \right\rangle = * \, \mathbf{d} * X^{\flat_{\mathrm{dpp}}} \tag{6.1.1}$$

and if $X \in \mathfrak{X}_d(K)$ then

$$\langle \operatorname{div}(X), \star\sigma^n \rangle = * \, \mathbf{d} * X^{\flat_{\mathrm{pdd}}} \, . \tag{6.1.2}$$

Thus for a dual vector field, divergence is a primal 0-form, and for a primal vector field divergence is a dual 0-form. $\Diamond$

The divergence defined as above satisfies a discrete divergence theorem. This is proved for a dual vector field in the following lemma and theorem. For a primal vector field, we only sketch the proof. We will now prove the discrete divergence theorem for dual vector fields over dual n-cells, starting with the result over a single dual n-cell.

Lemma 6.1.2 (Divergence Theorem on a Dual n-cell). *Let K be a primal mesh, not necessarily flat, and* *of dimension n, and σ^0, a vertex in it. Let $X \in \mathfrak{X}_d(\star K)$ be a dual vector field on the complex. Then*

$$(6.1.3) \qquad |\star\sigma^0| \;\; \langle \operatorname{div}(X), \sigma^0 \rangle = \sum_{\sigma^1 \succ \sigma^0} \; \sum_{\sigma^n \succ \sigma^1} |\star \sigma^1 \cap \sigma^n| \;\; \left(X(\star\sigma^n) \cdot \frac{\vec{\sigma}^1}{|\sigma^1|} \right) .$$

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

Proof. First we indicate why we call this a divergence theorem. Here $\vec{\sigma}^1/|\sigma^1|$ is a unit normal perpendicular to the boundary of the region $\star\sigma^0$ and pointing outwards. This region is the Voronoi region of the vertex σ^0 where $\operatorname{div}(X)$ is being evaluated. The quantity $|\star \sigma^1 \cap \sigma^n|$ is the length of the part of the dual edge of σ^1 that is in the simplex σ^n. Thus equation (6.1.3) is a statement of the divergence theorem over the Voronoi region $\star\sigma^0$, i.e., the integral of divergence over this region equals the the flux of X through the boundary of this region.

In this proof we will write $\flat$ as a shorthand for $\flat_{\mathrm{dpp}}$. Since $\operatorname{div}(X) = *\,\mathbf{d}\,{*}X^\flat$, as expected, the divergence is a scalar. In particular because the flat used is DPP-flat and X is a dual vector field, $X^\flat$ is a primal 1-form and so due to the two Hodge stars, $\operatorname{div}(X)$ is a primal 0-form. Thus we can compute it at a primal vertex, σ^0. This is the quantity

$$\left\langle \operatorname{div}(X), \sigma^0 \right\rangle = \left\langle *\,\mathbf{d}\,{*}X^\flat, \sigma^0 \right\rangle .$$

Using the definition of Hodge star we get

$$\frac{1}{|\sigma^0|} \left\langle *\,\mathbf{d}\,{*}X^\flat, \sigma^0 \right\rangle = \frac{1}{s\,|\star\sigma^0|} \left\langle *\,*\,\mathbf{d}\,{*}X^\flat, \star\sigma^0 \right\rangle .$$

Here s is the sign $\pm$ as discussed in the Hodge star definition for 0- and n-simplices in Chapter 4. Assume, without loss of generality, that the orientation of K is the one that makes $s = (-1)^{n-1}$. Then, since $|\sigma^0| = 1$, we get

$$\begin{aligned} \left\langle \operatorname{div}(X), \sigma^0 \right\rangle &= \frac{(-1)^{n-1}}{|\star\sigma^0|} \left\langle *\,*\,\mathbf{d}\,{*}X^\flat, \star\sigma^0 \right\rangle \\ &= \frac{(-1)^{n-1}}{|\star\sigma^0|} \left\langle \mathbf{d}\,{*}X^\flat, \star\sigma^0 \right\rangle \\ &= \frac{(-1)^{n-1}}{|\star\sigma^0|} \left\langle {*}X^\flat, \partial(\star\sigma^0) \right\rangle . \end{aligned}$$

The second equality is by application of definition of Hodge star and the last one above is by application of discrete Stokes' theorem. But by Def. 3.6.8 of dual boundary,

$$\partial(\star\sigma^0) = \sum_{\sigma^1 \succ \sigma^0} \star(s_{\sigma^1}\sigma^1)$$

where the sign $s_{\sigma^1} = \pm 1$ is chosen to that the edges $s_{\sigma^1}\;\sigma^1$ all point inwards or outwards, depending on the orientation of K as explained Def. 3.6.8. In our case, the orientation has been chosen so that they will all point outwards. See Def. 4.1.1 and Def. 3.6.8 for an explanation.

For simplicity of notation in the calculation that follows, we will use σ^1 instead of $s_{\sigma^1}\sigma^1$. That is, we will assume that the edges σ^1 have been oriented so that they all point outwards. Now we can use the linearity of the pairing of forms and chains and write

$$\begin{aligned}\frac{(-1)^{n-1}}{|\star\sigma^0|}\left\langle *X^\flat, \partial(\star\sigma^0)\right\rangle &= \frac{(-1)^{n-1}}{|\star\sigma^0|}\left\langle *X^\flat, \sum_{\sigma^1\succ\sigma^0}\star\sigma^1\right\rangle \\ &= \frac{(-1)^{n-1}}{|\star\sigma^0|}\sum_{\sigma^1\succ\sigma^0}\left\langle *X^\flat, \star\sigma^1\right\rangle .\end{aligned}$$

Another use of the definition of discrete Hodge star now gives

$$\frac{1}{|\star\sigma^0|}\sum_{\sigma^1\succ\sigma^0}\left\langle *X^\flat, \star\sigma^1\right\rangle = \frac{1}{|\star\sigma^0|}\sum_{\sigma^1\succ\sigma^0}\frac{|\star\sigma^1|}{|\sigma^1|}\left\langle X^\flat, \sigma^1\right\rangle .$$

Now we can use the definition of DPP-flat operator and we get that

$$\begin{aligned}\frac{1}{|\star\sigma^0|}\sum_{\sigma^1\succ\sigma^0}\frac{|\star\sigma^1|}{|\sigma^1|}\langle X^\flat, \sigma^1\rangle &= \frac{1}{|\star\sigma^0|}\sum_{\sigma^1\succ\sigma^0}\frac{|\star\sigma^1|}{|\sigma^1|}\sum_{\sigma^n\succ\sigma^1}\frac{|\star\sigma^1\cap\sigma^n|}{|\star\sigma^1|}X(\star\sigma^n)\cdot\vec{\sigma}^1 \\ &= \frac{1}{|\star\sigma^0|}\sum_{\sigma^1\succ\sigma^0}\sum_{\sigma^n\succ\sigma^1}\frac{|\star\sigma^1\cap\sigma^n|}{|\sigma^1|}X(\star\sigma^n)\cdot\vec{\sigma}^1 \\ &= \frac{1}{|\star\sigma^0|}\sum_{\sigma^1\succ\sigma^0}\sum_{\sigma^n\succ\sigma^1}|\star\sigma^1\cap\sigma^n|\left(X(\star\sigma^n)\cdot\frac{\vec{\sigma}^1}{|\sigma^1|}\right)\end{aligned} \tag{6.1.4}$$

where σ^1 all point outwards. Thus we have finally that

$$|\star\sigma^0|\ \langle\operatorname{div}(X), \sigma^0\rangle = \sum_{\sigma^1\succ\sigma^0}\ \sum_{\sigma^n\succ\sigma^1}|\star\sigma^1\cap\sigma^n|\ \left(X(\star\sigma^n)\cdot\frac{\vec{\sigma}^1}{|\sigma^1|}\right)$$

which we wanted to show. ■

Theorem 6.1.3 (Divergence Theorem on a Dual n-Chain). *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.*

Proof. It is enough to show that for two adjacent dual n-cells the contributions due to the shared dual edge cancel in the RHS of equation (6.1.3). Consider two such adjacent dual n-cells. Let v_0 and v_1 be the two vertices of which these are the dual cells. Since the cells are adjacent, there is an edge $[v_0, v_1]$ and its dual is the only shared face. That edge appears with opposite signs for the two versions of equation 6.1.3 corresponding to v_0 and v_1. The coefficients are otherwise the same. Thus the term corresponding to that edge cancels. ■

Corollary 6.1.4 (Uniqueness of DPP-flat). *The discrete divergence theorem on a dual n-cell is true if and* *only if the factors in the DPP-flat definition, Def. 5.5.2, are*

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

Proof. Suppose in the proof of Lemma 6.1.2 above we replace the definition of $X^{\flat_{\mathrm{dpp}}}$ in equation (6.1.4) by one that uses arbitrary factors b_{σ^n}. Thus we have, in the proof of Lemma 6.1.2, that

$$\begin{aligned}\left\langle \operatorname{div}(X), \sigma^0 \right\rangle &= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \frac{|\star\sigma^1|}{|\sigma^1|} \sum_{\sigma^n \succ \sigma^1} b_{\sigma^n} X(\star\sigma^n) \cdot \vec{\sigma}^1 \\ &= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \sum_{\sigma^n \succ \sigma^1} |\star\sigma^1| b_{\sigma^n} \left(X(\star\sigma^n) \cdot \frac{\vec{\sigma}^1}{|\sigma^1|} \right).\end{aligned}$$

Since the divergence theorem must be true for any dual vector field X we can choose one which is 0 everywhere except in one $\sigma^n \succ \sigma^0$. Then the divergence theorem is true iff $|\star\sigma^1 \cap \sigma^n| = |\star\sigma^1| b_{\sigma^n}$ for some $\sigma^1 \prec \sigma^n$, which implies that

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

Since σ^n was arbitrary, this proves the desired uniqueness. ■

Remark 6.1.5. Divergence of dual vector field in primal is 0: If divergence is computed by Def. 6.1.1, for a dual vector field inside a primal n-simplex, the DPD-flat is used. An easy calculation shows that then the divergence at the center of the simplex is 0, because in the calculation, there is a sum of the dot product of a vector with the dual edges which are scaled so that the sum is 0. Thus one gets the correct answer in this case. To compute the divergence inside a primal simplex but for a primal vector field, one uses a PDD-flat and this results in the following Lemma. ♢

Lemma 6.1.6 (Divergence Theorem on a Primal n-simplex). *Let K be a flat primal mesh of dimension n, and σ^0 a vertex in it. Let $X \in \mathfrak{X}_d(K)$ be a primal vector field on the complex. Then*

$$|\sigma^n| \ \left\langle \operatorname{div}(X), \star\sigma^n \right\rangle = \sum_{\sigma^{n-1} \prec \sigma^n} |\sigma^{n-1}| \left(\sum_{\sigma^0 \prec \sigma^{n-1}} X(\sigma^0) \right) \cdot \frac{\star\sigma^{n-1}}{|\star\sigma^{n-1}|}\,. \tag{6.1.5}$$

where the orientation of σ^n is such that the dual edges $\star\sigma^{n-1}$ point outwards. If the given orientation is the other one then RHS is multiplied by -1.

Sketch of proof. The proof consists of application of the definitions, as in the proof of Lemma 6.1.2. The only difference is that PDD-flat is used. Thus the vector field is interpolated to be constant in the Voronoi dual of each primal vertex. ■

Theorem 6.1.7 (Divergence Theorem on a Primal n-chain). *Let c be a primal n-chain which, as a set, is a simply connected subset of $|K|$. Then the discrete divergence theorem is true over this set.*

Sketch of proof. It is enough to show this for two adjacent primal n-simplices. It follows due to the fact that the shared face is oriented oppositely by the adjacent simplices while the vector field data is the same. This causes a cancellation giving us the proof over the two simplices. ■

Corollary 6.1.8 (Uniqueness of PDD-flat). *The discrete divergence theorem on a primal n-simplex is true if and only if the factors in the PDD-flat definition in Section 5.6 are 1.*

Proof. Similar to the proof of Cor. 6.1.4. ■

Now we will give the formal definition of divergence via the volume form. We have not worked out the resulting discrete formula in all cases, but in 2D, it appears to give the same result as the definition used above.

Definition 6.1.9. Let X be a discrete primal vector field on a flat complex K and σ^0 a vertex in K. Extend X to $\bar{X}$ in *any* smooth fashion to a neighborhood of the boundary vertices of the one-ring $\mathrm{St}(\sigma^0)$ around σ^0. Then the discrete divergence on the one-ring is defined by

$$\left\langle \mathrm{div}(X), \sigma^0 \right\rangle |\mathrm{St}(\sigma^0)| := \left.\frac{d}{dt}\right|_{t=0} |\varphi_t(\mathrm{St}(\sigma^0))|$$

where φ_t is the affine simplicial homeomorphism extended from from the flow of $\bar{X}$ restricted to the vertices. ♢

We intend to explore this definition in future work. The nice property of this is that the metric enters only via the volume form as it should.

6.2 Gradient

In smooth theory the gradient of a function is $(\mathbf{d}\, f)^\sharp$. Thus it converts the metric independent quantity into a metric dependent one. For a primal 0-form the gradient can easily be computed in the interior of the primal simplex by first interpolating the 0-form from the vertices to the interior using the affine, barycentric interpolation functions, and then taking the gradient. Since the interpolation is affine, the gradient is a constant vector and we can associate it with the dual of the simplex. This is the primal-dual gradient defined below. For the primal-primal gradient, one has to necessarily combine the information from the one ring around a vertex in some way, and for now we propose an ad hoc method using the primal-primal sharp.

As we mentioned in Section 5.8, the right way to define sharp is to interpolate 1-forms first. But we have not done that in this thesis, and instead we have given an ad hoc definition. Similarly one can give ad hoc definitions for dual-dual and dual-primal sharps and consequently for those gradients. But we will not do that here. In summary, the only reliable gradient we give here is the obvious one, the primal-dual gradient. We note however, that our primal-primal gradient, when interpreted for regular nonsimplicial 2D rectangular mesh, gives a standard, finite difference formula for the gradient. The primal-dual and primal-primal gradients are defined below.

Definition 6.2.1. Let K be a primal mesh of dimension n and $f \in \Omega_d^0(K)$ a discrete primal 0-form, i.e., a real valued function on the vertices of K. Then the **discrete primal-dual gradient** of f written $\operatorname{grad}_{\mathrm{pd}} f$ or $\nabla_{\mathrm{pd}} f$ is defined as $(\mathbf{d} f)^{\sharp_{\mathrm{pd}}}$. That is, using Definition 5.7.1 of discrete $\sharp$ its value on $\star\sigma^n$ is:

$$\left\langle (\mathbf{d}\, f)^{\sharp_{\mathrm{pd}}}, \star\sigma^n \right\rangle := \sum_{\sigma^0 \prec \sigma^n} (f(\sigma^0) - f(v)) \nabla\phi_{\sigma^0,\sigma^n} \tag{6.2.1}$$

where v is a vertex of σ^n and we state without proof that the definition is independent of which v is chosen. Given a vertex $v \in K$ the **discrete primal-primal gradient** of f is defined as $(\mathbf{d}\, f)^{\sharp_{\mathrm{pp}}}$ by

$$(\nabla_{\mathrm{pp}} f)(v) := \sum_{\sigma^1 = [v,\sigma^0]} \left[f(\sigma^0) - f(v) \right] \sum_{\sigma^n \succeq [v,\sigma^0]} \frac{|\star v \cap \sigma^n|}{|\sigma^n|} \;\nabla\phi_{\sigma^0,\sigma^n}\,. \tag{6.2.2}$$

The outer sum is over all 1-simplices $[v,\sigma^0]$ containing the given vertex v and the inner sum is over all σ^n containing the 1-simplex $[v,\sigma^0]$. The volume factors are in dimension n. The maps ϕ_{σ^0,σ^n} are the primal-primal interpolation functions. $\diamondsuit$

6.3 Curl

In vector calculus, curl is usually defined in dimension 3 and sometimes as a scalar in dimension 2. In the smooth exterior calculus notation these are, $*\,\mathbf{d}\, X^\flat$ in dimension 2 and $(*\,\mathbf{d}\, X^\flat)^\sharp$ in dimension 3, where X is a smooth vector field in $\mathbb{R}^2$ or $\mathbb{R}^3$ respectively. In geometric mechanics the use of curl may be replaced by $\mathbf{d}$ of a 1-form. One example is vorticity in fluid mechanics, which is $\mathbf{d}\, u^\flat$ in geometric theory of fluid mechanics, but $\operatorname{curl} u$ in the more common engineering literature. Notice that the sharp is not required in the geometric mechanics definition of vorticity. In any case, having a discrete curl in exterior calculus is useful for translating equations that have been written using curl. Due to the multiplicity of discrete sharps and flats there will be many definitions of discrete curls. We have not explored all these, and give only one definition each in the 2D and 3D case.

We first define the 2D curl and show that the DEC definition results in the same formula, modulo an area factor, as one found by Polthier and Preuss [2002]. This is the content of Rem. 6.3.2.

Definition 6.3.1. Let K be a primal mesh of dimension 2 and $X \in \mathfrak{X}_d(\star K)$ a dual vector field. Then the **discrete 2D dual-primal curl** is defined by

$$\operatorname{curl}_{\mathrm{dp}} X = *\,\mathbf{d}\, X^{\flat_{\mathrm{dpd}}}\,.$$

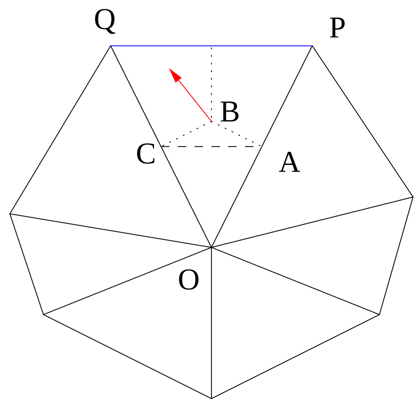


Figure 6.1: Curl in 2D

Remark 6.3.2. DEC 2D curl compared to Polthier and Preuss [2002]: The DEC definition of the 2D dual-primal curl coincides with one found by Polthier and Preuss [2002], modulo an area factor that their definition does not have. Consider the configuration shown in Fig. 6.1. According to Polthier and Preuss [2002], the discrete curl in 2D that assigns vectors to primal nodes is

$$\left\langle \operatorname{curl}(X), \sigma^0 \right\rangle = \frac{1}{2} \sum_{\sigma^2 \succ \sigma^0} X(\star\sigma^2) \cdot \vec{\sigma}^1(\sigma^2)$$

where $\sigma^1(\sigma^2)$ is the outer edge of triangle σ^2. Let us compute the DEC version of the 2D curl. For simplicity of notation we will use $\flat$ instead of $\flat_{\mathrm{dpd}}$. Since $* \mathbf{d} X^\flat$ is a 0-form, we can evaluate it at a vertex σ^0. In Fig. 6.1 this is marked as the point O whose one-ring is shown in that figure. Let the complex shown in the figure be oriented by orienting each triangle counter clockwise. By definition of discrete Hodge star we have

$$\frac{1}{\sigma^0} \left\langle \star \mathbf{d} X^\flat, \sigma^0 \right\rangle = \frac{1}{-|\star\sigma^0|} \left\langle \mathbf{d} X^\flat, \star\sigma^0 \right\rangle .$$

Then, by discrete Stokes' theorem we have

$$\left\langle \operatorname{curl} X, \sigma^0 \right\rangle = \frac{1}{-|\star\sigma^0|} \left\langle X^\flat, \partial(\star\sigma^0) \right\rangle .$$

By the definition of dual boundary, and because of the orientation chosen for the complex we get

$$\left\langle \operatorname{curl} X, \sigma^0 \right\rangle = \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \left\langle X^\flat, \partial(\star\sigma^0) \right\rangle$$

where the negative sign has canceled with the one coming from the dual boundary definition and all the σ^1 are pointing outwards.

The flat to be used is the DPD-flat. This consists of simply taking the dot product of the vector inside each triangle with the dual edges, when evaluating $X^\flat$ on the dual edges. This is because in DPD-flat the dual vector field inside the triangle is interpolated to be constant inside the triangle. Thus the above RHS becomes

$$\frac{1}{|\star\sigma^0|}\sum_{\sigma^1}\sum_{\sigma^2\succ\sigma^1} X(\star\sigma^2)\cdot(\star\sigma^1\cap\sigma^2)\,.$$

Collecting terms by the triangles we get

$$\left\langle \operatorname{curl} X, \sigma^0\right\rangle = \frac{1}{|\star\sigma^0|}\sum_{\sigma^2\succ\sigma^0}\sum_{\sigma^1\prec\sigma^2} X(\star\sigma^2)\cdot(\star\sigma^1\cap\sigma^2)\,.$$

In the case of the triangle shown with the dual edges in Fig. 6.1, the term $\sum_{\sigma^1\prec\sigma^2} X(\star\sigma^2)\cdot(\star\sigma^1\cap\sigma^2)$ in the RHS above becomes simply

$$X(B)\cdot\overrightarrow{AB} + X(B)\cdot\overrightarrow{BC}\,.$$

The term according to Polthier and Preuss [2002] should be

$$\frac{1}{2}\,X(B)\cdot\overrightarrow{PQ}\,.$$

But

$$X(B)\cdot\overrightarrow{AB} + X(B)\cdot\overrightarrow{BC} = X(B)\cdot(\overrightarrow{AB}+\overrightarrow{BC}) = X(B)\cdot\overrightarrow{AC} = \frac{1}{2}\,X(B)\cdot\overrightarrow{PQ}$$

where the last equality is due to the elementary geometric fact that the length of the edge joining midpoints of two sides is half the remaining side of the triangle and in the same direction as it. Thus the DEC formula is the same as the one given in Polthier and Preuss [2002] except that we have an additional factor of $1/|\star\sigma^0|$. $\Diamond$

For the 3D curl one needs to define sharp operator. We have given a primal-dual sharp for exact forms and a primal-primal sharp in Chapter 5. Of these, only the primal-dual sharp for exact forms is satisfactory. Thus the correct formulation of 3D discrete curl will have to wait a better development of sharp, which will possibly involve interpolation of 1-forms. For completeness we give here the definition of a discrete 3D curl using the usual smooth exterior calculus definition of curl.

Definition 6.3.3. Let K be a flat simplicial complex of dimension 3. Let $X\in\mathfrak{X}_d(K)$ be a discrete primal vector field. Then the **discrete 3D curl** is defined by

$$\operatorname{curl}(\mathbf{X}) = (*\mathbf{d}(\mathbf{X}^\flat))^\sharp$$

where the operators $*$, $\flat$ and $\sharp$ on RHS are the discrete operators. $\Diamond$

Remark 6.3.4. Curl and vector calculus identities: Recall that in smooth exterior calculus the identity $\operatorname{div}\circ\operatorname{curl} = 0$ follows from the fact that $\mathbf{d}^2 = 0$. This is because $\operatorname{div}(\operatorname{curl}(X)) = \mathbf{d}*([*(\mathbf{d}X^\flat)]^{\sharp\flat})$ and $\sharp$ is the inverse of $\flat$. However as we pointed out in Section 5.9, in the discrete case we have to use the right combination of $\sharp$ and $\flat$. For example, in this chapter we have used a dual-primal flat and a primal-primal

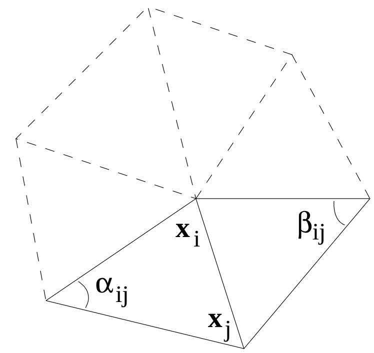


Figure 6.2: The variable names used in formula (6.4.1) for the Laplace-Beltrami of a triangle mesh, found by Meyer et al. [2002]. The complex does not have to be flat.

sharp. The composition has no chance of being identity. We point out that various vector calculus identities are true in our vector field decomposition work Tong et al. [2003]. The proof is reproduced in Section 9.3. Thus the information about the right flat and sharp to use is probably hidden in that work. $\diamondsuit$

6.4 Laplace-Beltrami

The Laplace-Beltrami operator is the generalization to curved surfaces, of the usual Laplacian of flat space. In the smooth case the Laplace-Beltrami operator on smooth functions is defined to be $\nabla^2 = \mathrm{div} \circ \mathrm{curl} = \boldsymbol{\delta} d$. See, for example, page 459 of Abraham et al. [1988]. In the smooth case the Laplace-Beltrami on functions is a special case of the more general Laplace-deRham operator $\Delta : \Omega^k(M) \to \Omega^k(M)$ defined by $\Delta = \mathbf{d}\boldsymbol{\delta} + \boldsymbol{\delta}\mathbf{d}$.

In this section we show that this definition of Laplace-Beltrami leads to a well-known formula for discrete Laplace-Beltrami found by Meyer et al. [2002]. The formula that they found was

$$\Delta f(\mathbf{x}_i) = \frac{1}{2\mathcal{A}} \sum_{j \in N_1(i)} (\cot\ \alpha_{ij} + \cot\ \beta_{ij})\ \ (f(\mathbf{x}_i) - f(\mathbf{x}_j)) \tag{6.4.1}$$

where the angles and points shown are marked in Fig. 6.2. The term $\mathcal{A}$ stands for an area around the point $\mathbf{x}_i$. Meyer et al. [2002] also showed that the use of the Voronoi area around the vertex is optimal in some sense.

Recently, Castrillon Lopez and Fernandez Martinez [2003] showed us that the Laplace-Beltrami we derive can be obtained from a discrete variational principle, by extremizing a discrete Dirichlet energy. This shows that, at least in this case of harmonic maps, discretizing the smooth Lagrangian and obtaining the discrete Euler-Lagrange equations gives the same result as first obtaining the Euler-Lagrange equations and then discretizing them. Thus in this case the application of variational principle commutes with discretization via DEC.

Example 6.4.1. Laplace-Beltrami on a triangle mesh: As an example we compute here Δf on a primal vertex σ^0 where $f \in \Omega^0_d(K)$ and K is a (not necessarily flat) triangle mesh in $\mathbb{R}^3$. Suppose that K is oriented by orienting all its triangles counterclockwise. Since $\boldsymbol{\delta} f = 0$ by definition, we have that

$$\begin{aligned} \left\langle \Delta f, \sigma^0 \right\rangle &= \left\langle \boldsymbol{\delta} \mathbf{d} f, \sigma^0 \right\rangle \\ &= -\left\langle * \mathbf{d} * \mathbf{d} f, \sigma^0 \right\rangle . \end{aligned}$$

Now by using the definition of discrete Hodge star followed by the discrete Stokes' theorem we get

$$\begin{aligned} \left\langle * \mathbf{d} * \mathbf{d} f, \sigma^0 \right\rangle &= \frac{|\sigma^0|}{-|\star \sigma^0|} \left\langle \mathbf{d} * \mathbf{d} f, \star \sigma^0 \right\rangle \\ &= \frac{-1}{|\star \sigma^0|} \left\langle * \mathbf{d} f, \partial(\star \sigma^0) \right\rangle . \end{aligned}$$

The explanation for the use of signed volume $-|\star \sigma^0|$ was given in Rem. 4.1.2. Thus

$$\left\langle \Delta f, \sigma^0 \right\rangle = \frac{1}{|\star \sigma^0|} \left\langle * \mathbf{d} f, \partial(\star \sigma^0) \right\rangle .$$

By Def. 3.6.8 of the dual boundary,

$$\partial(\star \sigma^0) = \sum_{\sigma^1 \succ \sigma^0} \star(s_{\sigma^1} \sigma^1)$$

where $s_{\sigma^1} = \pm 1$ is a sign, that depends on the orientation of K and σ^1. In dimension 2, with triangles of K oriented counterclockwise, the definition of dual boundary dictates that the edges $s_{\sigma^1} \sigma^1$ are all pointing outwards. For simplicity, as usual, in the following we will set σ^1 to be $s_{\sigma^1}\, \sigma^1$, which means that all edges incident on σ^0 are now all pointing outwards. Thus,

$$\begin{aligned} \left\langle * \mathbf{d} f, \partial(\star \sigma^0) \right\rangle &= \left\langle * \mathbf{d} f, \sum_{\sigma^1 \succ \sigma^0} \star \sigma^1 \right\rangle \\ &= \sum_{\sigma^1 \succ \sigma^0} \left\langle * \mathbf{d} f, \star \sigma^1 \right\rangle . \end{aligned}$$

Now another use of the definition of discrete Hodge star gives

$$\left\langle * \mathbf{d} f, \star \sigma^1 \right\rangle = \frac{|\star \sigma^1|}{|\sigma^1|} \left\langle \mathbf{d} f, \sigma^1 \right\rangle .$$

But then by discrete Stokes' theorem we have that

$$\left\langle \mathbf{d} f, \sigma^1 \right\rangle = f(v) - f(\sigma^0)$$

where $\sigma^1 = [\sigma^0, v]$. Putting all this together we get that

$$\left\langle \Delta f, \sigma^0 \right\rangle = \frac{1}{|\star \sigma^0|} \sum_{\sigma^1 = [\sigma^0, v]} \frac{|\star \sigma^1|}{|\sigma^1|} (f(v) - f(\sigma^0)) . \tag{6.4.2}$$

Then a geometric calculation shows that the above expression is the same as the formula (6.4.1) found by Meyer et al. [2002], without using discrete exterior calculus. As mentioned before, this formula is also obtained by a discrete variational principle as shown to us recently by Castrillon Lopez and Fernandez Martinez [2003]. ♦

6.5 Summary and Discussion

In our future work the divergence will be defined via the Lie derivative of the volume form, as outlined in Def. 6.1.9. For such a development, the vector field is extended in any smooth fashion, to the neighborhood of vertices, and the mesh is moved with the flow of the vector field. The vectors can actually be placed at any point, not just at the dual or primal vertices. Of course, then one would have to decide, what volume is being used in that case – for example the convex hull of the points. If the vectors are placed at the primal vertices, this definition of divergence can be pursued even in the current setting of DEC, without interpolation of forms, since the volume form is defined everywhere. In hindsight, this is really the approach to divergence we should have taken, since the metric dependence of divergence should only be through the volume form. It should not have anything to do with Hodge duality, dual meshes or flat operator. The definition we used, should actually be a theorem in the new setting.

In the interpolation view of DEC that we envision in the future, and as outlined in Section 1.5, the sharp would be defined after interpolating 1-forms. This should yield a better definition of the 3D curl, that satisfies various vector calculus identities. Similarly, that should yield a better primal-primal gradient, since in the interpolation point of view, operators are defined even pointwise.

That said, we should point out that the definition of divergence we have given yields a nice divergence theorem. Also, the formula in dimension 2, seems to be the same as the one obtained by the new, change of volume point of view of divergence outlined above. The 2D curl we derive has been found by others, without the use of DEC. The primal-dual gradient is a good definition, it even uses the idea of interpolation and the primal-primal gradient yields a gradient on regular nonsimplicial meshes, as shown in Section 9.4.

Chapter 7

Wedge Product

Results: As in the smooth case, the discrete wedge product we will construct is a way to build higher degree forms from lower degree ones. Some common applications of the wedge are, for example in defining the Lagrangian for harmonic maps, as $\mathbf{d}\, f \wedge * \,\mathbf{d}\, f$. In spacetime electromagnetism in vacuum, starting with a 1-form A one defines the Lagrangian using $\mathbf{d}\, A \wedge * \,\mathbf{d}\, A$. Thus the wedge product is of practical significance in important applications. In this thesis we give two different definitions for the primal-primal wedge, one of which is due to Castrillon Lopez [2003], and we state some of the properties that our primal-primal wedge satisfies.

Shortcomings: For a complete treatment, the dual-dual and primal-dual discrete wedge products should be defined. We only give speculative suggestions for the other cases here. One definition of primal-primal wedge we give, uses the metric. This use of metric is not satisfying because in the smooth theory, the definition does not use the metric. Furthermore, the discrete wedge should commute with discrete pullbacks. The metric dependent definition doesn't. Recently Castrillon Lopez [2003] showed us a definition of discrete wedge which does not use the metric *and* which commutes with discrete pullbacks. We include it here for completeness.

7.1 Primal-Primal Wedge

For information about the smooth case see the first few pages of Chapter 6 of Abraham et al. [1988]. We give two definitions of a primal-primal wedge here. The first definition is the one we had been working with until recently. The second definition was suggested to us recently by Marco Castrillion and it has the nice property that it is natural under pullbacks, i.e., his definition commutes with discrete pullbacks. This is an example of how naturality under pullbacks can be used as a criterion for selecting definitions in the discrete case, even when the operator being defined, like the wedge, is on only one manifold. The other obvious advantage of his definition is that metric is not used in the definition. His definition is Def. 7.2.1.

Definition 7.1.1. Given a primal discrete k form $\alpha^k \in \Omega^k_d(K)$ and a primal discrete l form $\beta^l \in \Omega^l_d(K)$ the **discrete primal-primal wedge product** $\wedge : \Omega^k_d(K) \times \Omega^l_d(K) \to \Omega^{k+l}_d(K)$ defined by the evaluation on a $k+l$ simplex $\sigma^{k+l} = [v_0, \ldots, v_{k+l}]$ as follows,

$$\left\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \right\rangle := \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{\left|\sigma^{k+l} \cap \star v_{\tau(k)}\right|}{\left|\sigma^{k+l}\right|} (\alpha \smile \beta)(\tau(\sigma^{k+l})) \tag{7.1.1}$$

where S_{k+l+1} is the permutation group and its elements are thought of as permutations of the numbers $0, \ldots, k+l$. Here $\operatorname{sign}(\tau)$ is the sign of the permutation τ, being $+1$ if τ is even and -1 if it is odd. The notation $\tau(\sigma^{k+l})$ stands for the simplex $[v_{\tau(0)}, \ldots, v_{\tau(k+l)}]$. Finally the notation $(\alpha \smile \beta)(\tau(\sigma^{k+l}))$ is borrowed from algebraic topology (see, for example, page 206 of Hatcher [2002]) and is defined as

$$(\alpha \smile \beta)(\tau(\sigma^{k+l})) := \langle \alpha, \left[v_{\tau(0)}, \ldots, v_{\tau(k)}\right] \rangle \langle \beta, \left[v_{\tau(k)}, \ldots, v_{\tau(k+l)}\right] \rangle .$$

$\Diamond$

The above expression looks complicated but the idea behind it, and its computation is really simple. What it amounts to, is evaluating the forms α and β on the k and l simplices emanating from each vertex of the simplex σ^{k+l} on which the wedge product is being evaluated. The sign of the permutation τ is there to provide the anti commutativity property. The volume factor is provided to make the computation democratic, by giving an appropriate weight to each vertex of σ^{k+l}. The following example of wedge product between two 1-forms should clarify the notation.

Example 7.1.2. Let α and β be two 1-forms whose wedge product has to be computed, so $k = l = 1$. The definition above gives the value of $\alpha \wedge \beta$ on a triangle $\sigma^2 = [v_0, v_1, v_2]$. According to the definition above the permutation group to be used is $S_{1+1+1} = S_3$. Thus τ are elements of the set of permutations of $\{0, 1, 2\}$. We will write the elements of S_3 as 1-0-2, 2-0-1, 0-1-2, 2-1-0, 1-2-0 and 0-2-1 with the obvious interpretation. The signs of these are $-$, $+$, $+$, $-$, $+$ and $-$ respectively. Let the volume factors appearing in (7.1.1) be denoted by C_0, C_1 and C_2, i.e., let

$$C_i = \frac{|\sigma^2 \cap \star v_i|}{|\sigma^2|} .$$

Then

$$\begin{aligned} \langle \alpha \wedge \beta, [v_0, v_1, v_2] \rangle = \frac{1}{2} [&-C_0 \langle \alpha, [v_1, v_0] \rangle \langle \beta, [v_0, v_2] \rangle + C_0 \langle \alpha, [v_2, v_0] \rangle \langle \beta, [v_0, v_1] \rangle \\ &+ C_1 \langle \alpha, [v_0, v_1] \rangle \langle \beta, [v_1, v_2] \rangle - C_1 \langle \alpha, [v_2, v_1] \rangle \langle \beta, [v_1, v_0] \rangle \\ &- C_2 \langle \alpha, [v_0, v_2] \rangle \langle \beta, [v_2, v_1] \rangle + C_2 \langle \alpha, [v_1, v_2] \rangle \langle \beta, [v_2, v_0] \rangle] \end{aligned} \tag{7.1.2}$$

Thus the formula says to go around the 3 vertices of the triangle evaluating α and β on the two edges

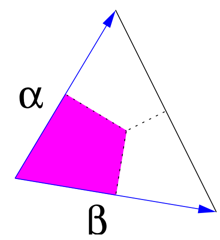


Figure 7.1: Pictorial depiction of 1 term in the sum in equation (7.1.2).

emanating from the vertex, then switching the arguments with an appropriate sign. The weighting factor is the area of the triangle corner obtained by intersecting the Voronoi cell of the vertex with the triangle divided by the area of the triangle. A pictorial depiction of 1 term in the equation above is in Fig. 7.1. ♦

The definition Def. 7.1.1 discussed above has some nice properties and some undesirable properties. If a smooth volume k-form and a volume l-form are discretized and their primal-primal wedge computed on a $(k+l)$-simplex, the result is the volume of the simplex. Also, this wedge satisfies most of the properties of the smooth wedge. Specifically the following lemma is true.

Lemma 7.1.3. *The discrete wedge product* $\wedge : \Omega_d^k(K) \times \Omega_d^l(K) \to \Omega_d^{k+l}(K)$ *satisfies the following properties:*

(i) **Anti-commutativity** $\alpha^k \wedge \beta^k = (-1)^{kl} \beta^l \wedge \alpha^k$.

(ii) **Leibniz rule** $\mathbf{d}(\alpha^k \wedge \beta^l) = (\mathbf{d}\alpha^k) \wedge \beta^l + (-1)^k \alpha^k \wedge (\mathbf{d}\beta^l)$.

(iii) **Associativity for closed forms** *For* $\alpha^k \in \Omega_d^k(K)$, $\beta^l \in \Omega_d^l(K)$, $\gamma^m \in \Omega_d^m(K)$, *such that* $\mathbf{d}\alpha^k = 0$, $\mathbf{d}\beta^l = 0$, $\mathbf{d}\gamma^m = 0$, *we have that,* $(\alpha^k \wedge \beta^l) \wedge \gamma^m = \alpha^k \wedge (\beta^l \wedge \gamma^m)$.

Proof. See Desbrun et al. [2003]. ■

Remark 7.1.4. Lack of associativity: According to Givental [2003] this lack of associativity in general, and a special status for closed forms, is not an accident. Putting the "democratic weighting" aside, the wedge definition works for any simplicial complex (such as singular cochains, for instance). It is known that it is in principal impossible to make a universal definition anti-commutative *and* associative. This phenomenon has been studied a lot in algebraic topology or homological algebra and gives rise to the concepts of Massey products and homotopy-associative algebras.

In our situation, one can define on the chain complex $(C^*, \mathbf{d})$ a sequence of operations: the binary operation $a, b \mapsto ab$ (the wedge product), some triple operation $a, b, c \mapsto [a, b, c]$ etc. such that the deviation of each operation from some kind of associativity property is measured by the differential of the previous operation. The key example is:

$$(ab)c - a(bc) = \mathbf{d}[a,b,c] - [\mathbf{d}\,a,b,c] - [a,\mathbf{d}\,b,c] - [a,b,\mathbf{d}\,c]\,.$$

The signs correspond to even a, b, c and in general should be changed by the factors

$$(-1)^{\deg(a)} \text{ and } (-1)^{\deg(a)+\deg(b)}$$

in the last two summands. This implies that the product is associative on the cohomology i.e. when a, b, c are closed, then $(ab)c - a(bc)$ is exact. Our statement that it is not just exact but 0 is a bit surprising but not impossible in this context. $\Diamond$

Remark 7.1.5. Wedge product and interpolation of forms: It has been pointed out by Sen et al. [2000] that if the wedge product is defined by first interpolating the discrete forms by using the Whitney maps, the resulting wedge product is still non-associative. Intuitively, this lack of associativity, and the lack in our case, stem from the fact that one is not defining the wedge product pointwise. Thus it seems that one must not only interpolate, but also specify, say, a vertex at which the evaluation must take place, to have a good chance of getting associativity. This point of view seems to appear in Hiptmair [2002a] and we intend to explore this in future work. $\Diamond$

Remark 7.1.6. Absence of naturality under pullback: Consider a simplex σ^n and an affine map $\varphi : \mathbb{R}^n \to \mathbb{R}^n$. Then in general the circumcenter is *not* invariant under such maps. That is, in general $\varphi(c(\sigma^n)) \neq c(\varphi(\sigma^n))$. Now suppose that we are given two simplicial complexes with a simplicial homeomorphism φ between them. If we use Def. 7.1.1 for the wedge then in general the wedge will not commute under discrete pullback. That is, in general we will *not* have that

$$\langle \varphi^*(\alpha \wedge \beta), \sigma \rangle = \langle \alpha \wedge \beta, \varphi(\sigma) \rangle \ .$$

This appears to be not a good sign for that discrete definition, since the above property in the smooth theory should follow from the change of variables theorem. Fortunately, the alternative definition presented in the next section does satisfy this property. $\Diamond$

7.2 Alternative Primal-Primal Wedge

Now we give the other definition of primal-primal wedge, shown to us recently by Castrillon Lopez [2003], which has the nice properties of not using the metric and of being natural under discrete pullbacks.

Definition 7.2.1 (Castrillon Lopez [2003]). Given a primal discrete k form $\alpha^k \in \Omega^k_d(K)$ and a primal discrete l form $\beta^l \in \Omega^l_d(K)$ the natural (in the sense of commuting with discrete pullbacks) **discrete primal-primal wedge product** $\wedge : \Omega^k_d(K) \times \Omega^l_d(K) \to \Omega^{k+l}_d(K)$ defined by the evaluation on a $k + l$ simplex $\sigma^{k+l} = [v_0, \ldots, v_{k+l}]$ as follows,

$$\left\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \right\rangle := \frac{1}{(k+l+1)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau)(\alpha \smile \beta)(\tau(\sigma^{k+l}))\,. \tag{7.2.1}$$

$\diamondsuit$

Remark 7.2.2. Comparison of factors: In the above definition, equation (7.2.1) can be rewritten as

$$\begin{aligned}\left\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \right\rangle &= \frac{1}{(k+l+1)(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau)(\alpha \smile \beta)(\tau(\sigma^{k+l})) \\ &= \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{1}{k+l+1} (\alpha \smile \beta)(\tau(\sigma^{k+l}))\,.\end{aligned}$$

Comparing this with equation (7.1.1) we find that the factor

$$\frac{|\sigma^{k+l} \cap \star v_{\tau(k)}|}{|\sigma^{k+l}|}$$

in that definition has been replaced by

$$\frac{1}{k+l+1}\,.$$

Thus a metric dependent factor has been changed into a constant factor. This is what makes Def. 7.2.1 natural under discrete pullback. Note also that

$$\sum_{\tau \in S_{k+l+1}} \frac{|\sigma^{k+l} \cap \star v_{\tau(k)}|}{|\sigma^{k+l}|} = \sum_{\tau \in S_{k+l+1}} \frac{1}{(k+l+1)!} = 1$$

a property that is useful in proving properties of the discrete wedge. $\diamondsuit$

7.3 Summary and Discussion

In the last two sections we have discussed the primal-primal wedge product in some detail. We defined it in two ways, one of which due to Castrillon Lopez [2003] has the nice feature of being defined without the use of metric and of commuting with discrete pullbacks. Since forms can be dual as well, for a complete treatment of discrete wedge product we should define dual-dual and primal-dual wedges. In this section we give only some preliminary suggestions for these definitions and do not study the properties of these wedge products.

Given a dual discrete k form $\hat{\alpha}^k \in \Omega^k_d(\star K)$ and a dual discrete l form $\hat{\beta}^l \in \Omega^l_d(\star K)$ the **discrete dual-dual wedge product** $\wedge : \Omega^k_d(\star K) \times \Omega^l_d(\star K) \to \Omega^{k+l}_d(\star K)$ might be defined (modulo some factors that have been left out) by the evaluation on a $k+l$ dual cell $\hat{\sigma}^{k+l} = \star\sigma^{n-k-l} = \star[v_0, \ldots, v_{n-k-l}]$ as follows.

$$\begin{aligned}\langle \hat{\alpha}^k \wedge \hat{\beta}^l, \hat{\sigma}^{k+l} \rangle =& \langle \hat{\alpha}^k \wedge \hat{\beta}^l, \star\sigma^{n-k-l} \rangle \\ =& \sum_{\sigma^n \succ \sigma^{n-k-l}} \operatorname{sgn}(\sigma^{n-k-l}, [v_{k+l}, \ldots, v_n]) \sum_{\tau \in S_{k+l}} \operatorname{sign}(\tau) \\ & \cdot \langle \hat{\alpha}^k, \star[v_{\tau(0)}, \ldots, v_{\tau(l-1)}, v_{k+l}, \ldots, v_n] \rangle \langle \hat{\beta}^l, \star[v_{\tau(l)}, \ldots, v_{\tau(k+l-1)}, v_{k+l}, \ldots, v_n] \rangle\end{aligned}$$

where $\sigma^n = [v_0, \dots, v_n]$, and we have without loss of generality assumed that $\sigma^{n-k-l} = \pm[v_{k+l}, \dots, v_n]$. Here we have left out the factor to be used, and that is for future work.

As mentioned in the preamble of this chapter, in some important applications, the Lagrangian can be written as $\alpha \wedge *\alpha$. These are a complementary primal-dual pair, i.e., their degrees sum to n. The cochain obtained by such a wedge product of a k and $(n-k)$-form could be defined on the support volumes of all the k-simplices. Recall that these tile the underlying space $|K|$.

Let $\alpha^k \in \Omega_d^k(K)$ be a primal k-form and $\hat{\beta}^{n-k} \in \Omega_d^{n-k}(\star K)$ a dual $(n-k)$-form. Thus α and $\hat{\beta}$ are a complementary primal-dual pair. The **discrete primal-dual wedge product** $\wedge : \Omega_d^k(K) \times \Omega_d^{n-k}(\star K) \to \Omega_d^n(V_k(K))$ can be defined by the evaluation on the support volume of a k-simplex as follows. Here $\Omega_d^n(V_k(K))$ are the cochains on the n-cells that are the support volumes of k-simplices. The value of

$$\left\langle \alpha^k \wedge \hat{\beta}^{n-k}, V_{\sigma^k} \right\rangle$$

will likely involve terms like

$$\left\langle \alpha^k, \sigma^k \right\rangle \; \left\langle \hat{\beta}, \star\sigma^k \right\rangle .$$

One obvious weighting factor to use for such a term might be

$$\frac{\frac{1}{2}\frac{1}{n}|\sigma^k| \; |\star\sigma^k \cap \sigma^n|}{V_{\sigma^k}} .$$

Here the numerator is the volume of that part of support volume V_{σ^k} that is formed by σ^k and its dual and lies inside some σ^n. But again these factors are metric dependent, which may not be good.

However, recently Castrillon Lopez and Fernandez Martinez [2003] used a similar construction in the special case of $n = 2$ and $k = 1$ to do a discrete variational derivation of the Euler-Lagrange equation for $\mathbf{d}\, f \wedge * \mathbf{d}\, f$. The solutions of these are harmonic maps on a surface. Their variational derivation yielded the same Laplace-Beltrami operator that we defined in Chapter 6. They have shown that starting from a smooth Lagrangian, one can derive the equation for harmonic maps and discretize it, or discretize the Lagrangian and derive the discrete equation for harmonic maps using DEC. In both cases the resulting discrete Euler-Lagrange equations are the same.

Chapter 8

Interior Product and Lie Derivative

Results: In this thesis, we are trying to build a discrete exterior calculus which treats vector fields and forms as separate entities, as does smooth theory. One motivation is that Lie derivatives of forms and vector fields are two very different things. This is expanded upon in Sec. 8.1 below. In this chapter we will discuss interior product and Lie derivatives of forms. First, we will derive an identity relating smooth interior product to Hodge star and wedge products. This yields an algebraic, discrete interior product. However since in the discrete theory we are only concerned with integrals of forms we can use the notion of extrusion of a manifold by the flow of a vector field to define integral of interior product. This is an idea of Bossavit [2003] and it leads to another definition of discrete interior product. A similar distinction exists in our discrete Lie derivative definition. Use of the Cartan homotopy formula leads to an algebraic definition of Lie derivative, and a flow-out formula that we prove, leads to another, flow based definition. In this Chapter we argue that interpolation of forms becomes a must for a proper definition of Lie derivative.

Shortcomings: Our algebraic definition of interior product uses metric information in the form of Hodge star and flat. We prove here that in the smooth case this metric dependence cancels out. But we don't know if this cancellation happens in the discrete case also. We have not studied carefully which properties are satisfied by the two definitions of interior product we give here. Nor have we studied if the two are the same in the discrete case.

A wedge product is involved in the algebraic definition. Thus the Lie derivative of a wedge product ends up with a wedge of three forms, if the algebraic definition is used. Due to the lack of associativity for general forms, one risks losing the important property of Leibniz rule for Lie derivative, except perhaps, for closed forms. This was pointed out to us by Alan Weinstein. We give here the discrete version of the flow-out formula for Lie derivative, to the extent possible without interpolation of forms. This is one of the key examples that shows the importance of interpolation of forms. In fact Bossavit [2003] uses the interpolation approach approach for interior product. But we haven't seen a Lie derivative development like this. Neither have the properties of such an interior product been studied in detail.

The smooth definition of Lie derivative, and hence this interpolated one, depends on derivatives. Hence, ultimately, the discrete definition for higher degree forms may turn out to be independent of the extension (interpolation) used. Finally, we do not discuss the Lie derivatives of vector fields at all in this thesis.

8.1 Separation of Forms and Vector Fields

In Chapter 5 we defined discrete vector fields and the discrete sharps and flats for going between 1-forms and vector fields. One use for sharps and flats is of course, to be able to translate vector calculus into exterior calculus, allowing one to discretize equations written in vector calculus notation. But there is another, more important reason for defining sharps and flats. As mentioned in Chapter 5, this is that in mechanics some quantities are *defined* using these operators. An example from Chapter 5 worth repeating for emphasis, is that of vorticity in fluid mechanics. In geometric treatment of fluid mechanics vorticity is defined as $\mathbf{d}\, u^\flat$. Here u is the velocity field of the fluid, a genuine vector field which is not a proxy for a 1-form.

In many applied fields, vector calculus has been given prominence over differential forms even when forms would have been more appropriate and simpler to use. In 3D, time-dependent electromagnetism, the quantities of interest should be modeled by differential forms, not vector fields. When the Maxwell system is written like this, the *only* place where metric plays a role, is in the constitutive, material dependent relationships $d = *_\epsilon e$ and $b = *_\mu$, where e and h are 1-forms and d and b are two forms. When Maxwell's equations are written in terms of vector fields, which is the more common formulation, then *all* the fields that appear are proxies for 1-forms and 2-forms.

In $\mathbb{R}^3$, this prevalent confusion between 1-forms, 2-forms and vector fields, all of which have a basis size of 3, takes the following form. For example, given a vector field F on $\mathbb{R}^3$ given by

$$F = F_1 \frac{\partial}{\partial x} + F_2 \frac{\partial}{\partial y} + F_3 \frac{\partial}{\partial z}$$

we can identify it with the 1-form $F^\flat = F_1 dx + F_2 dy + F_3 dz$. With the standard inner product on $\mathbb{R}^3$ we can identify F also with the 2-form $*(F^\flat) = F_3 dx \wedge dy - F_2 dx \wedge dz + F_1 dy \wedge dz$. Most previous works on DEC like theories that do talk about vector fields, do so in this way, by using vector fields as proxies for differential forms. One exception is the work of Bossavit [2003]. The cost of this choice, and the importance of the exterior calculus approach, has become clear in computational electromagnetism. Many researchers in that field have explained this in their papers and books. For excellent treatments see for example Bossavit [1991]; Mattiussi [2000].

Our motivation for keeping forms and vector fields distinct is our introduction of a discrete Lie derivative into the theory. Lie derivative of a tensor is its derivative along the flow of a vector field. Arnol′d [1989] has also called it the fisherman's derivative (page 198 of Arnol′d [1989]) :

> the flow carries all possible differential-geometric objects past the fisherman, and the fisherman sits there and differentiates them.

See Abraham et al. [1988] for a thorough treatment of Lie derivatives of tensors and vector fields. Lie derivatives of forms and vector fields are very different things. For example, if α is a 1-form and X a vector field in $\mathbb{R}^3$ then in general

$$(\pounds_X \alpha)^\sharp \neq \pounds_X (\alpha^\sharp)\,.$$

Similarly, if β is a 2-form then in general

$$(*(\pounds_X \beta))^\sharp \neq \pounds_X ((*\beta)^\sharp)\,.$$

Thus if one was to identify 1-forms α or 2-forms β with their corresponding vector fields $\alpha^\sharp$ and $(*\beta)^\sharp$ then the Lie derivative along a vector field X would turn out to be *wrong*. This is why in certain applications it is very important to keep the distinction between forms and vector fields.

8.2 Algebraic Discrete Interior Product or Contraction

Interior product is an operator that allows one to combine a vector field and a form. For a smooth manifold M the interior product of a vector field $X \in \mathfrak{X}(M)$ with a $k+1$ form $\alpha \in \Omega^{k+1}(M)$ is written as $\mathbf{i}_X \alpha$ and for vector fields $X_1, \ldots, X_k \in \mathfrak{X}(M)$ the interior product in smooth exterior calculus is defined by

$$\mathbf{i}_X \alpha(X_1, \ldots, X_k) = \alpha(X, X_1, \ldots, X_k)\,.$$

Thus it is an operator that does not depend on the metric. We will first define the interior product by using an identity that is true in smooth exterior calculus. Since we have not seen this identity we state it here with proof. As the proof shows, the metric dependence cancels out in the smooth case.

Lemma 8.2.1. *Given a smooth manifold M of dimension n and a vector field $X \in \mathfrak{X}(M)$ and a k-form $\alpha \in \Omega^k(M)$ we have that*

$$\mathbf{i}_X \alpha = (-1)^{k(n-k)} * (*\alpha \wedge X^\flat)\,. \tag{8.2.1}$$

Proof. For properties of the interior product that we use in this proof see page 429 of Abraham et al. [1988]. Recall that $\mathbf{i}_X$ is $\mathbb{R}$-linear. Moreover, for a smooth function $f \in \Omega^0(M)$ we have that $\mathbf{i}_{fX}\alpha = f\mathbf{i}_X\alpha$. This is due to the multilinearity of α. As a result it is enough to show the result in terms of basis elements. In particular let $\tau \in S_n$ be a permutation of the numbers $1, \ldots n$ such that $\tau(1) < \ldots < \tau(k)$ and $\tau(k+1) < \ldots < \tau(n)$. Since the identity (8.2.1) to be proved is a pointwise statement, pick a chart on M around an arbitrary point $x \in M$ and let $e_1, \ldots, e_n$ and $e^1, \ldots, e^n$ be respectively the bases for the tangent and cotangent spaces T_xM and T_x^*M. Let $X = e_{\tau(j)}$ for some $j \in \{1, \ldots, n\}$ and let $\alpha = e^{\tau(1)} \wedge \ldots \wedge e^{\tau(k)}$.

Then it is enough to show that

$$\mathbf{i}_{e_{\tau(j)}} e^{\tau(1)} \wedge \ldots \wedge e^{\tau(k)} = (-1)^{k(n-k)} * (*(e^{\tau(1)} \wedge \ldots \wedge e^{\tau(k)}) \wedge e^{\tau(j)}) \,. \tag{8.2.2}$$

It is easy to see that the LHS is 0 if $j > k$ and it is

$$(-1)^{j-1}(e^{\tau(1)} \wedge \ldots \wedge \widehat{e^{\tau(j)}} \wedge \ldots \wedge e^{\tau(k)})$$

otherwise. Here $\widehat{e^{\tau(j)}}$ means $e^{\tau(j)}$ is omitted from the wedge product. Now on the RHS of (8.2.2) we have that

$$*(e^{\tau(1)} \wedge \ldots \wedge e^{\tau(k)}) = \operatorname{sign}(\tau)(e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)}) \,.$$

Thus RHS is equal to

$$(-1)^{k(n-k)} \operatorname{sign}(\tau) * (e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)} \wedge e^{\tau(j)})$$

which is 0 as required if $j > k$. So assume that $1 \leq j \leq k$. We need to compute

$$*(e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)} \wedge e^{\tau(j)}) \,.$$

This is

$$s\, e^{\tau(1)} \wedge \ldots \wedge \widehat{e^{\tau(j)}} \wedge \ldots \wedge e^{\tau(k)}$$

where the sign $s = \pm 1$ to be determined is the one that makes

$$s\, e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)} \wedge e^{\tau(j)} \wedge e^{\tau(1)} \wedge \ldots \wedge \widehat{e^{\tau(j)}} \wedge \ldots \wedge e^{\tau(k)} = \mu$$

for the standard volume form $\mu = e^1 \wedge \ldots \wedge e^n$. This shows that $s = (-1)^{j-1}(-1)^{k(n-k)} \operatorname{sign}(\tau)$. (This technique to determine signs of wedge product involving permuted basis elements also appears on page 412 of Abraham et al. [1988]). Thus RHS = LHS as required. ■

Definition 8.2.2 (Algebraic). Let K be a simplicial complex, $X \in \mathfrak{X}_d(K)$ a primal discrete vector field and $\alpha \in \Omega^p_d(\star K)$ a dual p-form. Then the **discrete primal-dual interior product** is defined as

$$\mathbf{i}_X \alpha := (-1)^{p(n-p)} * (*\alpha \wedge X^\flat) \,.$$

A discrete **dual-primal** interior product can be defined analogously. ◊

A valid criticism of such a definition is the metric dependence. We saw in the proof of Lemma 8.3.2 that the metric dependence cancels out in the smooth case. But we don't know if the same is true in the discrete case. This will be studied in future work. In the next section we give a different definition of interior product.

This has appeared in Bossavit [2003] and is given here for completeness.

8.3 Interior Product via Extrusion

Recently, Bossavit [2003] described the importance of interior product in some applications in electromagnetism and gave a very interesting definition, based on the idea of extruding objects under the flow of a vector field. We develop this here for completeness and because this led us to a similar definition of Lie derivative which will be given in a later section. We point out however, that we only know how to give the definition in special cases. In particular, the vector field must be primal, and it must lie along primal edges. For a general primal vector field, we only know how to give the definition for a particular n-simplex. In that case, the vector at a primal vertex can be decomposed uniquely into vectors along the edges, since the edges emanating from a vertex, form a basis for the plane of the n-simplex. In the case of a full one-ring, the decomposition will not be unique. To get a general definition, we have to interpolate forms, which we intend to explore in future work. Now we give some preliminaries.

Definition 8.3.1. Let M be a smooth manifold of dimension n and $X \in \mathfrak{X}(M)$ a smooth vector field on it. Let S be a submanifold (dimension k, with $k < n$). As S is carried by the flow for a time t, it stays a submanifold if t is less than the lifetime of every point on S. We will call such a submanifold at time t the **flowed-out submanifold** and denote it by S_t. We will call the manifold obtained by sweeping S along the flow of X for time t as the **extrusion** of S by X for time t and denote it by $\mathrm{E}_X(S,t)$. $\diamondsuit$

Lemma 8.3.2 (Bossavit [2003]).

$$\int_S \mathbf{i}_X \beta = \left.\frac{d}{dt}\right|_{t=0} \int_{\mathrm{E}_X(S,t)} \beta \,. \tag{8.3.1}$$

Sketch of proof. Prove instead that

$$\int_0^t \left[\int_{S_\tau} \mathbf{i}_X \beta \right] d\tau = \int_{\mathrm{E}_X(S,t)} \beta \,.$$

Then by first fundamental theorem of calculus the desired result will follow. To prove the above, take coordinates on S and carry them along with the flow and define the transversal coordinate to be the flow of X. This is the proof that Bossavit [2002a] sketches. $\blacksquare$

Using the identity in equation (8.3.1) we shall define a discrete interior product like Bossavit [2003]. The idea is to define the discrete interior product by using a discretization of equation (8.3.1). The discrete version then is not an identity to be proved but true by definition. We don't claim that such a discretization converges to the smooth identity. As in the rest of the thesis, we leave such convergence questions for future work.

Now let $X \in \mathfrak{X}_d(K)$ be a discrete primal vector field and $\beta \in \Omega_d^{k+1}(K)$, a primal discrete $(k+1)$-form. Using $\mathbb{R}^N$ in place of M and a k-simplex $\sigma^k \in K$ in place of the submanifold S we get the following discrete version of equation (8.3.1)

$$\left\langle \mathbf{i}_X \beta, \sigma^k \right\rangle = \left. \frac{d}{dt} \right|_{t=0} \left\langle \beta, \mathrm{E}_X(\sigma^k, t) \right\rangle \ . \tag{8.3.2}$$

We will define the interior product on a primal $(k+1)$-simplex $\sigma^{k+1} \succ \sigma^k$. Since the interior product is linear w.r.t X it is enough to give the definition in terms of a basis vector of the plane of σ^{k+1}. The corner basis of σ^{k+1} consists of k vectors that span σ^k and 1 vector along an edge σ^1. We will now derive the discrete definition for $\mathbf{i}_{\vec{\sigma}^1} \beta$ from the discretized identity 8.3.2. It will be clear from the derivation that if any of the other basis elements are chosen, which all span the plane of σ^k, the interior product will be 0. This is the discrete analogue of the property that $\mathbf{i}_X \circ \mathbf{i}_X = 0$. As mentioned at the start of this Section, the vector fields allowed in our definition are restricted to be along edges.

We will do the derivation by first interpolating the primal vector which is $\vec{\sigma}^1$ based at σ^0 and 0 on all other nodes. Parameterize the edge σ^1 with $t \in [0, 1]$. Assume without loss of generality that σ^0 is the origin of $\mathbb{R}^{k+1}$, in which σ^{k+1} is embedded. Let $\vec{x} = (x_0, \ldots, x_k)$ be coordinates on $\mathbb{R}^{k+1}$. In these coordinates, the vector field along σ^1 is $\dot{\vec{x}}(t) = \vec{\sigma}^1 \, (1-t)$. Since $\vec{x}(0) = 0$, the solution of this system of ODEs is $\vec{x}(t) = \sigma^1 \, (t - (t^2)/2$.

Now $\mathrm{E}_{\vec{\sigma}^1}(\sigma^k, t)$ is a $(k+1)$-simplex that is a subset of σ^{k+1}. It also has the same base as σ^{k+1} and this base is σ^k. In fact it is the simplex obtained by joining the point $\vec{x}(t) \in \mathbb{R}^{k+1}$ to all the points in σ^k by straight lines. Now we will assume that the value of a discrete form on part of a simplex is proportional to the ratio of volumes of that part and the full simplex. With this assumption, we have

$$\begin{aligned} \frac{\left\langle \beta, \mathrm{E}_{\vec{\sigma}^1}(\sigma^k, t) \right\rangle}{\left\langle \beta, \sigma^{k+1} \right\rangle} &= \frac{|\mathrm{E}_{\vec{\sigma}^1}(\sigma^k, t)|}{|\sigma^{k+1}|} \\ &= \frac{(1/(k+1)) \quad |\sigma^k| \quad h(t)}{(1/(k+1)) \quad |\sigma^k| \quad h} \end{aligned}$$

where $h(t)$ is the height of $\vec{x}(t)$ above σ^k and h is the height of the other end point of σ^1 above σ^k. By geometry, this ratio of heights $h(t)/h$ is

$$\begin{aligned} \frac{h(t)}{h} &= \frac{\|\vec{x}(t)\|}{\|\sigma^1\|} \\ &= \frac{\|\vec{\sigma}^1\|}{|\sigma^1|} \left(|t - \frac{t^2}{2}| \right) \ . \end{aligned}$$

Thus, for $t \leq 1$

$$\frac{\left\langle \beta, \mathrm{E}_{\vec{\sigma}^1}(\sigma^k, t) \right\rangle}{\left\langle \beta, \sigma^{k+1} \right\rangle} = \frac{1}{\sigma^{k+1}} \left\langle \beta, \sigma^{k+1} \right\rangle \left(t - \frac{t^2}{2} \right)$$

and so taking time derivative of both sides and setting $t = 0$ we get

$$\left\langle \mathbf{i}_{\vec{\sigma}^1} \beta, \sigma^k \right\rangle = \frac{1}{|\sigma^{k+1}|} \left\langle \beta, \sigma^{k+1} \right\rangle \ .$$

Thus interior product of an edge vector $\vec{\sigma}^1$ with a $(k+1)$-form, evaluated on a simplex σ^k, is the average value on the $(k+1)$-simplex built from the edge σ^1 and the simplex σ^k.

8.4 Algebraic Lie Derivative

Once the interior product has been defined, one can *define* the Lie derivative by the Cartan magic formula. In this, if the algebraic definition of interior product is used, then there is a potential problem with Leibniz property of the Lie derivative. The algebraic definition Def. 8.2.2 involves a wedge product. Since the wedge product is not associative, except for closed forms, the Leibniz property of Lie derivative might not hold. This is the property that

$$\pounds_X(\alpha \wedge \beta) = \pounds_X(\alpha) \wedge \beta + \alpha \wedge \pounds_X(\beta)\,.$$

This possibility was pointed out to us by Weinstein [2003]. We don't know whether this is a problem in practice or not, but indeed Leibniz property of the Lie derivative is an important property, and its lack probably *will* be a problem in applications. Nevertheless we give the algebraic definition below.

Definition 8.4.1. Let K be a simplicial complex, $X \in \mathfrak{X}_d(K)$ a primal discrete vector field and $\omega \in \Omega_d^p(\star K)$ a dual p-form. Then the **discrete primal-dual Lie derivative** is defined using the interior product and the Cartan magic (or homotopy) formula (see Abraham et al. [1988] as

$$\pounds_X \omega := \mathbf{i}_X \mathbf{d}\omega + \mathbf{d}\mathbf{i}_X \omega\,.$$

$\Diamond$

8.5 Lie Derivative From Flow-Out Formula

An alternative to the algebraic approach detailed above is a method based on flowing out simplices similar to the idea for interior product sketched above. It appears as if, for Lie derivative, this approach cannot be carried through without interpolation of forms, which is something we intend to do in the future. We use this as an argument that interpolation of forms may be required for a proper definition of a discrete Lie derivative. It may turn out, that the resulting formula is independent of the interpolation, but at least its derivation seems to require interpolation of forms. We develop the discrete formula of the Lie derivative, based on this flow-out approach, to the point where we see that the interpolation is required. It appears that even this, can be done only for special vector fields, that lie along primal edges. This is a strong argument in favor of interpolation of forms.

Below, we give an identity from the smooth case from which the discrete definition of a flow-out Lie derivative follows if interpolation of forms is allowed. But then one can argue that the smooth formula for Lie derivative should be used with the interpolated forms. This would allow all primal vector fields, and not just those along edges. We agree with this argument and intend to pursue the interpolation approach in future work. For completeness however, we now state and prove the identities referred to above.

Lemma 8.5.1. *Let S, S_t be as above and β be a k-form on M. Then*

$$\int_S \pounds_X \beta = \left.\frac{d}{dt}\right|_{t=0} \int_{S_t} \beta \,. \tag{8.5.1}$$

Proof. By the Lie Derivative Theorem (Theorem 6.4.1 of Abraham et al. [1988]) we have that for any $\tau \leq t$

$$F_\tau^*(\pounds_X \beta) = \frac{d}{d\tau} F_\tau^* \beta \,.$$

Integrating both sides from 0 to t and using the fact that $F_0^*\beta = \beta$ we get

$$\int_0^t F_\tau^*(\pounds_X \beta) d\tau = F_t^*\beta - \beta \,.$$

In the above equation both sides are k-forms on M and are functions of t, so they are time dependent k-forms on M. Being k-forms on M they can be integrated on a k-dimensional submanifold of M. Integrating both sides on S we get

$$\int_S \int_0^t F_\tau^*(\pounds_X \beta) d\tau = \int_S F_t^* \beta - \int_S \beta \,.$$

Now interchange the order of integration on the LHS and on RHS use the fact that $\int_S F_t^* \beta = \int_{S_t} \beta$. This yields

$$\int_0^t \int_{S_\tau} \pounds_X \beta d\tau = \int_{S_t} \beta - \int_S \beta \,.$$

Both sides are real valued functions of t. Taking derivative w.r.t t of both sides and using the first fundamental theorem of calculus we get

$$\int_{S_t} \pounds_X \beta = \frac{d}{dt} \int_{S_t} \beta \,.$$

Evaluating both sides at $t = 0$ we get the desired result. ∎

To derive a discrete definition of Lie derivative from the flow-out formula (8.5.1) we sketch the idea with an example. Suppose the mesh consists of 1 tetrahedron $[v_0, v_1, v_2, v_3]$ and we are given a discrete primal 1-form α. Let X be the primal vector field taking the value $\vec{\sigma}^1$ at v_1, where $\vec{\sigma}^1$ is the vector along the edge $[v_1, v_2]$. See Fig. 8.1. At the other nodes, X is 0. We are interested in computing the Lie derivative $\pounds_X \alpha$ and evaluating it on the edge $[v_0, v_1]$.

By a reasoning exactly similar to the one carried out in the case of the extrusion based formula for interior product, we get to a step that requires the computation of the value of the 1-form α on the edge $[v_0, \vec{x}(t)]$ where $\vec{x}(t)$ is a point along the edge $[v_1, v_2]$. Then a time derivative of this value has to be taken. Due to this, it may turn out that the answer finally only depends on the value of α on $[v_0, v_1]$ and the vector along $[v_1, v_2]$. Nevertheless, we see here that the intermediate step requires the interpolation of α so it can be evaluated

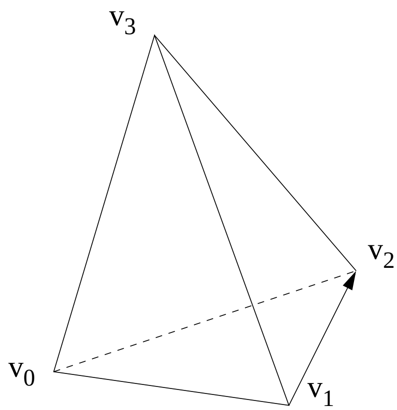


Figure 8.1: The configuration for computing the flow-out formula of Lie derivative of a 1-form. The vector field is nonzero only at v_1 and has the length and direction of the edge $[v_1, v_2]$. It is linearly interpolated to be 0 at vertex v_2. This is the restriction, to an edge, of the barycentric interpolation of the vector field inside the tetrahedron. We wish to evaluate the Lie derivative of a 1-form on the edge $[v_0, v_1]$.

on $[v_0, \vec{x}(t)]$ which lies inside the triangle $[v_0, v_1, v_2]$ and somewhere between the primal edges $[v_0, v_1]$ and $[v_0, v_2]$. But once interpolation of forms is accepted as a method, one might as well just use the definition of the smooth Lie derivative. This is the plan we intend to pursue further in our future work. We sketch the idea using 0-forms.

Remark 8.5.2. Interpolation Lie Derivative for Zero Forms: Consider for example a flat 2D mesh and the vector field X to be a primal vector field. Define

$$(\pounds_X f)(\sigma^0) = \left.\frac{d}{dt}\right|_{t=0} \varphi_t^* \bar{f}(\sigma^0)$$

where $\bar{f}$ is an arbitrary smooth extension of f and φ_t is the flow of an arbitrary smooth extension of $\bar{X}$. Thus

$$\begin{aligned}(\pounds_X f)(\sigma^0) &= \left.\frac{d}{dt}\right|_{t=0} (f \circ \varphi_t) \\ &= (\mathbf{d}\, f)(\sigma^0) \cdot X(\sigma^0)\,.\end{aligned}$$

Here we have not done anything more than use the definitions from smooth theory. Thus everything is defined pointwise, and the result only depends on the given discrete data and is independent of the extension used. $\diamondsuit$

8.6 Summary and Discussion

This Chapter presents the strongest arguments in favor of an interpolation approach. Here we have seen that in the case of interior products and Lie derivatives, the purely discrete approach can be pushed only so far. One can get algebraic definitions, for both, but the lack of associativity can rule out the important Leibniz property of Lie derivative, except perhaps for closed forms. The extrusion and flow-out based definitions also have limitations. Firstly, only special vector fields are allowed. Secondly, for the Lie derivative defined like this, the intermediate calculation seems to require the interpolation of forms. Once interpolation of forms is allowed however, it makes sense to use the smooth definitions of various operators to give the discrete definitions. This leads to an alternative development of the metric independent part of DEC, and we will pursue this in future work. In Rem. 8.5.2 we sketched the idea for doing this with 0-forms.

Chapter 9

Other Work

In this chapter we describe some of the other, related work that we have done recently. Some of this is work which does not yet fall directly into DEC. The rest is in DEC but very speculative and very preliminary. The first few sections describe template matching, discrete shells, and vector field decomposition. These are included here because our future work on these topics is likely to be influenced by our DEC work. Moreover, some of these have influenced our thinking on DEC. The last few sections describe some preliminary and speculative work, like some basic calculations on lattices and on nonsimplicial meshes. Also included, are some early thoughts on building general discrete tensors into DEC.

9.1 Template Matching

Deformable template matching is a technique for comparing images with applications in computer vision, medical imaging and other fields. It has been reported on extensively in the literature. See for example, the references in Hirani et al. [2001]. Template matching is based on the notion of computing a deformation induced distance between two images. The "energy" required to do a deformation that takes one image to the other defines the distance between them. The deformations are often taken to be diffeomorphisms of the image rectangle, i.e smooth maps with smooth inverse. The energy can be defined using various metrics on the space of diffeomorphisms.

In this way of posing the problem, template matching is similar to the way fluid mechanics is formulated. In fluid mechanics, averaged equations have been shown to have the property that length scales smaller than a certain parameter in the equation are averaged over correctly and don't need to be resolved in a numerical solution. See Marsden and Shkoller Marsden and Shkoller [2001] for details. Motivated by this, in Hirani et al. [2001] we derived the Averaged Template Matching Equation (ATME) :

$$\mathbf{v}_t + (\operatorname{div}\mathbf{u})\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{v} + (\mathbf{D}\mathbf{u})^T\mathbf{v} = 0 \tag{9.1.1}$$

$$\mathbf{v} = (1-\alpha^2\Delta)\mathbf{u} \tag{9.1.2}$$

According to Holm [2003] this equation can be written in div, grad, curl form.

Our hope in deriving the ATME was that it would allow matching while ignoring features smaller than a fixed size. This property has not yet been verified but some progress has been made in the analysis of the equation in one and two spatial dimensions. For example, in Chapman et al. [2002] we showed how natural boundary conditions lead to the reduction of the boundary value problem of template matching, to a parameterized initial value formulation. Specifically, we derived the form that the initial velocity must take to take one image to the other while satisfying the ATME. This initial condition was a piecewise smooth, continuous function with a jump in the derivative at edges of the image.

Independently, Fringer and Holm [2001] and Holm [2003] have analyzed and computed the solutions of the ATME and related equations in one and two spatial dimensions. In 1D they found that the initial condition we derived (which they called a peakon) leads to stable solutions in which the initial peakons move like solitons. Any other initial condition that they tried immediately broke up into peakons that proceeded to move around and collide elastically. More interestingly, recently they have discovered solutions in the two spatial dimension case. These turn out to be one dimensional string like peakons that move and collide in very interesting soliton like ways. The crucial step in the numerical solution was the use of mimetic discretization of the ATME when it is written using div, grad and curl. Mimetic discretization (Hyman and Shashkov [1997a]) is related to a basic form of DEC involving only discrete forms and on logically rectangular meshes. Our development of DEC should now allow the solutions to be computed on simplicial, irregular meshes. Another way to write the ATME is using Lie derivatives, and again, DEC should prove useful in discretizing that.

9.2 Discrete Shells

The work described in this section is joint work with Mathieu Desbrun, Eitan Grinspun and Peter Schröder. See Grinspun et al. [2003] for details. A shell is a thin flexible structure whose rest configuration is non-flat. Previously such models required complex continuum mechanics formulations and correspondingly complex algorithms but we have derived a shell model in the discrete setting of triangle meshes.

The stored energy functional for a discrete shell consists of a membrane part, that measures area and length changes, and a flexural part that accounts for the energy stored by out of plane bending. The key new part of our work in discrete shells is the measurement of bending strain by the difference between the shape operator on the reference configuration and the *pullback* of the shape operator on the deformed configuration. We use the commuting of trace and pullback to obtain a simple expression for the strain. Here we state and prove this elementary result. This proposition was also proved independently by Grinspun and Desbrun [2003].

Proposition 9.2.1. *Let $\varphi : \overline{M} \to M$ be a diffeomorphism. Here $\overline{M}$ is the reference configuration of the shell and M is the current. Let $\overline{S}$ and S be the shape operators on $\overline{M}$ and M respectively. Then* $\mathrm{Tr}\,(\varphi^* S) =$

$\varphi^*(\mathrm{Tr}\, S)$.

Proof. For a point $\bar{x} \in \overline{M}$ we have by definition and by the inverse function theorem that

$$\begin{aligned}\varphi^* S &= T_{\varphi(\bar{x})}\varphi^{-1} \circ S \circ T_{\bar{x}}\varphi \\ &= [T_{\bar{x}}\varphi]^{-1} \circ S \circ T_{\bar{x}}\varphi\end{aligned}$$

where T is the tangent map (derivative). Thus

$$\begin{aligned}\mathrm{Tr}\,(\varphi^* S) &= \mathrm{Tr}\left([T_{\bar{x}}\varphi]^{-1} \circ S \circ T_{\bar{x}}\varphi\right) \\ &= \varphi^*\left(\mathrm{Tr}\, S\right)\ .\end{aligned}$$

■

What this proposition allows one to do is to compare these traces at corresponding points of the reference and deformed configurations. This is because now we can compute

$$\mathrm{Tr}\left(\varphi^* S - \overline{S}\right) = \mathrm{Tr}\,(\varphi^* S) - \mathrm{Tr}\,\overline{S}$$

which makes sense only because of the proposition above. Discrete shells is an example of a subject in which we take the approach that everything be defined on the discrete mesh. Thus, future development of this will benefit from a development of DEC.

9.3 Discrete Multiscale Vector Field Decomposition

The work described in this section is joint work with Mathieu Desbrun, Santiago Lombeyda and Yiying Tong (Tong et al. [2003]). In Section 8.1 we have mentioned that in DEC we keep the distinction between differential forms and vector fields. But there are applications in which the use of vector field proxies for forms is acceptable. One such application is the discrete decomposition of vector fields.

There is a Hodge decomposition theorem for smooth manifolds without boundaries that states that for any k-form $\omega \in \Omega^k(M)$ there exist unique $\alpha \in \Omega^{k-1}(M)$, $\beta \in \Omega^{k+1}(M)$ and $\gamma \in \Omega^k(M)$ such that $\omega = \mathbf{d}\alpha + \boldsymbol{\delta}\beta + \gamma$ and $\Delta\gamma = 0$. There is also a generalization of this theorem for manifolds with boundary. For details see pages 538– 541 of Abraham et al. [1988]. If we use vector field proxies for elements of $\Omega^1(M)$ we get that any vector field can be decomposed into a gradient (curl-free), curl (divergence-free) and harmonic parts.

We have developed an algorithm for vector field decomposition for discrete vector fields on a 3D simplicial mesh. The decomposition is done variationally and also leads to a definition of discrete divergence and discrete curl. The curl-free part of a vector field ξ is the critical point of the functional: $\int_K (\nabla f - \xi)^2\ dV$

and the divergence-free part is the critical point of the functional: $\int_K (\nabla \times V - \xi)^2 \; dV$. This vector field decomposition work was done without using the DEC framework, but it was our first hint that interpolation should play a role in DEC. We will denote the discrete divergence and curl by Div and Curl and the gradient and curl of interpolated fields by ∇ and $\nabla\times$.

Definition 9.3.1. Let K be a flat simplicial complex of dimension 3, $W \in \mathfrak{X}_d(\star K)$ a dual discrete vector field and v a given vertex. Then define

$$(\mathrm{Div}\ W)(v) := \sum_{\sigma^3 \succ v} |\sigma^3| \; \nabla\phi_{v,\sigma^3} \cdot W(\star\sigma^3) \tag{9.3.1}$$

$$(\mathrm{Curl}\ W)(v) := \sum_{\sigma^3 \succ v} |\sigma^3| \; \nabla\phi_{v,\sigma^3} \times W(\star\sigma^3)\,. \tag{9.3.2}$$

In this Section, Div and Curl are our notations for discrete divergence and discrete curl. $\Diamond$

The following proposition was proved by Yiying Tong in Tong et al. [2003] and is reproduced here in DEC notation for completeness.

Proposition 9.3.2 (Tong et al. [2003]). *Let K be a flat simplicial complex of dimension 3, and $\tilde{V} \in \mathfrak{X}_d(\star K)$ a dual discrete vector field. Denote by V a piecewise affine vector field obtained by linearly interpolating $\tilde{V}$ in the interior of each tetrahedron using the primal-primal interpolation functions. Let $\tilde{f}$ be a primal discrete 0-form and f a piecewise affine function obtained by linearly interpolating f in the interior of each tetrahedron. Then away from the boundary of K, the discrete operators* Div *and* Curl *satisfy the following identities :*

$$\mathrm{Div}(\nabla \times V) = 0 \tag{9.3.3}$$

$$\mathrm{Curl}(\nabla f) = 0\,. \tag{9.3.4}$$

Here $\nabla\times$ and ∇ are the usual smooth curl and gradient operators.

Proof. First we need a simple result about volumes of tetrahedra. For a tetrahedron σ^3 let a, b be two of its vertices and let $\vec{\sigma}^1_{ab}$ be the edge vector that does not contain these vertices, oriented along the direction $\nabla\phi_{a,\sigma^3} \times \nabla\phi_{b,\sigma^3}$. For conciseness we have written ϕ_a for ϕ_{a,σ^3} etc. Then

$$|\sigma^3| \; \nabla\phi_a \times \nabla\phi_b = \frac{\vec{\sigma}^1_{ab}}{6}\,.$$

To see this let σ^2 be the face opposite to a, θ the dihedral angle at edge $\vec{\sigma}^1_{ab}$, and h_a, h_b the heights of vertices a and b above their respective opposite faces. Then

$$|\sigma^3| \; \nabla\phi_a \times \nabla\phi_b = \frac{1}{3}|\sigma^2| \, h_a \;\; \frac{1}{h_a}\frac{1}{h_b} \; \sin\theta \frac{\vec{\sigma}^1_{ab}}{|\sigma^1_{ab}|} = \frac{\vec{\sigma}^1_{ab}}{6}\,.$$

Now to prove (9.3.3) note that for any vertex p :

$$\begin{aligned}
\mathrm{Div}(\nabla \times V)(p) &= \sum_{\sigma^3 \succ p} \nabla \phi_{p,\sigma^3} \cdot (\nabla \times V)|_{\sigma^3} \;\; |\sigma^3| \\
&= \sum_{\sigma^3 \succ p} \nabla \phi_{p,\sigma^3} \cdot \left(\sum_{\substack{a \prec \sigma^3 \\ a \neq p}} \nabla \phi_{a,\sigma^3} \times V(\star a) \right) |\sigma^3| \\
&= \sum_{\sigma^3 \succ p} \sum_{\substack{a \prec \sigma^3 \\ a \neq p}} V(\star a) \cdot \left(\nabla \phi_{p,\sigma^3} \times \nabla \phi_{a,\sigma^3} \right) |\sigma^3| \\
&= \sum_{\sigma^3 \succ p} \sum_{\substack{a \prec \sigma^3 \\ a \neq p}} V(\star a) \cdot \frac{\vec{\sigma}^1_{pa}}{6} = 0 \,.
\end{aligned}$$

The third equality is from a basic identity about scalar triple products and the second last one is from the result about tetrahedral volume derived above. This resulting sum is null, because the oriented edges $\vec{\sigma}^1_{pa}$ form a loop around p. To prove (9.3.4) we use similar reasoning and show that

$$\begin{aligned}
(\mathrm{Curl}(\nabla f))(p) &= \sum_{\sigma^3 \succ p} \nabla \phi_{p,\sigma^3} \times (\nabla f)|_k \;\; |\sigma^3| \\
&= \sum_{\sigma^3 \succ p} \sum_{\substack{a \prec \sigma^3 \\ a \neq p}} \left(\nabla \phi_{p,\sigma^3} \times \nabla \phi_{a,\sigma^3} \right) f(a) \;\; |\sigma^3| \\
&= \sum_{\sigma^3 \succ p} \sum_{\substack{a \prec \sigma^3 \\ a \neq p}} f(a) \;\; \frac{\vec{\sigma}^1_{pa}}{6} = 0 \;\; .
\end{aligned}$$

Thus we have shown that the vector calculus identities in equation (9.3.3) and (9.3.4) are true. ∎

The discrete divergence Div here, is related to the dual-primal divergence of DEC, but is taken over the full one-ring, rather than the Voronoi dual of a vertex. In the first identity proved above, we have thus, a composition of primal-dual curl followed by a dual-primal divergence. In the second identity the composition is of a primal-dual gradient followed by a dual-primal curl. Thus in this work we have been able to find the pairs of operators that can be composed.

It was our vector field decomposition work described in this Section, that first suggested to us the usefulness of interpolation of forms and vector fields. The idea of interpolation and its role in current and future DEC is discussed in Section 1.5 and in various places in the thesis. Also, it is in this vector field decomposition that we have found a nice definition of 3D curl that satisfies the usual vector calculus identities. This means that the hints for defining a sharp and a flat that are inverses of each other, might be found in this work.

9.4 Regular Nonsimplicial Meshes

In this section we report some very preliminary ideas about regular nonsimplicial meshes, like square and rectangular meshes and a regular hexagonal mesh in 2D. Note that these are not simplicial complexes, although they are cell complexes. If we only include the edges and vertices, as in lattices, then indeed the mesh becomes a dimension 1 simplicial complex.

For example consider vertices at integer pair locations on the plane and edges between nodes that are distance one from each other. If the square area is not included, but only the edges and vertices are, then this complex *is* a simplicial complex of dimension 1. The dual of a vertex is the plus shaped region starting from the vertex and going halfway along the 4 edges incident on the node. The dual of an edge is the midpoint of the edge. One can include even longer distance interaction. For example, if edges of length 2, or diagonal edges etc. are also included, the complex is still a simplicial complex of dimension 1.

For such a mesh which is of dimension 1, it makes sense to compute gradients along the edges. This is the primal-dual gradient and the result is placed in the middle of the edges, which are the duals of edges. In the primal-dual gradient formula (6.2.1), in the dimension 1 case, the term $\nabla\phi_{\sigma^0,\sigma^1}$ is a vector along the edge σ^1 pointing towards σ^0. Note that here σ^0 is in σ^1. The vector has length $1/|\sigma^1|$. Thus one will get the usual definition of gradient along the edges. It does not make sense to compute operators like the two dimensional Laplacian because the complex is of dimension 1.

Now we will consider the regular meshes not as dimension 1 lattices, but with the areas or volumes included. In 2D, a square or rectangular the mesh such as above is a dimension 2 cell complex but it is not a simplicial complex. In what follows we consider a 2D square mesh and a 2D hexagonal mesh. We compute the gradient for the 2D square mesh. We do this by simply applying a formula analogous to (6.2.2) which was for simplicial case. The gradients of the shape functions are replaced by corresponding normals. The result is a standard formula for gradients on uniform meshes. Although we don't show a similar computation for a rectangular grid, we have checked that the correct gradient formula results from such a procedure on the rectangular grid as well. The Laplacian on such grids is also reproduced by the DEC formula for Laplacian. Similarly we compute Laplacian on a hexagonal grid by using the DEC formula for Laplacian and find a standard formula for the Laplacian on such grids.

These calculations are being presented just as curiosities, not as a suggestion for extending DEC to non-simplicial cases.

Example 9.4.1. Gradient on a square mesh in 2D:

Consider a flat uniform mesh with square cells of side length h such as the one shown in Figure 9.1. Let f be a 0-form on this, i.e., real values defined at the nodes of the mesh. We will simply use the formula (6.2.2) for discrete gradient and replace quantities that don't make sense in a nonsimplicial mesh by the

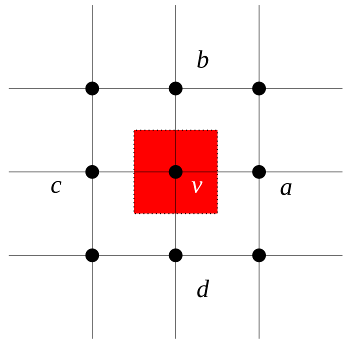


Figure 9.1: Portion of a grid on which gradient is to be defined. The dashed region is the Voronoi cell of the vertex v. The length of the side of each square is h and a,b, etc. are names of the nodes.

corresponding geometric quantity. With such replacements the formula becomes :

$$(\nabla f)(v) = \sum_{\sigma^1=[v,\sigma^0]} \big[f(\sigma^0) - f(v)\big] \sum_{c^2 \succ \sigma^1} \frac{|\star\, v \cap c^2|}{|c^2|}\ \vec{n}_{\sigma^0,c^2}\,. \tag{9.4.1}$$

Here $\sigma^1 = [v, \sigma^0]$ is an edge containing the vertex v and σ^0, c^2 is a square cell in the mesh, assumed to be of size $|c^2| = h^2$. Let $\hat{e}_x$ and $\hat{e}_y$ be unit vectors in the horizontal and vertical directions. The normal $\vec{n}_{\sigma^0,c^2}$ replaces the gradient of the shape function that appeared in the simplicial case in formula (6.2.2). If in the figure of the mesh shown here the square c^2 is the northeast square adjacent to v, then for example,

$$\vec{n}_{a,c^2} = \frac{\hat{e}_x}{h}\,.$$

The Voronoi cell $\star v$ shown as shaded in the figure, also has area h^2 whereas the quantity $|\star v \cap c^2| = h^2/4$ is the area of the overlap region between the dashed square and any one of the primal mesh squares adjacent to v. We will use the shorthand f_x for $f(x)$. The first sum in formula (9.4.1) is over edges that contain v. These are the four edges going to vertices a,b,c and d from v. For each such edge, say $[v, a]$ the second sum is over all squares c^2 that contain this edge. For $[v, a]$ these are the two squares above and below the edge $[v, a]$. Thus for each edge there will be 2 terms and hence 8 terms in total. This gives :

$$\begin{aligned}(\nabla f)(v) = {} & 2\,(f_a - f_v)\,\frac{h^2/4}{h^2}\ \frac{\hat{e}_x}{h} + 2\,(f_b - f_v)\,\frac{h^2/4}{h^2}\ \frac{\hat{e}_y}{h} + \\ & 2\,(f_c - f_v)\,\frac{h^2/4}{h^2}\ (-\frac{\hat{e}_x}{h}) + 2\,(f_d - f_v)\,\frac{h^2/4}{h^2}\ (-\frac{\hat{e}_y}{h}) \\ = {} & \frac{f_a - f_c}{2h}\hat{e}_x + \frac{f_b - f_d}{2h}\hat{e}_y\end{aligned}$$

which is a standard discrete approximation of the gradient on a uniform square mesh. We state without proof that this works for a rectangular grid as well. ♦

Example 9.4.2. Laplacian on a hexagonal mesh: Refer to Fig. 9.2. We want to compute the discrete

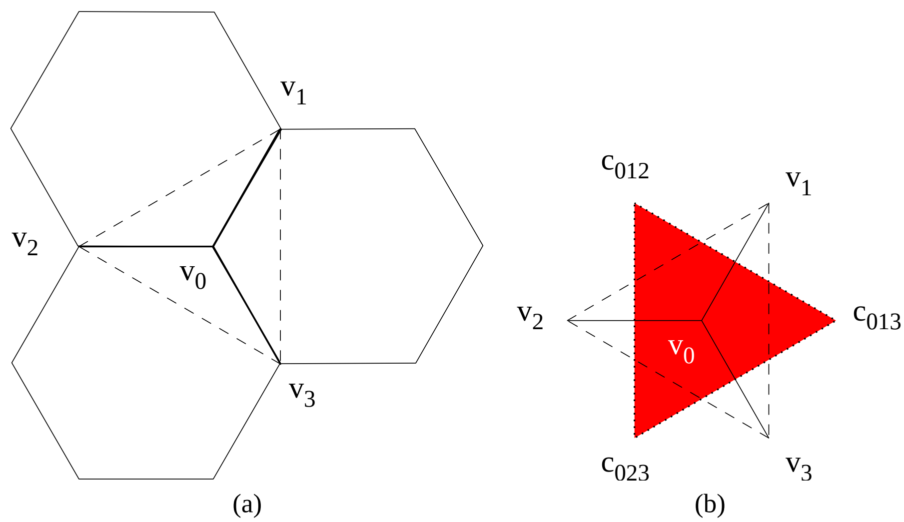


Figure 9.2: (a) Hexagonal grid; (b) The Laplacian is computed at point v_0. Since the triangles $v_0 v_1 v_2$ etc. are not well-centered, the circumcenters c_{012} etc. lie outside them, but the computation of Laplacian still yields the correct discrete Laplacian on hexagonal grids.

Laplacian at the vertex v_0. If f is a 0-form, we will simply use the DEC formula for Laplace-Beltrami of f. We will use the simplicial complex formed from the "stencil" consisting of v_0, v_1, v_2 and v_3. The complex consists of the three triangles inside the dashed lines shown in Fig. 9.2 (b). The Voronoi dual $\star v_0$ is shown as shaded. Note that the 3 triangles in the primal mesh are not well-centered. But we will still use the DEC formula (6.4.2) for Laplace-Beltrami.

Thus we want to compute

$$\langle \Delta f, v_0 \rangle = \frac{1}{|\star v_0|} \sum_{\sigma^1 = [v_0, \sigma^0]} \frac{|\star \sigma^1|}{|\sigma^1|} (f(\sigma^0) - f(v_0)) \,.$$

The quantity $|\star v_0|$ is the area of the shaded triangle in Fig. 9.2 (b). If h is the length of each side of the hexagonal mesh, this area is

$$|\star v_0| = \frac{3\sqrt{3}}{4} h^2 \,.$$

The dual edges that appear in the Laplacian formula above, are the sides of the shaded triangle in the figure. For a hexagonal mesh with each edge h, these dual edges have length $\sqrt{3}h$. Thus we have

$$\langle \Delta f, v_0 \rangle = \frac{1}{h^2} \left(\frac{4}{3} f(v_1) + \frac{4}{3} f(v_2) + \frac{4}{3} f(v_3) - 4 f(v_0) \right)$$

which is the finite difference formula for discrete Laplacian on a hexagonal grid appearing, for example, in Iserles [1996]. ♦

9.5 General Discrete Tensors

For a complete theory of discrete exterior calculus, one must also include general tensors. The tensors we have included so far are forms, which are antisymmetric tensors. But there are numerous applications that involve other types of tensors. One example is elasticity. For example, the stress tensor there is not a differential form. Perhaps, one way to build general tensors into the discrete theory is to define tensors by taking discrete tensor products of discrete 1-forms. This would require a discrete pairing between forms and vectors. For example one could build a (2,0)-tensor from 1-forms α and β, by defining the general tensor $\alpha \otimes \beta$ by its evaluation on vector fields U and V by

$$(\alpha^1 \otimes \beta^1)(U, V) = \alpha(U)\beta(V)\,.$$

We have proposed a discrete pairing of forms and vector fields in Section 5.10. That is not very satisfactory because of the use of metric operator sharp, to define an operator of natural pairing between forms and vector fields, which should be metric independent. Perhaps with interpolation of forms that we are envisioning in our future work, one can get a more natural definition of pairing, and hence of general tensors.

9.6 Summary and Discussion

The first three Sections of this Chapter are geometric computations on discrete meshes, and as such will benefit from an implementation and further development of DEC. Some of these have also influenced our work on DEC, for example, by pointing out the need for interpolation.

The speculative work we have described here are just some simple hints about how we might extend DEC to include general tensors and how some simple finite difference formulas can be reproduced by using the DEC formula, even when the mesh in question is not simplicial.

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