

A multivector data structure for differential forms and equations

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Abstract

We use tools from algebraic topology to show that a class of structural differential equations may be represented combinatorially and thus by a computer data structure. In particular, every differential k -form may be represented by a formal k -cochain over a cellular structure that we call a starplex, and exterior differentiation is equivalent to the coboundary operation on the corresponding k -cochain. Furthermore, there is a one to one correspondence between this model and the classical finite cellular model supported by the Generalized Stokes' Theorem, and translation between the two models can be completely automated.

Our results point the way to a common combinatorial and data structure well-suited for a physical modeling computer algebra that unifies finite and infinitesimal, symbolic and numeric, geometric and physical descriptions of distributed phenomena. We illustrate the advantages of our approach by a prototype interactive physics editor that uses the computer algebra to automatically translate intuitive geometrical/physical descriptions of balance conditions created by the user into the corresponding symbolic differential and integral equations.

1 Introduction

1.1 Motivation

Much of scientific computing and engineering analysis deals with physical phenomena that are distributed in space and time and are typically modeled by partial differential equations. Symbolic descriptions of partial differential equations have evolved over the years from the classical notations used by Leibnitz and Newton to vector and tensor calculus, and later to a more geometric calculus of differential forms and geometric algebra of multivectors. Each transformation in the evolution of the languages for differential equations is marked by the desire to make the language simpler, more precise, and/or more universal. Geometry and topology play a special role in this quest for the ideal language for several reasons:

- All symbolic quantities, but particularly spatial and temporal variables in differential equations have a well-defined *type*;
- Most differential equations are derived by postulating physical laws for small regions of assumed *dimension* and *shape*;
- Many differential equations are instances of the same *fundamental structural laws* or theorems, differing from each other only by the choice of coordinates, dimensionality, or selected labels.

Without going into widely discussed advantages and disadvantages of various symbolic descriptions, we note that the above geometric and topological information – quantity type, dimension, shape, and the fundamental law – is *implied* by the usual symbolic forms and notations, but it is not represented *explicitly* by any of them (with the notable exception of dimension in differential forms). Thus, the types of variables are usually implied by the associated units and operations; symbols x , y , r , θ , etc. signal choice of particular coordinate systems; and significant specialized experience is often needed in order to interpret and to relate given differential equations geometrically. The lack of an explicit structure to maintain the geometric and topological information manifests itself in several important ways.

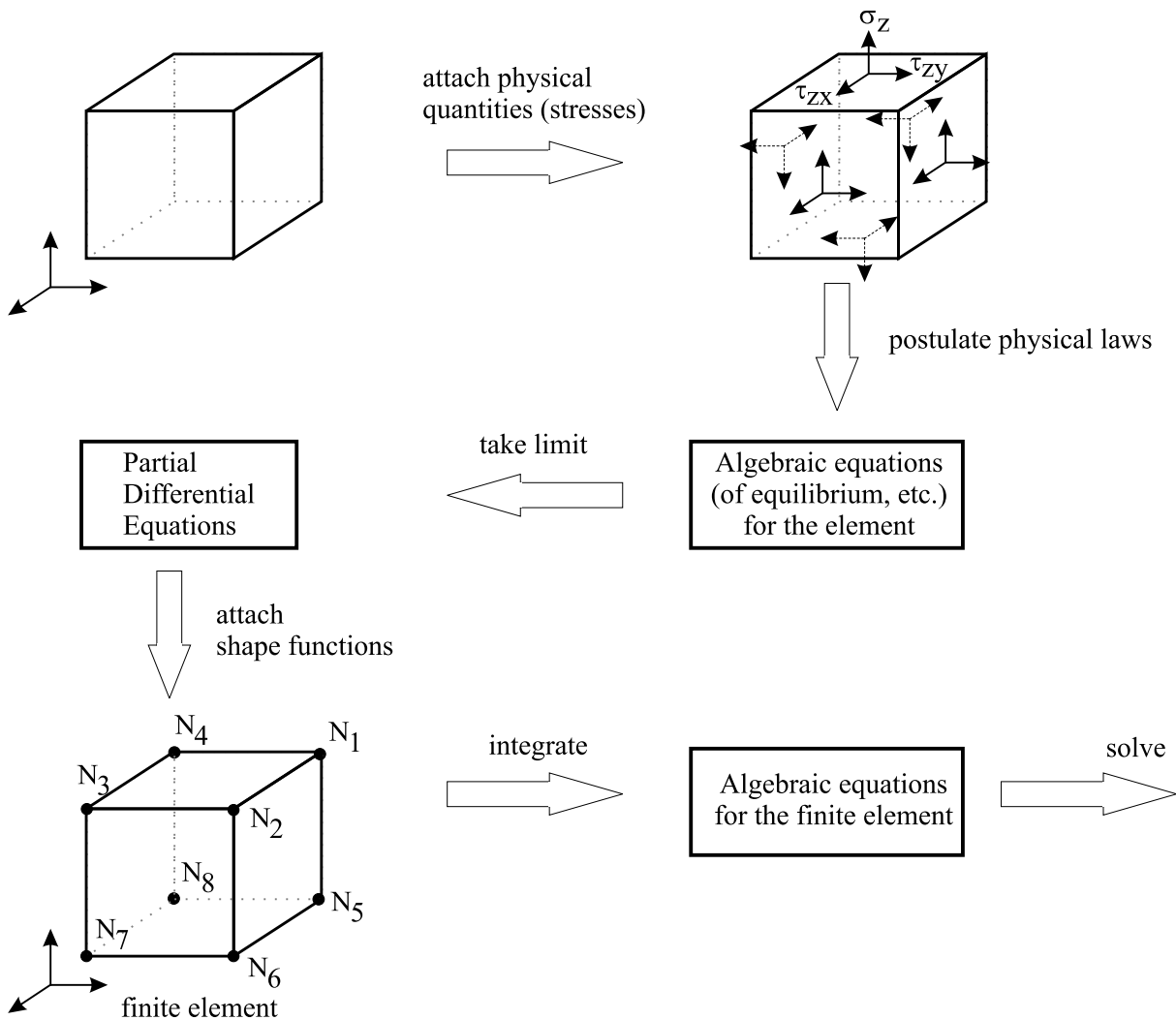


Figure 1.1: A traditional sequence of steps in modeling physical behavior.

Proliferation of models Figure 1.1 illustrates a typical sequence of steps in a traditional modeling process, starting with a model formulation and ending with a numerical approximation based on a spatial discretization. Such physical models of various distributed phenomena are being derived on a case-by-case basis, usually manually, and often repeating or rearranging a sequence of steps differing only in variable naming, choice of coordinate systems, or dimension. The underlying assumptions and models may be difficult to reconcile and relate, leading to artificial distinctions and inter-disciplinary barriers.

Communication barriers The symbolic notation of the differential and integral equations is reminiscent of Latin in the Middle Ages: on one hand, the commonly accepted and the standardized language facilitates broad scientific exchanges and enables great progress; on the other hand, its apparent complexity and narrow specialization (usually implied by the notation) effectively limits many scientists and engineers from participating in rigorous modeling and analysis of spatially distributed phenomena. Most physical laws follow from experimental observations and can be expressed algebraically or geometrically (right middle of Figure 1.1), but they must be translated into the languages of differential equations (left middle of the same figure) before they may be abstracted, modeled on a computer, and eventually solved.

Segregation of models and solutions Few differential equations can be solved exactly, and most common solution procedures rely on spatial and temporal discretization techniques that associate approximate physical quantities with the resulting geometric data structures (bottom row of Figure 1.1). Such data structures are usually associated with the solution method and not the first-principles differential model, and often appear to be incompatible with the form and structure of the original differential equations. Once again, this forces a case-by-case analysis, and prevents automatic translation of the analytical models into numerical approximation schemes.

In this paper, we use tools from algebraic topology to show that a class of structural differential equations may be represented combinatorially and thus by a computer data structure. Furthermore, there is a one to one correspondence between the new model and the classical finite cellular model supported by the Generalized Stokes' Theorem, and the translation between the two models can be completely automated. Our results point the way to a common combinatorial and data structure well-suited for a physical modeling computer algebra that unifies finite and infinitesimal, symbolic and numeric, geometric and physical descriptions of distributed phenomena. We illustrate the advantages of our approach by a prototype interactive physics editor program that accepts from the user intuitive geometrical/physical descriptions for the balance conditions, which do not require knowledge of associated symbolic descriptions, and automatically translates them into the equivalent symbolic differential and integral equations.

1.2 Historical remarks

The quest for classification and unification of physical quantities and theories has always been a central theme in science. James Clerk Maxwell was one of the first to express the desire to establish a formal analogy between various physical quantities based on their mathematical form [38]. The study of physical analogies has continued and intensified in 20th century (for example see [56]) fueled by developments in engineering and mathematics that we briefly summarize below.

Advances in electrical systems analysis and manufacturing led many to explore the possibility of extending this success to other physical, and in particular, mechanical domains [41, 43]. Nickle was one of the first to map mechanical dynamical systems into 'equivalent' analog electrical circuits whose response predicted that of the modeled mechanical system [41]. Similar ideas led Henry Paynter to developing his language of bond-graphs that describe multiple domain lumped-parameter systems and transformations between them in a graph language that can be automatically translated into a system of ordinary differential equations [46]. This electrical-network approach to modeling and simulation of mechanical systems culminated in the work of Gabriel Kron, a controversial electrical engineer, who showed how distributed mechanical systems may be modeled by multi-dimensional electrical networks and proposed an efficient method of "diakoptics" for solving them [33, 34]. Kron's disciples included Branin who recognized that the versatility of electrical networks is an indication of the combinatorial nature of the classical vector calculus [5], and Roth who identified the algebraic topology as that common structure responsible for the apparent analogies in physical theories [48, 49].

The quest for unification of physical theories has proceeded in parallel with development of mathematical theories aimed at identifying a common geometric structure and symbolic language for calculus. In the mid 19th-century, Hermann Grassmann and Sir William Hamilton came up with two different versions of a geometric calculus: Grassmann's so-called "calculus of extensions" and Hamilton's algebra of quaternions. Although Grassmann attempted to fit quaternions into the calculus of extensions on his own, William Clifford is generally credited with unifying the two, and geometric algebra is commonly called Clifford Algebra in recognition of the achievement [27, 42]. The significance of Clifford's Algebra was not immediately recognized and advocates of Grassmann and Hamilton followed along separate paths. Hamilton's work was eventually simplified by Josiah Gibbs and Oliver Heaviside into the modern version of vector calculus [47], although a conflicting account claims the simplification is from Grassmann's work [4]. What does appear certain is that Grassmann influenced Elie Cartan in his development of exterior differential forms [42, 51] that are becoming an increasingly accepted language for mathematics and physics at all levels [1].

One important advantage of differential forms over the usual expressions in vector calculus is that every form comes with an explicit declaration of dimensionality. This eliminates the possibility of symbolic manipulations which are possible in the vector calculus, but have no real meaning (such as $\mathbf{curl}(\mathbf{curl} \vec{f})$). A related advantage of differential forms is that, in contrast to vector calculus, differential forms generalize for any dimension n [58].

A movement towards further generalization appears to be taking shape. The geometric algebra [22, 23] is being advocated as a "universal" language for dealing with a variety of physical applications. Example problems in classical mechanics [24], electromagnetism, quantum mechanics and general relativity [2] have been published in the past

decade or so to indicate the broad applicability of this mathematical tool.

In his landmark manuscript [54], Tonti bridged the artificial gap separating engineering and mathematics by showing that most physical models may be classified based on their algebraic topological structure, with cochains (see the appendix) as the discrete *analogues* of differential forms [54, chapter 7]. Palmer and Shapiro [45] built on Tonti's work to propose a universal combinatorial structure and language for modeling and analysis of physical systems.

However, none of the proposed combinatorial structures are suitable for explicitly maintaining the necessary geometric and topological information in differential (or infinitesimal) statements of physical behavior. The main contribution of this work is to close this void by defining a structure which *does* maintain this information.

1.3 A multivector structure

Equations of differential forms contain the same information as more traditional (vector calculus) differential equations [12], along with the explicit dimensionality of elements. In this paper, we show that differential forms (and therefore other traditional symbolic differential expressions) may be represented using an explicit cellular structure that can be informally described as a *star pseudo-complex*. It is a proper subset of the usual cubical cell complex that is commonly used in spatial discretizations and approximations of distributed phenomena. Differential forms may be represented by cochains on such a structure, (exterior) differentiation corresponds to a modified coboundary operation, and the translation between infinitesimal differential and finite integral statements may be completely automated via the classical Stokes' Theorem and its dual described in Section 5.2.

The combinatorial structure of the constructed model explicates the known analogies between distinct physical domains and establishes a direct hierarchy between various models in terms of the assumed dimension and variable types. The described model immediately translates into a straightforward and intuitive computer data structure that enforces the strong typing of variables in the model and can be manipulated by users with minimal understanding of the underlying mathematics.

We eschew the use of geometric algebra in this paper, but we explain in Section 3.3 that our data structure is well-suited for representing the fundamental objects of geometric algebra, called *multivectors*. Accordingly, we use the term "multivector data structure," even though in this paper we restrict its use to differential forms and equations. That said, we would like the reader to recognize that multivectors are suitable to represent most other languages of mathematical physics. As described in [13, 14, 23, 24, 25] among others, these geometric objects facilitate the expression of laws currently written with tensors, differential forms, spinors, twistors and others. So our data structure is just as well-positioned to express tensorial descriptions as it is in our current presentation of differential forms; such versatility suggests that the multivector data structure is a powerful and promising choice for computer algebra systems applied to problems of mathematical physics.

The rest of the paper is organized as follows. The next section provides a cursory overview of k -vectors and their dual quantities, differential forms. The third section proposes an alternative representation for multivectors and differential forms which naturally leads to an explicit data structure. We then show how some of the typical differential form operations may be algorithmically performed on our proposed data structure in the fourth section. The fifth section shows how translation between finite and infinitesimal domains – steps necessary according to the middle and bottom rows of Figure 1.1 – may also be performed algorithmically on the multivector data structure. The concluding sixth section explains the significance and advantages of modeling with the multivector structure, and discusses a prototype implementation of an interactive physics editor.

2 Mathematical Preliminaries

The process in Figure 1.1 may be described in several formally equivalent ways. For the purposes of this paper, it is convenient to recognize that infinitesimal control elements of dimension k are k -vectors. For example, a line segment is a 1-vector, a 3D cube is a 3-vector, and so on. The physical quantities that are attached to the control elements are usually described by functions of k -vectors, called differential forms, representing distributions of the assumed quantities throughout the space. This section briefly summarizes the essential properties of k -vectors and differential forms as they are usually presented in the literature.

2.1 Intrinsic properties of k -vectors

A k -vector is an object with specific attributes of dimension, attitude, orientation, and magnitude [31]. The dimension of a k -vector is the integer k , representing the dimension of the region of space which the k -vector occupies. For the usual directed line segment depiction of a vector (a 1-vector), the attitude is the direction parallel to the straight line along which the vector lies. This obviously only makes sense when the 1-vector is embedded in n -space, with $n \geq 2$. Ignoring translations, attitude may be viewed as the 1-vector's span. Orientation of the 1-vector is usually depicted by an arrow that distinguishes the vector's tip and tail. Magnitude is the familiar attribute typically corresponding to 1-dimensional "volume" or length.

These attributes generalize to higher-dimensional k -vectors in a straightforward fashion. A 2-vector, or bivector, has an attitude which is the planar direction parallel to the plane in which it lies; its magnitude corresponds to area, and the orientation of a 2-vector is given by the circular sense of direction: clockwise or counterclockwise. A 3-vector is often called a trivector, and so on. A k -vector can have only one of two possible orientations, corresponding to the assumed sense of direction within its attitude; they are opposites of each other and can be represented by \pm symbols. Such an orientation is often called *inner* or intrinsic orientation. When a k -vector is embedded into a space of dimension greater than k , its *outer* orientation may also be induced from the orientation of the containing space [8, 31, 54]. We will avoid using outer orientation in this paper, but will rely on the concept of *relative* orientation (see the appendix) of the k -vectors to capture their orientation relative to the containing space.

Some 2- and 3-vectors inspired primarily by [31] are depicted in Figure 2.1. Specific geometry of a k -vector is of no importance; only the listed attributes are of consequence. Thus, two k -vectors are identical if they agree on attitude, orientation, and relative magnitude.

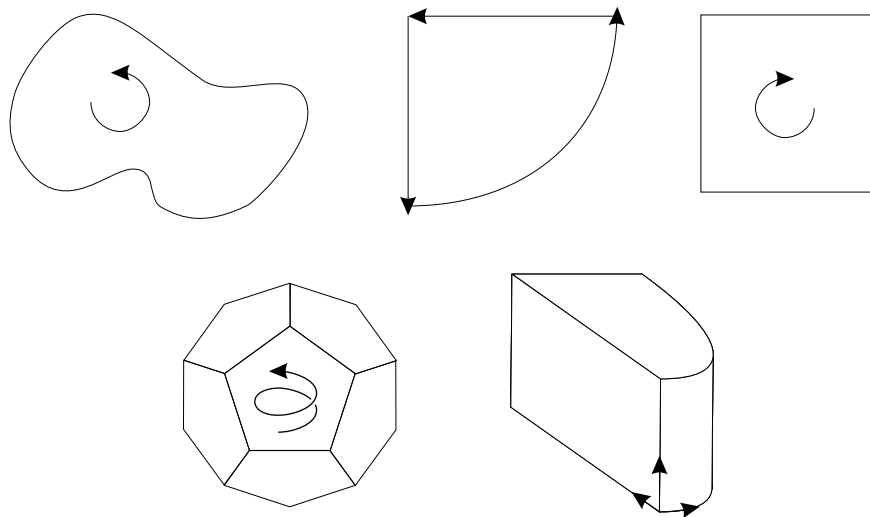


Figure 2.1: Graphical depictions of 2-vectors (top) and 3-vectors (bottom).

2.2 Algebraic properties of k -vectors

Simple arithmetic operations of addition and multiplication are defined for k -vectors. Addition and scalar multiplication are the familiar operations that preserve the vector's dimension: adding a pair of k -vectors produces another k -vector, and similarly scalar multiplication maintains the attitude of the original k -vector; of course magnitude and orientation may be changed by scalar multiplication.

Another important operation is the vector multiplication of a k -vector $\vec{\alpha}$ and a j -vector $\vec{\beta}$, where j may or may not equal k . This multiplication is denoted $\vec{\alpha} \wedge \vec{\beta}$ and, depending on the source, may be termed a wedge [52, 53], exterior [12, 17, 32] or outer [20, 24] product; some authors [31, 39] even use the terms interchangeably. For our purposes, the term *exterior* is preferable because of its role in defining the operation of exterior differentiation in Section 4.2.

Informally, exterior multiplication of two linearly independent 1-vectors sweeps one vector along the other producing a 2-vector of magnitude equal to the swept area and with attitude that is determined by the span of the attitudes of the 1-vectors, as illustrated in Figure 2.2. This informal description can be extended in a straightforward way for higher dimensions. In this way, any k -vector can be considered as a combination of k linearly independent 1-vectors.

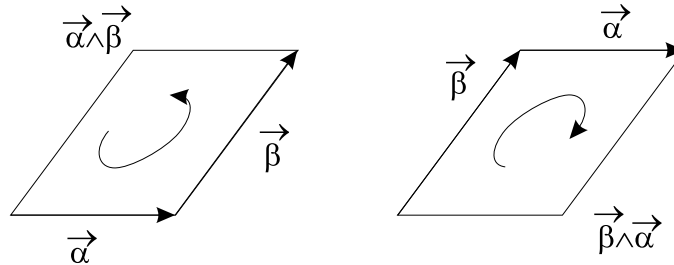


Figure 2.2: Multiplying a pair of 1-vectors. [31]

The orientation of the 2-vector resulting from the exterior product of a pair of 1-vectors is determined by the sense of direction implied by the path formed by the two 1-vectors. As suggested by Figure 2.2, the orientation of the k -vectors resulting from vector multiplication depends on the order of the operands – changing the order reverses the orientation. This implies that the multiplication is anticommutative; specifically $\vec{\alpha} \wedge \vec{\beta} = -\vec{\beta} \wedge \vec{\alpha}$ for $\vec{\alpha}$ and $\vec{\beta}$ both 1-vectors. It thus follows that a 1-vector multiplied by itself results in zero: $\vec{\alpha} \wedge \vec{\alpha} = -\vec{\alpha} \wedge \vec{\alpha} = 0$. The associative and distributive properties hold as in conventional algebra.

With the above operations of addition and scalar multiplication, the space of k -vectors is a linear space. This means we can define a basis and then write any other element as a linear sum of these basis elements. The attitude of a k -vector is naturally associated with a linear (sub)space. For a particular basis (coordinate system), the attitudes of the basis 1-vectors are the directions of each of the coordinate axes. Then all k -vectors defined in terms of the particular basis have attitudes that are spanned by the basis 1-vectors. The attitude which results from the exterior multiplication is the attitude which is spanned by the attitudes of both operands. More generally, the basis of the n -dimensional space may be formed by choosing linearly independent basis k -vectors. Simple counting arguments show that in n -space there are exactly $\binom{n}{k}$ basis k -vectors.

2.3 Differential forms

For a more complete discussion of differential forms without bias, see [12] or [50]; [15] and [58] approach the topic with some amount of comparison to the more traditional vector calculus; those wishing to see more in the way of applying differential forms to particular physical applications would do well to read [8], [17], [39] or [52]; lastly, [26] shows how forms fit into the framework of geometric calculus.

In the modeling scenario of Figure 1.1, differential forms can be used to state the differential relationships and equations. Equally important is the recognition that differential forms are, “the things which occur under integral signs” [17]. Perhaps the most intuitive and more relevant description of differential forms is that they represent local densities of distribution for the physical quantities of interest [8, 59]. These densities are associated with infinitesimal control elements (k -vectors) and vary from point to point. In other words, differential forms are functions of k -vectors.

Another popular interpretation of the differential forms found in literature views them operationally as objects which are introduced to “measure” vectors when a metric is absent. The depiction of forms in Figure 2.3 suggests how this works. The magnitude of a vector is the number of 1-forms it pierces; a bivector’s magnitude is the number of 2-forms it slices/covers; a trivector has magnitude equal to the number of 3-forms enclosed [31, 32, 39]. Visualization of higher dimensions is difficult, but the measurement proceeds in the same way.

This operational view illustrates well the duality between k -forms and k -vectors, which implies that there is a one-to-one correspondence between them. Furthermore, this correspondence suggests that properties of the differential k -forms may be viewed in terms of the properties of the dual k -vectors. Thus, every k -form has an attitude, orientation, and magnitude (but no well-defined shape). The linear space structure of k -forms indicates how higher-dimensional

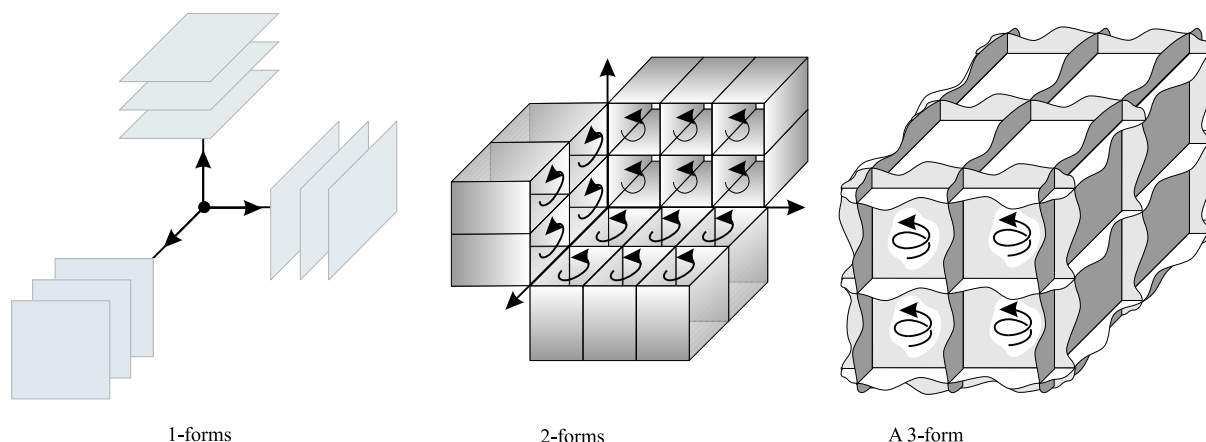


Figure 2.3: Graphical depiction of forms. [39, 32, 31]

forms may be formed from lower-dimensional ones using exterior product. And of course, there are exactly $\binom{n}{k}$ basis k -forms in an n -dimensional space [12, 50].

For example, in the familiar three-dimensional Euclidean space, there are $\binom{3}{0} = 1$ zero-forms, $\binom{3}{1} = 3$ one-forms, $\binom{3}{2} = 3$ two-forms, and $\binom{3}{3} = 1$ three-forms. The basis forms corresponding to each of these dimensions might be $\{1\}$, $\{dx, dy, dz\}$, $\{dx \wedge dy, dy \wedge dz, dz \wedge dx\}$ and $\{dx \wedge dy \wedge dz\}$. Example forms with these bases might be:

$$a \quad (0\text{-form}) \quad (2.1)$$

$$b_1 dx + b_2 dy + b_3 dz \quad (1\text{-form}) \quad (2.2)$$

$$c_1 dx \wedge dy + c_2 dy \wedge dz + c_3 dz \wedge dx \quad (2\text{-form}) \quad (2.3)$$

$$edx \wedge dy \wedge dz \quad (3\text{-form}) \quad (2.4)$$

Notationally, the addition in equations (2.2) and (2.3) should be interpreted in the usual formal sense, as the basis forms are directional placeholders and cannot be added any more than one may add \hat{i} and \hat{j} .

There is a similar binomial expansion of the number of basis forms with $n = 4$; 1 zero-form, 4 one-forms, 6 two-forms, 4 three-forms and 1 four-form. The basis one-forms here might be dx, dy, dz, dt and higher dimensional basis forms are again exterior product combinations of the basis one-forms. These should obviously correspond to bases for space-time; in general, any n -dimensional space can be represented in similar fashion.

3 The Multivector Structure

The precise relationship between k -forms, k -vectors and Figure 1.1 may not be obvious for several reasons. Both the control element in Figure 1.1 and its representation by a k -vector appear distinctly homogeneous in dimension k . The usual coordinate-free views of k -vectors reflected in images of Figure 2.1 and of the dual k -forms in Figure 2.3 deemphasize the combinatorial nature of the respective linear spaces, obscuring the relationship between vectors and forms of different dimensions. This is in sharp contrast to the typical modeling scenario that requires associating physical quantities with distinct dimensional portions of the control elements (volumes, surfaces, edges) and formulating physical laws that explicitly relate such quantities. Balance statements, for example, equate the quantities associated with the boundary of the control element with those stored or generated in its interior.

In this section, we propose an alternative, more explicit, combinatorial view of k -vectors and k -forms that naturally leads to a data structure for representing vectors and forms, as well as physical laws that relate forms of different dimensions.

3.1 The star pseudo-complex (starplex)

It may appear natural to think that the cubical control element in Figure 1.1 should be represented by a cubical cell complex as defined in the appendix. However, the combinatorics of the cube does not match that of the k -vector: there are $2^{n-k} \binom{n}{k}$ k -cells in a cubical n -complex. Intuitively, it is clear that the unit 3D cube corresponds to the unit 3-vector, the square faces of the cube correspond to the unit 2-vectors, the edges of the cube correspond to the unit 1-vectors, and cube's vertices are 0-vectors in the three-dimensional space. But there are too many of them: we need only $\binom{n}{k}$ k -vectors to define a k -dimensional basis in 3-space. In other words, we need a cellular structure constructed from one 0-cell (vertex), three 1-cells (edges), three 2-cells (faces), and one 3-cell (volume). Such a structure is shown at the right of Figure 3.1. It consists of the right number of the unit k -cells that are assembled together in the usual cell complex fashion, in the sense that the topological boundary of every k -cell *contains* the union of all incident lower-dimensional cells. But it is *not* a proper cell complex because the boundary of every k -cell is not a union of cells in the structure.

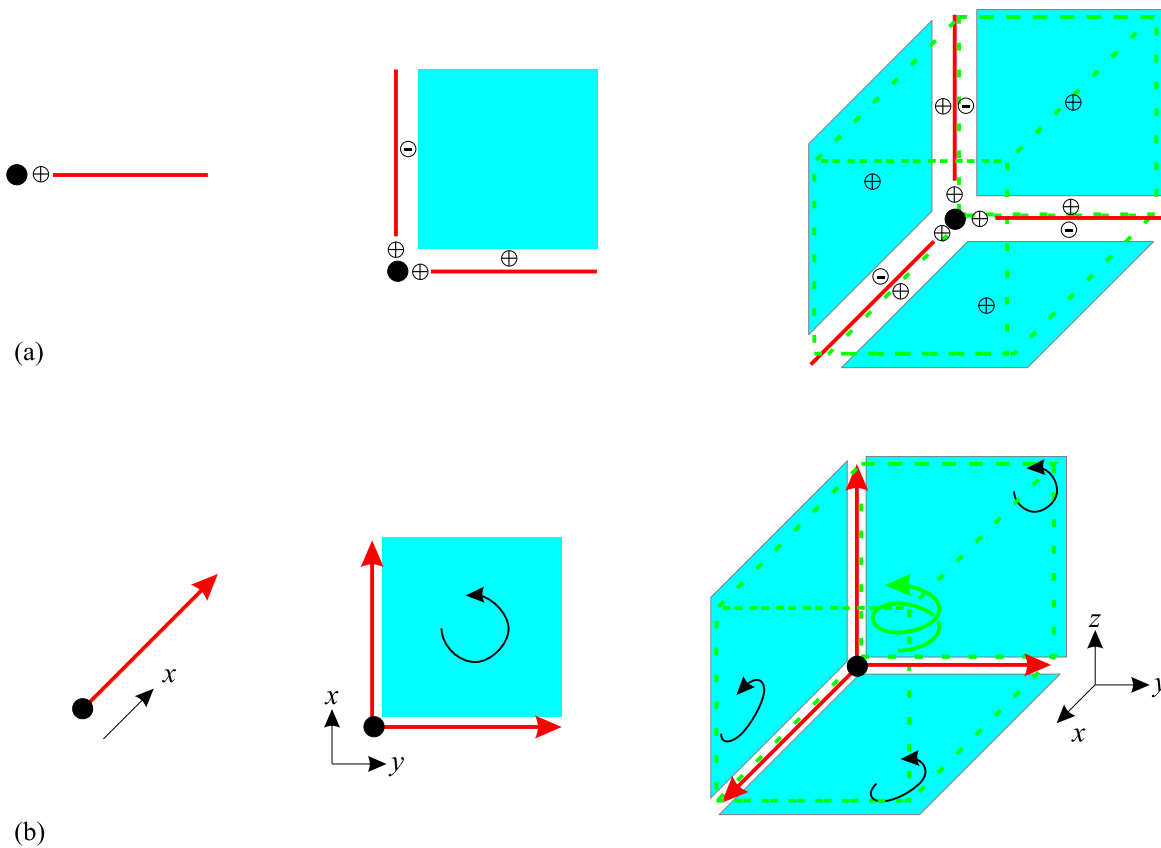


Figure 3.1: Star pseudo-complexes of dimension 1 (left) 2 (middle) and 3 (right). (a) The signs indicate relative orientation between the cells and their cofaces; (b) All cells are given explicit intrinsic orientation.

To be more precise, the collection of cells in Figure 3.1 is a combinatorial model of a 0-cell on a cubical n -complex with a single n -cell. Using the standard language of the combinatorial topology (see the appendix for definitions), this neighborhood is called a *star* of the 0-cell and is defined by all higher-dimensional cells incident on the 0-cell. To underscore the cellular nature of the neighborhood, the identified collection of cells may be properly called a *star pseudo-complex*, or *starplex* for short. The noteworthy features of the starplex are 1) that it is a subset of the set of cells in a proper finite cubical n -complex, and 2) that it is combinatorially equivalent to a basis for general multivectors up to dimension n .

Recall that every k -vector possesses one of two distinct orientations. This orientation is conveniently represented

by the relative orientation of the cells in the starplex in the same manner relative orientation is usually defined on any finite cell complex : \oplus indicates that two adjacent cells agree in their (relative) orientation, and \ominus indicates the opposite (relative) orientation. With the convention that 0-cells always have positive (inner) orientation, the assignment of signs shown in Figure 3.1 (a) corresponds to the more intuitive picture shown of Figure 3.1 (b).

Each k -cell in the starplex corresponds to a basis k -vector, and the set of all k -cells corresponds to a k -dimensional basis. Adjacency between a k -cell and a $(k + 1)$ -cell implies that the corresponding $(k + 1)$ -vector can be defined by exterior product of the corresponding k -vector with another adjacent 1-vector. This idea is illustrated in Figure 3.2. Thus, the starplex represents *all* basis k -vectors of all dimensions between 0 and n .

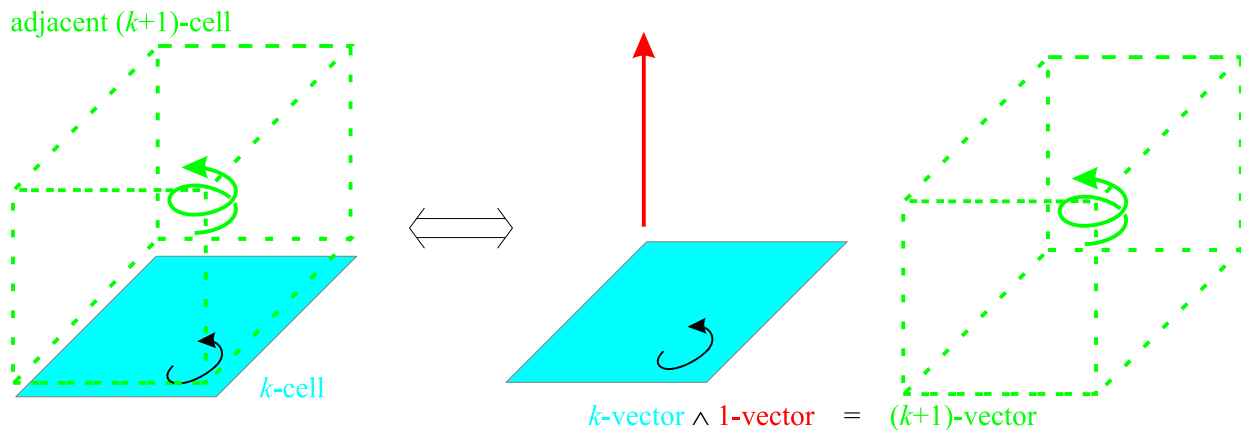


Figure 3.2: With the starplex, the exterior product is already built-in.

3.2 Embedding of basis via cell naming

The starplex structure captures the combinatorics of all k -vectors in n -dimensional space, but it is intrinsically coordinate free, because the same combinatorial structure is valid for any choice of bases: Cartesian, cylindrical, spherical, or general curvilinear basis as is suggested by the embeddings of its finite counterpart in Figure 3.3. To represent and compute with specific vectors and/or forms, a particular basis has to be chosen and represented. We will represent the basis by assigning an appropriate *name* (identifier, label) to every k -cell in the starplex. This, in turn, corresponds to embedding of the abstract k -cell as a particular basis k -vector. Since every basis k -vector is the exterior product of basis 1-vectors, naming the 1-cells immediately defines identifiers for all other k -cells for $2 \leq k \leq n$. For example, naming the three 1-cells to correspond to the Cartesian coordinate axes x , y , and z respectively, immediately identifies the three 2-cells as $x \wedge y$, $y \wedge z$, and $z \wedge x$ and the 3-cell as $x \wedge y \wedge z$.

By the duality noted in Section 2.3, the identical combinatorial structure of the starplex applies to basis k -forms. The 1-cells are named to correspond to a basis 1-form. For Cartesian coordinates, this becomes dx , dy , etc.; spherical coordinates would have dr , $d\theta$, and $d\phi$ as a basis. Higher dimensional cells are named by the exterior product of the incident 1-cells, e.g. a 3-cell incident to dx , dy and dt would be named $dx \wedge dy \wedge dt$ and so on.

3.3 Representing vectors or forms

Having chosen a basis, representing a particular k -vector or a k -form is a matter of choosing a coefficient for every named k -cell in the starplex and taking the formal sum of all terms (coefficient)*(basis k -cell). The coefficient of every term represents the magnitude and orientation of the corresponding basis k -cell whereas the attitude of the k -cell is implied by its name. Figure 3.4 depicts the forms of equations (2.1) - (2.4) together on the same structure.

Such a formal sum of (coefficient)*(basis k -cell) over all cells of a cell complex in essence defines a function and is called a cochain (see the appendix), provided that the coefficients come from some Abelian group or a linear vector space.¹ In other words, both k -vectors and k -forms may be represented by k -cochains over the starplex structure. The

¹Thus valid coefficients include scalars, vectors, tensors, functions on these, and any other additive types.

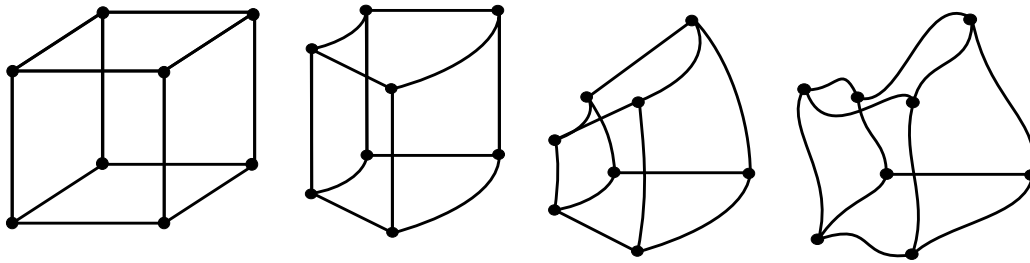


Figure 3.3: Embeddings of cubical 3-complexes.

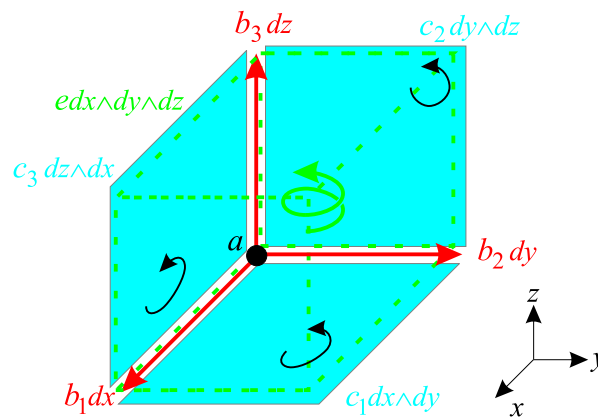


Figure 3.4: Representing forms with the multivector structure.

significance of this observation will become clear in the next section where we show that the structural physical laws are easily formulated by applying the coboundary operation on the corresponding k -cochains.

The reader will observe that our depiction of differential forms in Figure 3.4 is drastically different from the literature standard of Figure 2.3. One noticeable distinction is that Figure 3.1 explicitly shows k -cells (and therefore suggests representations for k -vectors and k -forms) of all dimensions from 0 to n – *in the same structure*. The aggregate object defined as the formal sum of k -vectors, $k = 0, 1, \dots, n$ plays a central role in the development of the universal geometric algebra and is called a *multivector* [14, 21, 20, 23, 24]. Hence the name for our data structure.

For computational purposes, we typically would like to express the forms in an orthonormal basis. In Cartesian coordinates, of course, this requires no change. Curvilinear coordinate systems force us to multiply some of the cochain coefficients by an appropriate factor in order to achieve normality. For example, to normalize the basis given above for spherical coordinates, we must include r in the coefficient of the $d\theta$ term and $r \sin \theta$ in the $d\phi$ term – and the product of these in any higher dimensional forms adjacent to both of these 1-forms. That we must include these as part of the coefficient, rather than cell name, will be shown in Section 6.3.

Note that assigning a null name to a cell is equivalent to omitting the corresponding cell from the cochain. Thus, the multivector structure is naturally represented on a *finite* unit cubical cell complex by assigning null names to all cells that are not in the starplex. More generally, it should be now clear that the cubical cell complex provides a single common data structure for representing any and all geometric and topological information about spatially distributed phenomena. Depending on the choice of cell coefficients, the cubical cell complex structure can support both numerical and symbolic models, as well as finite and infinitesimal control elements.

4 Operations and Physical Laws

We asserted earlier that the multivector structure will be useful in unifying and simplifying manipulation of physical models; now we supplement the multivector structure with several fundamental operations and illustrate how they can be used for formulating and expressing physical laws. We focus on the arguably one of the most fundamental physical laws – that of balance of an assumed physical quantity.

4.1 The balance law

Intuitively, a balance law is the simple requirement that:

$$\sum_{\text{boundary}} \left\{ \begin{array}{c} \text{amount of the} \\ \text{physical quantity} \\ \text{THROUGH} \\ \text{the boundary to the} \\ \text{INSIDE} \end{array} \right\} = \left\{ \begin{array}{c} \text{amount of the} \\ \text{physical quantity} \\ \text{DESTROYED or} \\ \text{STORED INSIDE} \\ \text{a region} \end{array} \right\} \quad (4.1)$$

where the boundary's role in distinguishing between the region's inside and outside is assumed. This intuitive law is surprisingly general, considering the simplicity of its statement. For one, note that it is not necessary to mention the particular shape or size of the boundary. This indicates that the law is a topological one. The type of physical quantity is not mentioned – balance might be of surface and body forces, mass flow, heat flow, and so on. For examples like mass flow, if there is no production or destruction of the quantity, the above balance simplifies further to a homogeneous equation of conservation; if the net sum of forces is zero, the balance becomes a static equilibrium statement; and so on.

The fact that the balance law is a topological notion suggests that it can be expressed in terms of operations on topological entities. Specifically, suppose the quantities are given as cochains on a complex which defines the region of space with its its boundary. Tonti, in [54, chapter 4], demonstrated that equation (4.1) may generally be written as

$$\delta(f) = g \quad (4.2)$$

where f is a k -cochain representing the quantity associated with the boundary cells and g is a $(k + 1)$ -cochain for the interior cell quantity production. The two cochains are related by the coboundary operation δ which, informally, sums the signed contributions of all boundary cells of f and assigns the resulting value to the incident cells of g (see the appendix). For each cell, the sign is determined by the relative orientation of incident cells. Branin [5] makes the same point in writing that gradient, curl and divergence are all topologically coboundary operators with the only difference of note being that the coboundary holds in the finite case whereas the vector calculus operators hold only in the limit.

Of course, the intuitive statement of equation (4.1), as well as Tonti's and Branin's observations regarding the coboundary process, hold only for finite regions. For the corresponding infinitesimal or differential statements, a limiting process must take the finite control element into infinitesimal – recall Figure 1.1 (middle row) once more – and transform the coboundary operation into the operation of *exterior differentiation*. While the analogy between the finite and infinitesimal models is well known [1, 60], the precise correspondence is often obscured by elegant symbolic transformations. We are now ready to describe how the balance law can be represented on the multivector data structure in terms of densities of the associated physical quantities, which also establishes direct relationships between the operations of coboundary, exterior differentiation, and the balance law. Storage or production terms in equation (4.1) are simply represented by attaching the appropriate coefficients to the 'volumetric' cells of indicated dimension. The main difficulty lies in expressing the flow of the quantity densities through the "boundaries" of the infinitesimal cells, because these boundaries are not in the starplex structure. In terms of classical differential forms, this notion is usually described by the process of exterior differentiation.

4.2 The exterior derivative d

The exterior derivative is commonly defined recursively in the literature. The base case is for 0-forms; for a scalar function (0-form) f , the exterior derivative is

$$df = \sum_i \frac{\partial f}{\partial x_i} dx_i \quad (4.3)$$

where $\frac{\partial f}{\partial x_i}$ is the partial derivative in the x_i direction and dx_i are linearly independent 1-forms. In other words, the exterior derivative of the 0-form is a 1-form, also known as the gradient of the scalar function f .

For a k -form ω , $k \geq 1$, the first step is to recognize that it is possible to write $\omega = \sum_i f_i \sigma_i$, where the f_i are functions (zero-forms) and the σ_i are orthogonal basis k -forms. Then we have

$$d\omega = \sum_i (df_i) \wedge \sigma_i = \sum_i \left(\sum_j \frac{\partial f_i}{\partial x_j} dx_j \right) \wedge \sigma_i \quad (4.4)$$

This general definition of the exterior derivative indicates that the result is the formal sum of the exterior products; each exterior product involves a 1-form and a k -form; therefore the dimension of the resulting form is always 1 more than the dimension of ω . That is, for any k -form ω , $d\omega$ is always a $(k+1)$ -form.

For a simple example, suppose $\omega_1 = f dx + g dy$ is a 1-form in Euclidean 2-space. So $\omega_1 = \sum_i f_i \sigma_i$ means

$$f_1 = f, \quad \sigma_1 = dx, \quad f_2 = g, \quad \sigma_2 = dy$$

and the exterior derivatives of the zero-forms f_i are

$$df_1 = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy, \quad df_2 = \frac{\partial g}{\partial x} dx + \frac{\partial g}{\partial y} dy$$

Then evaluating this in equation (4.4) is

$$\sum_i df_i \wedge \sigma_i = \left(\frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy \right) \wedge dx + \left(\frac{\partial g}{\partial x} dx + \frac{\partial g}{\partial y} dy \right) \wedge dy \quad (4.5)$$

$$= \frac{\partial f}{\partial x} dx \wedge dx + \frac{\partial f}{\partial y} dy \wedge dx + \frac{\partial g}{\partial x} dx \wedge dy + \frac{\partial g}{\partial y} dy \wedge dy \quad (4.6)$$

$$= \frac{\partial f}{\partial y} dy \wedge dx + \frac{\partial g}{\partial x} dx \wedge dy \quad (4.7)$$

$$= \left(\frac{\partial g}{\partial x} - \frac{\partial f}{\partial y} \right) dx \wedge dy \quad (4.8)$$

As expected, the exterior derivative of the 1-form is a 2-form that corresponds to the total (infinitesimal) quantity entering/exiting the two-dimensional cell $dx \wedge dy$ through its boundary; this is traditionally represented by the **curl** in vector calculus.

4.3 The exterior derivative d – a geometric interpretation

By the definition in equation (4.4), exterior differentiation is expressed through operations of partial differentiation and exterior product. The explicit representation of geometric and topological information simplifies the exterior differentiation process and at the same time explicitly relates it to the usual operation of coboundary. A correspondence between the exterior derivative d and the vector calculus **grad**, **curl** and **div** operations is commonly mentioned in the literature (for examples, see [12]) or [58]; at least one author relates these vector calculus operations with coboundary operation δ (see [5]); [1, chapter 15] and [54, chapter 7] combine these to show d and δ are “consistent” or “analogous”, whereas [60] writes that they “coalesce”. The multivector structure allows this correspondence to be made precise and algorithmic: the exterior derivative d is a simple extension of the coboundary process δ on the multivector structure.

This fact is relatively obvious in equation (4.3): except for the $\frac{\partial}{\partial x_i}$ operating on f , this is exactly how the definition of the coboundary given in the appendix would evaluate on a 0-form – a formal sum of a coefficient (the function f) attached to the adjacent 1-cells (the unit basis forms dx_i). Equation (4.4) generalizes this for higher dimension k ; notice that after expansion each exterior product operates on a basis k -form σ_i and 1-form $\frac{\partial f_i}{\partial x_j} dx_j$. This results in a $(k+1)$ -form and, as suggested in Figure 3.2, amounts to simply transferring the coefficient $\frac{\partial f_i}{\partial x_j}$ to the $k+1$ dimensional coface $dx_j \wedge \sigma_i$ of ω . Summation over all such exterior products has the effect of adding all coefficients attached to the same $(k+1)$ -dimensional cells. In other words, exterior differentiation operates precisely as coboundary on the coefficients differentiated with respect to the basis one-dimensional cells and are assigned to the corresponding cells of the starplex.

Because of our method of cell naming in Section 3.2, partial differentiation is a trivial symbolic process. The basis 1-cell names dx_j change syntactically to ∂x_j , and the directional derivatives are then $\frac{\partial}{\partial x_j}$ or, using notation we will define formally in Section 5, $\frac{\partial}{\text{cell name}}$. We shall use this notation when operating on the multivector data structure. Since we want to demonstrate equivalence with traditional formulations, we will rewrite some equations in more traditional vector calculus terms where appropriate.

The simple geometric interpretation is well hidden in the symbolic notations of equations (4.3) and (4.4). In terms of the multivector data structure, equation (4.3) – the exterior derivative of a 0-form – may be described in two steps:

1. transfer of the coefficient f from the 0-cell to the incident 1-cells dx_i , followed by
2. assign $\frac{\partial f}{\text{cell name}}$ for each 1-cell dx_i .

Exterior differentiation of a k -form – as in equation (4.4) – repeats this for a number of different coefficients and also requires a third step of forming the exterior products with the basis k -forms σ_i . In an orthogonal system, most of these exterior product terms will evaluate to 0; only those basis 1-cells dx_j that are linearly independent with σ_i produce non-zero coefficients. Thus, generalizing the base case, the exterior differentiation of a k -form may be summarized as a very simple and intuitive geometric procedure on the multivector structure:

1. for every k -cell, transfer the coefficient to every adjacent orthogonal 1-cell,
2. assign $\frac{\partial f}{\text{cell name}}$ for each 1-cell dx_i ,
3. transfer the result to the $(k+1)$ -cells spanned by the k -cell and adjacent orthogonal 1-cell and sum all the coefficients transferred to the same $(k+1)$ -cell.

This geometric procedure is shown in Figure 4.1 for the calculations carried out symbolically in equations (4.5) - (4.8). The $(k + 1)$ -form produced by the exterior differentiation is represented by the resulting $(k + 1)$ -cochain on the multivector structure; two further examples in Figure 4.2 illustrate exterior differentiation of a 1-form and a 2-form in Euclidean 3-space.

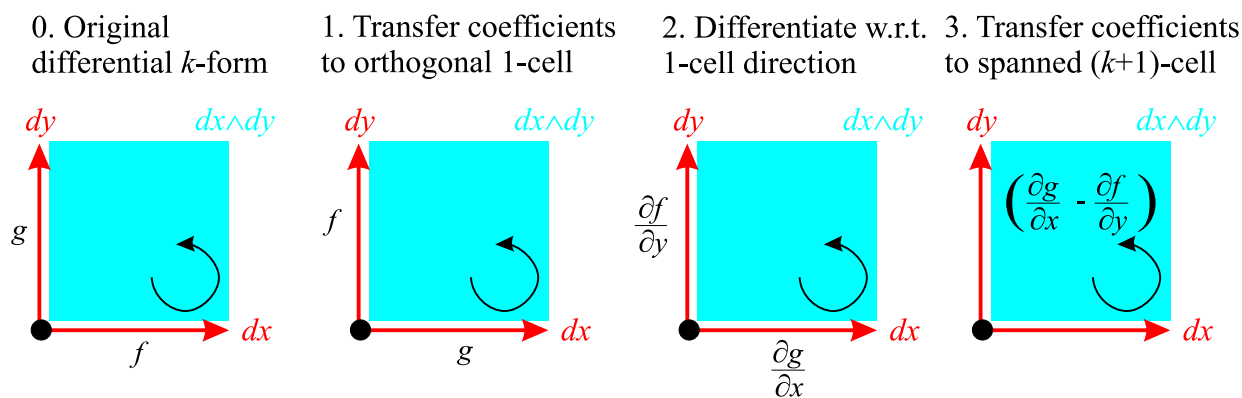


Figure 4.1: A pictorial representation of equations (4.5)-(4.8).

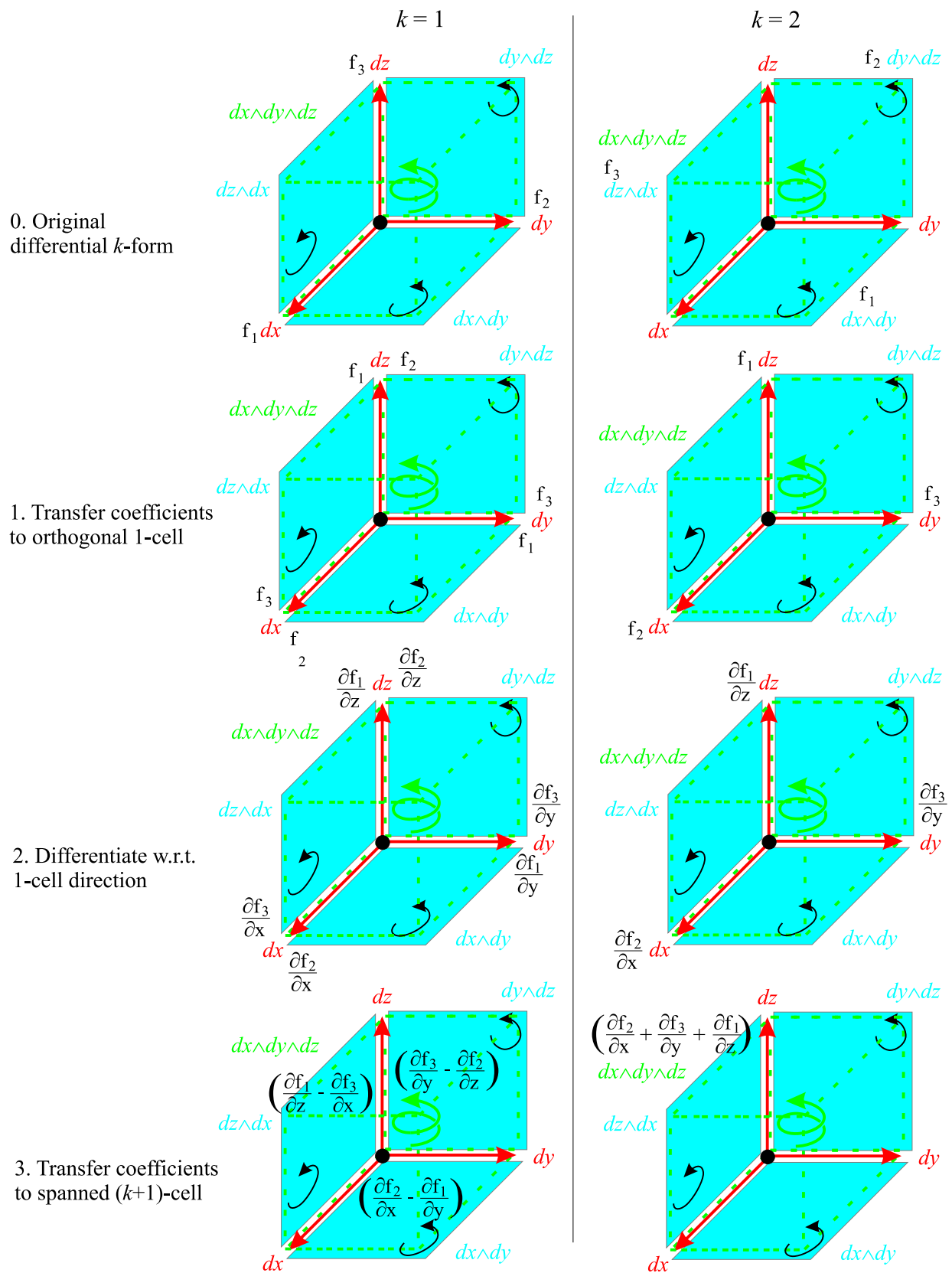


Figure 4.2: A pictorial representation of the exterior derivative with $n=3$.

5 Unification

By now it should be apparent that every physical balance law may be described in two distinct ways: in a finite integral sense on a finite cell complex, or in an infinitesimal differential sense on the starplex. Returning to Figure 1.1, we see that the transition between the finite and infinitesimal models occurs twice in a typical modeling scenario. The first time, in the middle row, a finite unit size control element is shrunk down through some limiting process into an infinitesimal model to help in problem *formulation*. Later, in the bottom row, the infinitesimal model is integrated back into a finite (usually not unit) one to facilitate numerical *solution* of the problem.

We are now in a position to explain how the translation between infinitesimal and finite statements may be completely automated using the Generalized Stokes' Theorem and its dual described below.

5.1 Stokes' Theorem: infinitesimal to finite

It is hard to imagine approaching most applied mathematics or mathematical physics problems without Stokes' Theorem in a central role [12, 39]. The *computational* significance can hardly be overstated as Stokes' Theorem, alternately expressed in specific dimensions as the Fundamental Theorem of Calculus, Green's or Gauss' Theorem, makes various calculations feasible. That the very proof of the theorem may be done as a computation is perhaps as persuasive an argument as any other that it is thoroughly intertwined with computations [53]. The *philosophical* significance of Stokes' Theorem is equally important. Its generality – it holds for *any* dimension, is independent of coordinate system [9], and is metric-free [36, 54] – provides a unification for the various problems it helps solve. In this sense, Stokes' Theorem can be called a fundamental link between analysis and topology [19].

For our limited purposes, Stokes' Theorem indicates precisely how to translate from the infinitesimal balance law (a differential relation between the differential forms) to the finite one (an integral equality expressed using coboundary operation on cochains). Let us take the typical formulation of the theorem $\int_{\partial R} \omega = \int_R d\omega$ and consider each side of the equation. The left hand side can be written as a two-step diagram:

$$\int_{\partial R} \omega = \left\{ \begin{array}{ccc} k - \text{cochain} & \xrightarrow{\delta} & (k + 1) - \text{cochain} \\ \int_{\text{cell by cell}} \uparrow & & \\ k - \text{form} & & \end{array} \right. \quad (5.1)$$

The first vertical transition corresponds to the usual operation of integration over the boundary ∂R of some region R . Given a k -form and a finite cell complex, integration takes place over every finite k -dimensional cell; the integral value represents the total physical quantity associated with the finite cell and is represented as a coefficient stored with the given cell. In other words, the result of the integration is a finite k -cochain. But recall that a k -form is also represented as a (coefficient)*(basis k -cell) in the multivector data structure and thus may be considered an infinitesimal k -cochain. It should be apparent that multivector representation of a differential form implies unambiguously and explicitly both the type of the coefficients and the dimension of the finite cochain. The second, horizontal, transition in the diagram (5.1) is the familiar coboundary process already described in Section 4. It simply transfers the coefficients from the all k -cells to all incident $(k + 1)$ -cells with the sign determined by the relative orientation between the cells; each $(k + 1)$ -cell gets a new coefficient equal to the sum of all transferred individual coefficients. The reader will notice that we have just restated the finite form of the balance law.

The right hand side of Stokes' Theorem may be represented by a similar diagram:

$$\int_R d\omega = \left\{ \begin{array}{ccc} & & (k + 1) - \text{cochain} \\ & & \uparrow \int_{\text{cell by cell}} \\ k - \text{form} & \xrightarrow{d} & (k + 1) - \text{form} \end{array} \right. \quad (5.2)$$

The first horizontal transition is the usual exterior differentiation operation whose representation on a multivector structure was described in Section 4.3. It is followed by a second vertical transition corresponding to integration of the resulting $(k + 1)$ -form over every finite $(k + 1)$ -dimensional cell of region R . The latter transition can be viewed as transition from infinitesimal $(k + 1)$ -cochain on the multivector data structure to the finite $(k + 1)$ -cochain representing an amount of some physical quantity over the discretized region R .

Combining the two diagrams, we see that Stokes' Theorem can be written with the commutative diagram

$$\begin{array}{ccc}
 k - \text{cochain} & \xrightarrow{\delta} & (k + 1) - \text{cochain} \\
 \int_{\text{cell by cell}} \uparrow & & \uparrow \int_{\text{cell by cell}} \\
 k - \text{form} & \xrightarrow{d} & (k + 1) - \text{form}
 \end{array} \tag{5.3}$$

which is a slight modification of a diagram found in [1, page 533]. The combined diagram may also be viewed as a transformation of the bottom row, expressing an infinitesimal balance statement, into the corresponding finite balance law expressed by the top row. In practical terms, Stokes' Theorem and the implied transformations corresponds to the numerical integration procedures indicated in the bottom row of Figure 1.1.

The discussion of Stokes' Theorem above introduced the notion of strong coefficient typing for the first time. A coefficient F attached to a finite size cell \mathbb{C} in the top row of diagram (5.3) represents a *total* quantity associated with \mathbb{C} . It is usually different from the form coefficients in the bottom row of the same diagram. The solitary, but crucial, exception being that 0-form coefficients have the same type as cochain coefficients. Coefficients g attached to an infinitesimal size cell represent the *density* of the same physical quantity over the volume of the cell. Since the cells for the bottom row of diagram (5.3) have different dimensions, namely k and $(k + 1)$, the form coefficients have different types. For example, with $k=1$, the k -form coefficients have type of quantity per length while the $(k + 1)$ coefficients are quantity per area. The vertical integration maps of diagram (5.3) provide a transformation from infinitesimal structure to finite structure, and therefore must change coefficient type from density to total quantity. Because the integration of k -forms is over k -cells, and similarly $(k + 1)$ -forms are integrated over $(k + 1)$ -cells, the change of type is exactly as required. The quantity per volume, when integrated over a volume, becomes simply a quantity.

5.2 The dual of Stokes' Theorem: finite to infinitesimal

The finite balance law is significant only because it is usually assumed to hold for *every* finite region in space. This assumption can be used to transform an integral equation into a differential relationship via a limiting process. That the vertical integration maps of diagram (5.3) may be reversed appears intuitively obvious; the resulting process may be described as "differentiation by a volume" [10]. To be more precise, we define the differentiation with respect to a cell C as:

$$\frac{\partial F}{\text{cell}} \stackrel{\text{def}}{=} \lim_{\|\mathbb{C}\| \rightarrow 0} \frac{F \cdot \mathbb{C}}{\|\mathbb{C}\|} \tag{5.4}$$

where F is a function that assigns a coefficient (value) to every k -cell F . In other words, F is a k -cochain, whose value on every k -cell is equal to the integral of some function f . This definition captures and expresses the standard notion of differentiation and subsumes the more common symbolic expressions relying on coordinate systems or metric.² It corresponds to a very precise theorem in [60, p. 166] stating every k -cochain limiting process yields a unique differential k -form.³ It is more common to rewrite equation (5.4) in an equivalent form [10, 12] as

$$\frac{\partial F}{\text{cell}} \stackrel{\text{def}}{=} \lim_{\|\text{cell } \mathbb{C}\| \rightarrow 0} \frac{1}{\|\mathbb{C}\|} \int_{\mathbb{C}} f(\vec{x}) d\mathbb{C} = f(x_0) \tag{5.5}$$

indicating explicitly that the limiting process transforms any cochain F into a differential form $f(x_0)$ evaluated at some point x_0 . If we apply $\frac{\partial}{\text{cell}}$ to the total quantities represented by a cochain on a finite cubical cell complex, we obtain the corresponding differential k -form – a function defined at every point of the finite cell. As written in equations (5.4) and (5.5), the limiting operation is completely coordinate-free and the direction of differentiation is implied to be the cell's attitude. Let us now apply the limiting procedure to a finite control element embedded using some orthogonal coordinate system. Recall from Section 3.2 that embedding infinitesimal cells with a coordinate

²We introduce a different notation for partial differentiation here; we feel that this is necessary since there is no good way to maintain consistency even within this text and certainly not with the conventions of previous literature. The symbol ∂ is already overloaded to represent either a partial derivative or the boundary operator. Although context would normally resolve ambiguities between the two, that is not the case here because we want to be able to differentiate with respect to a cell. Neither can we use symbol d , because it is usually used to denote the exterior derivative and calculus ordinary derivatives.

³The detailed proof is fairly complex and would take us beyond the scope of this paper.

system corresponds to naming cells in the multivector data structure according to the associated attitude. Therefore, the limiting operation $\frac{\partial}{\text{cell}}$ becomes $\frac{\partial}{\text{cell name}}$; for example, if cell names are dx and dy , $\frac{\partial}{\text{cell}}$ becomes $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$. Figure 5.1 illustrates how application of this limiting process to all cochains on a unit Cartesian cubical element produces a multivector representation of all differential forms at the origin of the corresponding starplex structure.

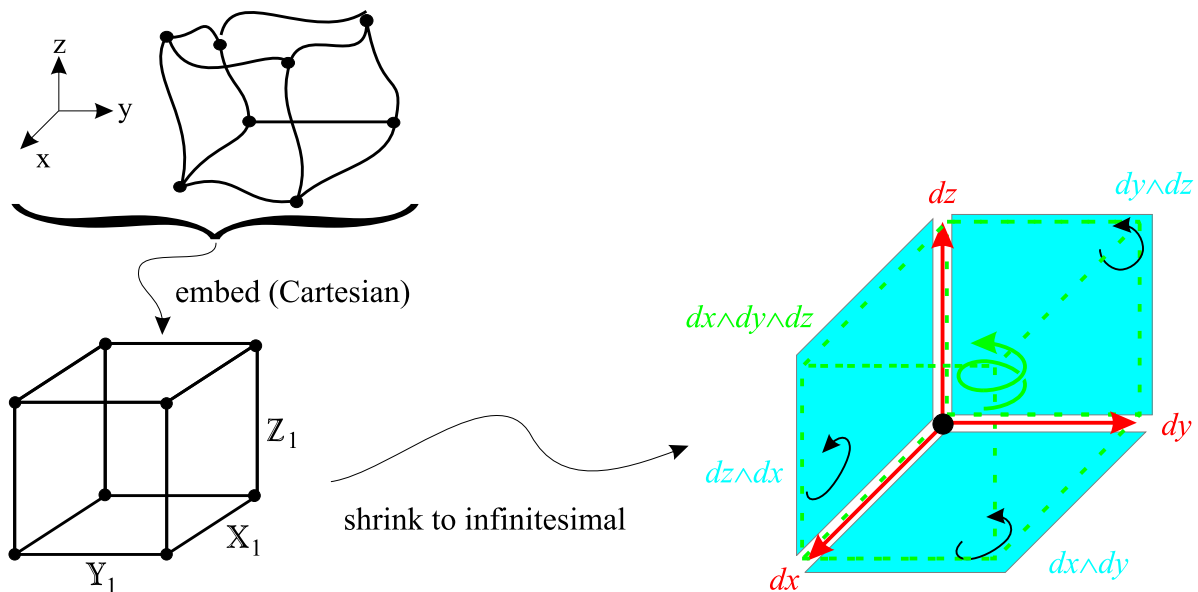


Figure 5.1: Mapping a cubical complex to a differential form.

With assumptions of cubical combinatorics and orthogonal corners, the limiting process may be visualized as a “collapse” of the finite cubical cell complex into the starplex representing the combinatorial neighborhood of the origin. Thus, all parallel cells of the same dimension collapse to a single cell of that dimension. Since there are precisely 2^{n-k} parallel k -cells in n -space, the limiting process perfectly adjusts the number of cells to match the number of forms. Note that this notation is also consistent with the use of the $\frac{\partial}{\text{cell name}}$ notation introduced in Section 4.3 for partial differentiation of coefficients attached to infinitesimal size cells.

Let us now assume that a finite balance law expressed by the top of row of diagram (5.3) holds for every region of space. Then applying the limiting process to all cochains yields the corresponding infinitesimal law expressed by the bottom row of the same diagram. This relationship may be concisely expressed by the following diagram, dual to Stokes' Theorem:

$$\begin{array}{ccc}
 k - \text{cochain} & \xrightarrow{\delta} & (k + 1) - \text{cochain} \\
 \frac{\partial}{\text{cell}} \downarrow & & \downarrow \frac{\partial}{\text{cell}} \\
 k - \text{form} & \xrightarrow{d} & (k + 1) - \text{form}
 \end{array} \tag{5.6}$$

Just as Stokes' Theorem requires integration over cells of various dimensions, this differentiation with respect to a cell is dependent on the cell's dimension. So the same $\frac{\partial}{\text{cell}}$ notation logically implies higher order derivatives for cells of dimension greater than 1; for a cell embedded with attitude the same as $dx \wedge dy \wedge dt$, $\frac{\partial}{\text{cell}}$ means $\frac{\partial^3}{\partial x \partial y \partial t}$. The somewhat surprising fact that such a diagram does not seem to appear in literature indicates that its utility is not clear. Let us transform the commutative diagram into a single equation by breaking it into two parallel paths from the

k -cochain to $(k + 1)$ -form, analogously to our analysis of Stokes' Theorem:

$$d\left(\frac{\partial f}{\text{cell}}\right) = \begin{cases} k - \text{cochain} \\ \frac{\partial}{\text{cell}} \downarrow \\ k - \text{form} \xrightarrow{d} (k + 1) - \text{form} \end{cases} \quad (5.7)$$

$$\frac{\partial}{\text{cell}}(\delta f) = \begin{cases} k - \text{cochain} \xrightarrow{\delta} (k + 1) - \text{cochain} \\ \downarrow \frac{\partial}{\text{cell}} \\ (k + 1) - \text{form} \end{cases} \quad (5.8)$$

or

$$d\left(\frac{\partial f}{\text{cell}}\right) = \frac{\partial}{\text{cell}}(\delta f) \quad (5.9)$$

The last equality makes it clear that there are two equivalent ways to formulate a differential balance law starting with a finite cell complex: the limiting process followed by exterior differentiation is equivalent to a coboundary statement followed the limiting process. In particular, the transformations between finite and infinitesimal balance laws on a typical control element amount to a simple syntactic substitution of cell names. In practical terms, this means that a balance law may be stated in terms of a convenient finite structure, for example using the finite cubical control element in Figure 1.1 or some other intuitive geometric structure. The translation of such a law to the language of differential forms can be completely automated; an example in Figure 5.2 shows all required transformations for the balance law expressed on a two-dimensional control element.

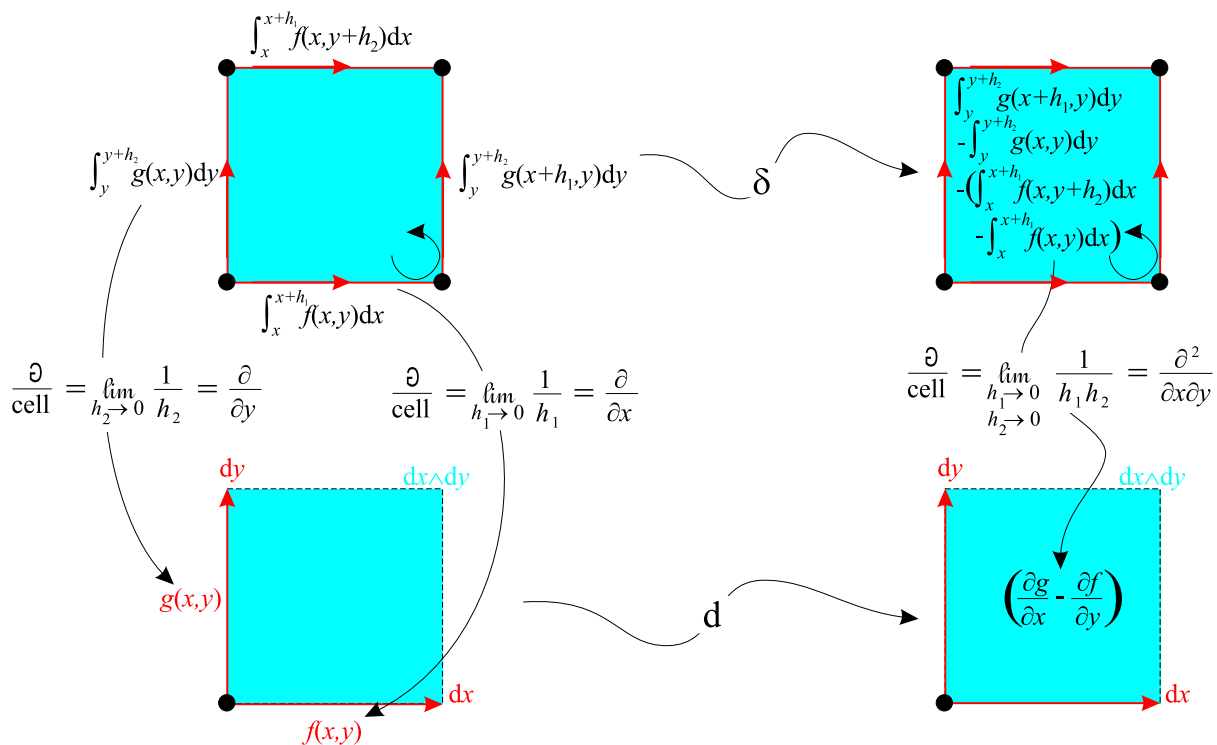


Figure 5.2: Dual of Stokes' Theorem on a two-dimensional cube.

6 Implications and Prototype

6.1 Advantages of the multivector structure

We now revisit the modeling process illustrated in Figure 1.1, to see how it may be supported by the multivector data structure. Because the whole process may now be restated in terms of the same combinatorial structure, the modeling sequence may be “collapsed” and represented by a set of transformations operating on the same structure, as shown in Figure 6.1. At the heart of the structure is a finite n -dimensional cubical cell complex and the corresponding starplex.

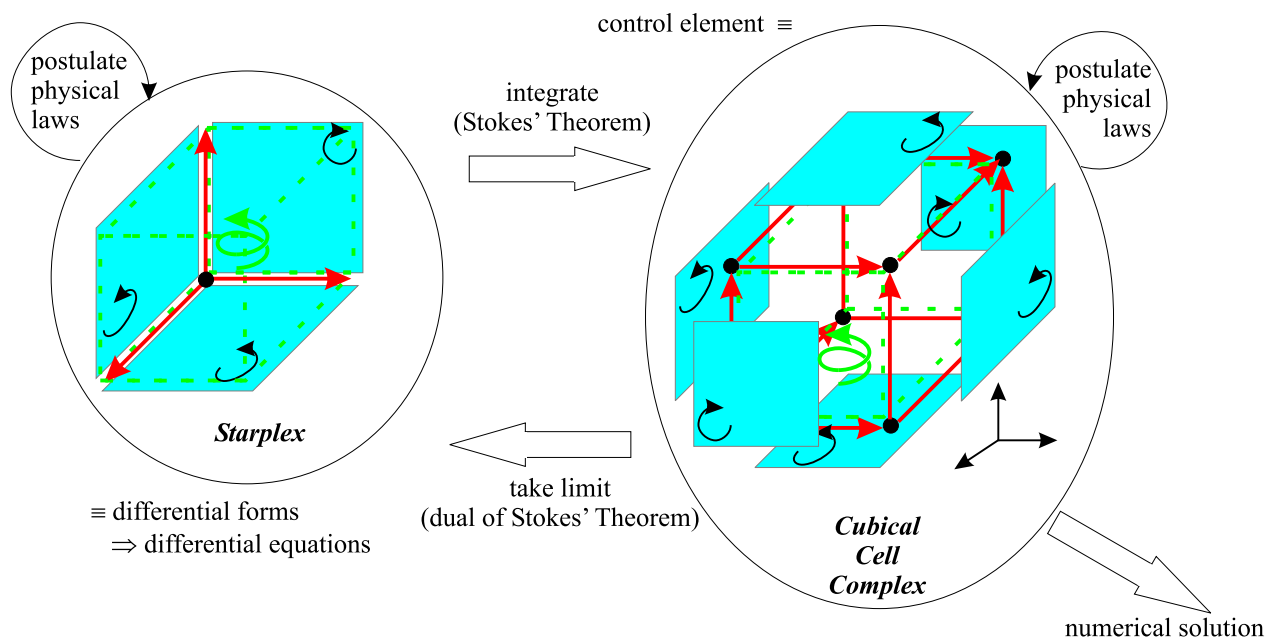


Figure 6.1: A new “sequence” of steps in modeling physical behavior – supported by the cubical cell complex. The infinitesimal statements are handled by a subset of the cubical cell complex – the starplex.

Coordinate systems are effected by naming the cells in the complex; postulated physical quantities are represented as appropriate cochains formed by attaching coefficients (scalars, vectors, etc.) to cells of the appropriate dimension. Physical laws may be expressed either in finite (integral) or infinitesimal (differential) form, as the translation between the two models is performed on demand. In contrast to the difficulties implied by the process in Figure 1.1, we observe:

- **Universality** As we showed in Section 4, all balance laws may be described by a coboundary or exterior derivative equation on the same multivector structure that explicitly reflects the usual analogies between physical theories. Changing coordinate systems amounts to syntactic change in the cell naming convention that is automatically propagated to symbolic expressions, if so desired (recall Section 3.2). Although we have not shown it here, [11] suggests that it is possible to create maps which reduce the dimension of a problem by reducing the dimension of the cell complex. Then a single model of dimension n would imply all the models of dimension $k < n$.
- **Strong Typing** By using cochains for our representation of physical quantities we automatically have strong coefficient typing – by virtue of the fact that the cochain coefficients must be from the same Abelian group and attached to the cells of the explicitly declared dimension. The strong typing of densities in the infinitesimal model eliminates possibility of nonsense operations such as $\text{curl}(\text{curl } f)$; the automatic translation via Stokes’ Theorem and its dual enforces the consistency of densities with the total quantities on the finite model. The proper typing of the total quantities is paramount in implementing consistent and standard interfaces between distinct software and multi-physics components.

- **Intuitiveness** The combinatorial and geometric appeal of the multivector structure naturally suggest an intuitive geometric language built over a computer algebra for defining and computing with physical models. We illustrate below by example that such a language should be easily accessible to users without specialized training or sophisticated mathematical background, because it does not require direct manipulation of differential forms or equations. The correctness of the model is enforced at all times, and the corresponding symbolic expressions may be generated automatically, if so desired.
- **Integration** Since the cubical cell complex structure is available at all stages in Figure 6.1, it may be used for both the model development in the early stages as a control element and in final stages for its solution as a discretization element (such as finite element). In particular, it should be possible to automate the translation from the model to some discretization scheme for its solution; in this case, the first principles model would be directly linked to its numerical solution.

To illustrate some of these attractive features, in the next section we describe a prototype implementation of an interactive physics editor using the multivector data structure. The editor allows creation and transformation of finite and infinitesimal models of balance in an intuitive and interactive fashion. Symbolic differential or integral equations may be generated automatically at the push of a button.

6.2 Prototype physical editor

The multivector structure translates into a straightforward implementation on a computer. The cubical cell complex may be represented using one of many known data structures for representing cells complexes, for examples see [7, 57]. Combinatorially, the starplex is a subset of a cubical cell complex, and is easily represented on the same structure by simply marking the extra cells as null. In addition to the information on incidence between the cells, each cell is a placeholder for its name and any number of associated coefficients. The resulting data structure can be visualized through a graphics interface, as shown by a screen capture of our implementation in Figure 6.2.

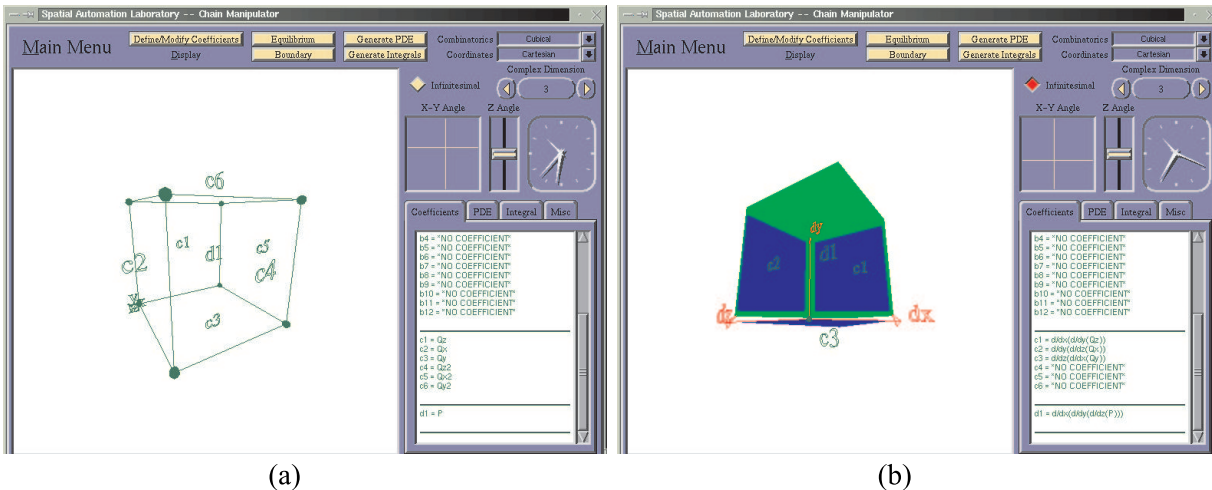


Figure 6.2: (a) A cubical 3-complex with some cochains defined. (b) The starplex and differential forms associated with (a).

With the implementation of classes for cells, cubical complexes, and coefficients, we can define k -cochains (and hence k -forms) to represent various physical quantities. For a particular choice of coefficients, the class of all k -cochains forms a linear vector space with addition and multiplication defined in a cell-by-cell fashion; for other useful operations on (co)chains see [44, 45]. Following Section 4.3, a balance law is represented by an algorithm that computes a $k + 1$ -dimensional cochain, given a k -cochain as input. If the input cochain is finite, the algorithm operates as the coboundary operation; the algorithm works as the exterior derivative operator if the input cochain is defined on an infinitesimal complex. In pseudo-code:

```

Procedure Balance (k-cochain/form)
For (number of (k + 1)-cells)
   $A_i = 0$ 
For (each cell  $\mathbb{C}$  of dimension k)
   $f =$  coefficient of  $\mathbb{C}$ 
  For (each coface  $\mathbb{C}'$  of  $\mathbb{C}$ )
     $i =$  index of  $\mathbb{C}'$ 
    If (complex is infinitesimal) //  $d$  of k-form
       $\mathbb{C}' =$  1-cell  $\perp \mathbb{C}$  s.t.  $\mathbb{C}' \wedge \mathbb{C} = \mathbb{C}$ 
       $f' = \frac{\partial f}{\text{name}(\mathbb{C}')}$ 
    Else //  $\delta$  of k-cochain
       $f' = f$ 
       $b = \sigma(\mathbb{C}, \mathbb{C}')$ 
       $A_i = A_i + b f'$ 
Return ( $\sum_i A_i \odot \mathbb{C}_i$ )

```

The **If ... Else** loop in the algorithm reinforces the statement in Section 4.3 that d is simply a slight variation of δ . Exterior differentiation requires $\binom{n}{k}$ iterations (the outer loop for each of the basis k -cells), with each iteration visiting all $n - k$ cofaces of k -cell \mathbb{C} . Thus, the total number of steps is $O((n - k)\binom{n}{k})$. For $k = n - 1$, this is $O(n)$ – substantially better than the $O(n\binom{n}{k}) = n^2$ symbolic differentiation procedure implied by equation (4.4).

Automatic switching between finite and infinitesimal models and laws is also straightforward. All such transformations amount to changing the embedded cell names, adjusting the type of the cell coefficients, and choosing the corresponding (finite or infinitesimal) coboundary operation, as described in Sections 5.1 and 5.2.

6.3 Examples

For a simple example, let us first consider three-dimensional mass balance in Cartesian space. We first define a control element and attached quantities – a cubical 3-complex with a 2-cochain and a 3-cochain defined as in Figure 6.2 (a). We now have the choice implied by equation (5.9): we can either shrink the control element to infinitesimal size and then apply the balance law, or we can declare the balance law on this finite structure, and have the editor generate the corresponding infinitesimal model. After we shrink the control element to infinitesimal size, the editor displays the corresponding infinitesimal model as shown in Figure 6.2 (b). When the user postulates a balance requiring that the sum of the 2-cell coefficients (with appropriate relative orientation) be equal to the 3-cell coefficient (Figure 6.3 (a)), the editor responds by generating the corresponding symbolic expressions, either in finite or infinitesimal form (Figure 6.3 (b)).

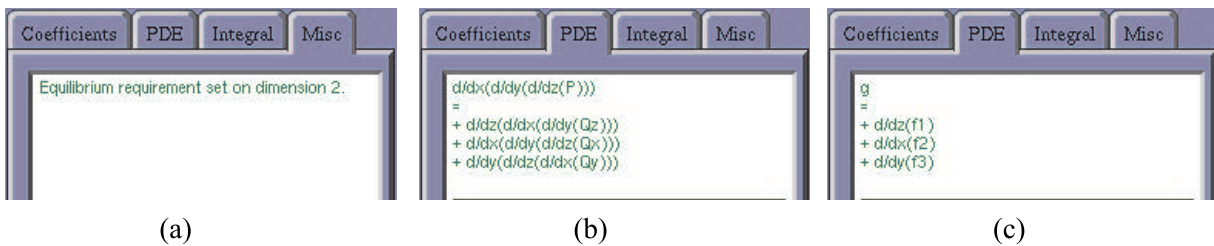


Figure 6.3: (a) Requiring balance, (b) a partial differential equation corresponding to balance on Figure 6.2 (b), and (c) a partial differential equation corresponding to balance of the differential form $f_1 dx \wedge dy + f_2 dy \wedge dz + f_3 dz \wedge dx$.

The generated partial differential equation displayed in Figure 6.3 (b)

$$\frac{\partial^3(Q_x + Q_y + Q_z)}{\partial x \partial y \partial z} = \frac{\partial^3 P}{\partial x \partial y \partial z} \quad (6.1)$$

is equivalent to the usual expression of the mass flow balance. To see this, note that each of the flows Q_{x_i} represents the entire quantity flowing through the face and can be written as

$$Q_{x_i} = \int \int \rho v_{x_i} dx_j dx_k,$$

where ρ is mass density and v is velocity. Similarly, if we allow mass density to vary over time, then

$$P = \int \int \int \left(-\frac{\partial \rho}{\partial t} \right) dx dy dz$$

Substituting expressions for coefficients Q_{x_i} and P into equation (6.1) we get the more familiar form of the same equation often derived by Taylor series expansion [18]:

$$\frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_y)}{\partial y} + \frac{\partial(\rho v_z)}{\partial z} = -\frac{\partial \rho}{\partial t}$$

We could also get this form of the equation directly, but we can only do this on the infinitesimal control element, because the coefficients ρv_{x_i} are intrinsically infinitesimal. If we take $f_i = \rho v_{x_i}$ and $g = -\frac{\partial \rho}{\partial t}$, the editor generates the equation shown in Figure 6.3 (c).

Suppose we now switch to cylindrical coordinates. The 2-cells of the infinitesimal structure are renamed to correspond to the orthogonal basis two-forms: $d\theta \wedge dz$, $dz \wedge dr$ and $dr \wedge d\theta$. The flow through the infinitesimal boundary would be $f_1 d\theta \wedge dz + f_2 dz \wedge dr + f_3 dr \wedge d\theta$, except we need to scale some cells in order to normalize the basis. The normalization for cylindrical coordinates includes a factor of r for every basis form involving $d\theta$. So the flow is actually

$$f_1 r d\theta \wedge dz + f_2 dz \wedge dr + f_3 r dr \wedge d\theta. \quad (6.2)$$

The editor reapplies the *same* balance law, following the infinitesimal version of the algorithm: it transfers $f_1 r$ to the orthogonal 1-cell, namely dr , and differentiates with respect to this direction to get $\frac{\partial}{\partial r}(f_1 r)$. Similarly, the other two terms of equation (6.2) produce $\frac{\partial}{\partial \theta}(f_2)$ and $\frac{\partial}{\partial z}(f_3 r)$. Transferring these coefficients to the coface and adding according to relative orientation results in

$$d(f_1 r d\theta \wedge dz + f_2 dz \wedge dr + f_3 r dr \wedge d\theta) = \left(\frac{\partial}{\partial r}(f_1 r) + \frac{\partial}{\partial \theta}(f_2) + \frac{\partial}{\partial z}(f_3 r) \right) dr \wedge d\theta \wedge dz$$

Once again, this expression is equivalent to the usual expression obtained by normalizing the coefficient of the three dimensional cell $dr \wedge d\theta \wedge dz$:

$$\left(\frac{1}{r} \frac{\partial}{\partial r}(f_1 r) + \frac{1}{r} \frac{\partial}{\partial \theta}(f_2) + \frac{\partial}{\partial z}(f_3) \right) r dr d\theta dz,$$

which the reader should recognize as the the differential forms version of $\vec{\nabla} \cdot \vec{f}$ in three dimensional cylindrical coordinates.

We emphasize that the above symbolic transformations are shown here only for the benefit of the reader; they are not needed for operation of the physics editor.

6.4 Conclusions and future work

We have used tools from algebraic topology to show that any balance law may be represented combinatorially – and thus on a computer data structure. This representation is valid for both finite and infinitesimal balance models and allows for complete automation of the process of formulating and subsequently solving balance problems. As a direct consequence, we have shown that it is possible to hide the underlying mathematics allowing for an intuitive computer program which can be used with minimal mathematical sophistication.

Most physical laws appear to be compositions of balance laws, constitutive (measured) relationships, and various structural transformations [54]. For example, proper formulation of laws that are commonly described using the Laplacian require switching to dual structure twice [3, 17, 32]. Constitutive laws, by definition, are not topological

as they require physical measurements. It has been suggested [16, 45, 55] that such laws may be formulated as additional constraints and transformations on embedded cochains representing distribution of physical quantities. Precise formulation of other structural and constitutive laws should greatly expand the scope and capabilities of the physics editor, including modeling of multi-physics problems.

The examples presented in Section 6.3 indicate how *symbolic* mathematical expressions of distributed phenomena may be automatically formulated from intuitive concepts. In fact, this is currently the extent of our prototype implementation. To take full advantage of the unification proposed in Figure 6.1, integration and numerical solution procedures need to be formulated in terms of the operations on numerically-valued cochains. Indeed, such formulations are beginning to appear in literature. For example, the algebraic-topological nature of finite volume method is explored [37], and advantages of finite difference operators that carefully respect the implied topological laws are discussed in [28, 29, 30]. All such properly formulated numerical procedures may be represented as a sequence of transformation of the cochains. Our work suggests that they can be also generated directly from the corresponding infinitesimal model represented on a multivector structure.

A fundamentally different, but equally important, line of enquiry relates to emergence and further development of geometric algebra [14, 20, 21, 23, 24]. We have explicitly recognized that the multivector structure corresponds to the notion of the number in this more general setting and subsumes other concepts, including tensors. With a modest effort, it should be possible to encode most or even all of the geometric calculus operations as algorithmic manipulations of coefficients on our data structure to gain the richness and power of that mathematical language in an intuitive geometric setting.

A Appendix: Concepts from Combinatorial Topology

This appendix briefly summarizes common concepts from algebraic topology that can be found in many standard texts [35, 40, 6]. Unfortunately, numerous topological invariance theorems also allow for wide variations in terminology. We hope that this summary will help the reader to follow the rest of the paper without ambiguities.

***k*-cell:** A set homeomorphic to a closed unit *k*-ball. The unit *k*-ball is a subset of $\mathbb{R}^k : \{x \in \mathbb{R}^k \mid \|x\|_2 \leq 1\}$. The equality here implies that our cells are closed. A **boundary** of a given cell \mathbb{C} is defined as

$$\partial(\mathbb{C}) \stackrel{\text{def}}{=} \{x \mid \|h(x)\|_2 = 1\}$$

where *h* is the homeomorphism mapping the cell \mathbb{C} to the unit *k*-ball.

Intrinsic orientation: The formal definition of orientation is technically complicated and may depend on the specific type of the cells in a complex (see for example [6, 40]). Informally, we assume that every cell is orientable; each of the two possible orientations corresponds to a sense of direction within the cell and is conveniently denoted by a ± 1 designation for a cell \mathbb{C} . It is also common to represent orientation by orderings of the boundary of a cell \mathbb{C} or to equate it with the handedness of the coordinate system associated with the cell. For 1-cells, orientation can be visualized by designating a “head” and a “tail”; for 2-cells, the orientation distinguishes between “clockwise” and “counterclockwise”; for 3-cells, it corresponds to the difference between left-handed and right-handed corkscrews. For 0-cells, we will arbitrarily define the orientation to always be positive. Intrinsic orientation has little significance of its own; its primary use is as an aid to define relative orientation below.

Complex: A collection *C* of cells that satisfy two properties:

- The boundary of each *k*-cell \mathbb{C} is a finite union of (*k* − 1)-cells in the set *C*: $\partial(\mathbb{C}) = \cup_j \mathbb{C}_j$.
- The intersection of any two cells $\mathbb{C}_i, \mathbb{C}_j$ in the set *C* is either empty or a unique cell in the set.

The dimension of the complex is the highest dimension of its cells. We will be particularly interested in a specific type of complex called a **cubical** cell-complex (see Figure A.1); an *n*-dimensional complex is cubical if every *n*-cell has exactly $2^{n-k} \binom{n}{k}$ *k*-cells in its boundary.

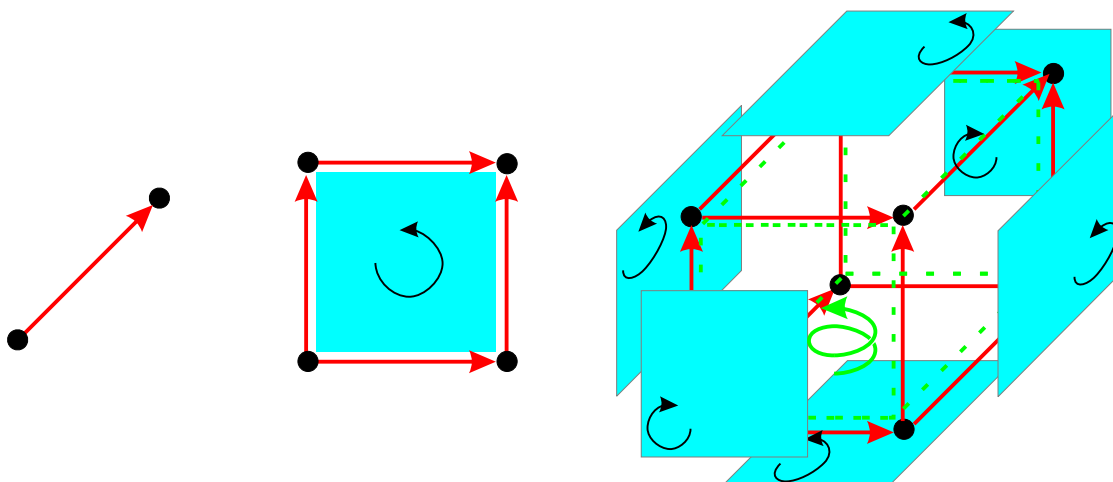


Figure A.1: The structure of 1-, 2- and 3- dimensional cubical complexes.

(Co)face: A k -cell \mathbb{C}_i is a coface of a $(k - 1)$ cell \mathbb{C}_j if \mathbb{C}_j is a cell in the boundary of \mathbb{C}_i . We also consider the reverse relationship and say that \mathbb{C}_j is a **face** of \mathbb{C}_i . Two examples of cofaces are pictured in Figure A.2. The left picture indicates the cofaces of a 0-cell; the right picture shows the cofaces of a 1-cell.

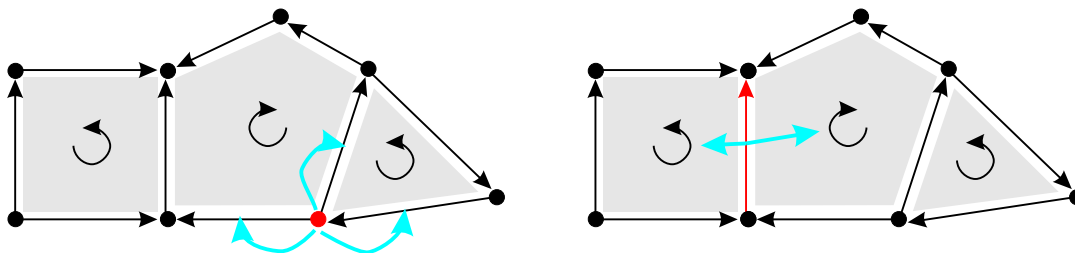


Figure A.2: Depiction of cofaces.

Star: For a cell \mathbb{C} of some complex C , the star of \mathbb{C} , denoted $St(\mathbb{C})$, is the union of adjacent cells \mathbb{C}_A of dimension greater than or equal to the dimension of \mathbb{C} . An equivalent statement would be to define

$$St(\mathbb{C}) \stackrel{\text{def}}{=} \{\mathbb{C}_i \in C \mid \mathbb{C} \in \partial(\mathbb{C}_i)\}$$

Note that all cofaces of \mathbb{C} are also in its star.

k -cochain: A function that assigns a coefficient g_i from some vector space G to every k -cell in a complex C ; it is usually represented by a formal sum:

$$\sum_{\mathbb{C}_i \in k\text{-cells}(C)} g_i \mathbb{C}_i$$

In particular, we are leaving open the possibility that the coefficients might be vectors, matrices or perhaps functions on some number of variables. The notion of a cochain technically subsumes the notion of a chain with integer valued coefficients, i.e. every such chain is also a cochain (but not vice versa). On a finite cell complex, the chains and cochains are isomorphic ([3, page 298]). Examples of cochains are pictured in Figure A.3; the left shows a 0-cochain and the right a 2-cochain.

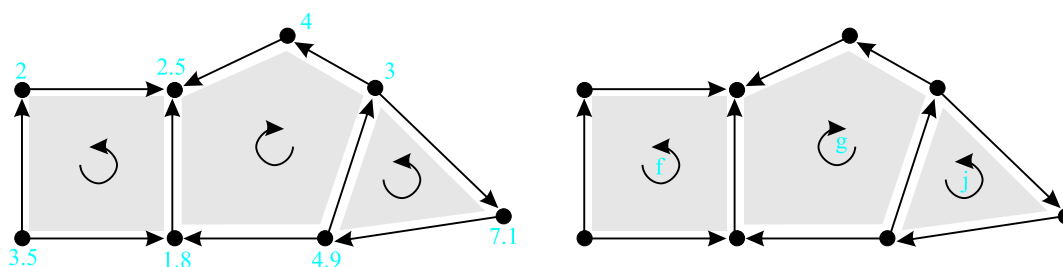


Figure A.3: Depiction of some cochains.

Relative orientation: The intrinsic orientation of a cell can be used to induce the intrinsic orientation of its (co)faces. When orientations are assigned independently to all cells, they may or may not agree. When they do agree, we say that the relative orientation between the two incident cells is positive; when they disagree, the relative orientation is negative. Our notation will be $\sigma(\mathbb{C}_i, \mathbb{C}_j)$ for the relative orientation between \mathbb{C}_i and \mathbb{C}_j . Pictorially, using the arrows of intrinsic orientation for each cell, when the arrows are in the same direction, the relative orientation is +1; when the arrows are in opposite directions, the relative orientation is -1. Orientation of 0-cells is defined to be positive relative to the “tail” of an incident oriented 1-cell and negative relative to the “head”. The relative orientations between some 1-cells and a 2-cell coface are shown in Figure A.4.

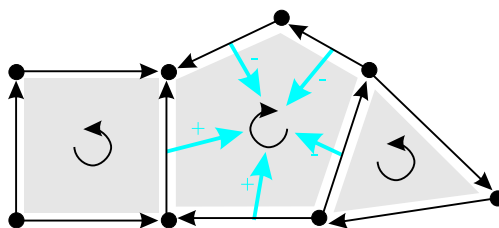


Figure A.4: Depiction of relative orientation.

Coboundary: An operation on a k -cochain ch defining a $(k + 1)$ -cochain by:

$$\delta(ch) \stackrel{\text{def}}{=} \sum_i g_i \mathbb{C}_i,$$

where \mathbb{C}_i are $(k + 1)$ -cells whose coefficients

$$g_i = \sum_{f \in \text{faces}(\mathbb{C}_i)} \sigma(f, \mathbb{C}_i) g_j$$

are determined by the signed (according to the relative orientation) sum of all coefficients g_j associated with the faces f of cell \mathbb{C}_i . An example of the coboundary operation producing a 2-cochain is pictured in Figure A.5. The definition of cochains given earlier mandates the coefficients be from the same group – all the coefficients in Figure A.5 are elements of \mathbb{R} (a and g are simply variables without specified value).

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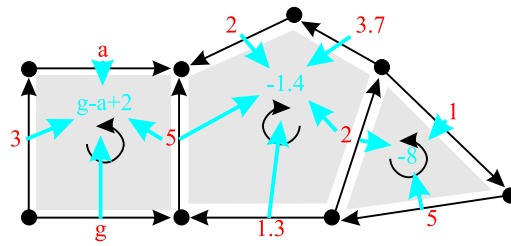


Figure A.5: Depiction of the coboundary operation.

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