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A Discrete Vector Calculus in Tensor Grids

Nicolas Robidoux · Stanly Steinberg

Abstract — Mimetic discretization methods for the numerical solution of continuum mechanics problems directly use vector calculus and differential forms identities for their derivation and analysis. Fully mimetic discretizations satisfy discrete analogs of the continuum theory results used to derive energy inequalities. Consequently, continuum arguments carry over and can be used to show that discrete problems are well-posed and discrete solutions converge. A fully mimetic discrete vector calculus on three dimensional tensor product grids is derived and its key properties proven. Opinions regarding the future of the field are stated.

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1. Introduction

Vector calculus is a powerful language for the formulation of continuum mechanics theories (fluids, materials, electromagnetism etc.). Basic conservation laws and constitutive laws (which model material properties), together with boundary and initial conditions, determine the state of the continuum system. Conservation laws generally do not depend on the details of constitutive laws; they do, however, depend on their structure. Additional conservation laws are obtained using vector calculus identities. These additional laws are key to the analysis of the initial boundary value problem describing the physical system and typically imply that it is well-posed.

The main contribution of this paper is the coherent integration of a number of ideas repeatedly rediscovered by researchers aiming to improve numerical methods. A discrete vector calculus theory with analogs of the important results of continuum calculus is presented. This discrete calculus can be used to discretize any problem expressed using continuum vector calculus. Then, the analysis of a continuum system, in particular, the analysis of its stability, carries over to the discrete system. The numerical analysis of the method's accuracy, however, cannot be performed with classical Taylor series analysis; alternative methods must be used.

Mimetic discrete differential operators are exact [118, 119, 123], that is, their truncation error vanishes, because the continuum fields are discretized (projected onto the discrete) using suitably averaged values of the scalar and vector fields. As a result, the truncation

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Nicolas Robidoux

Department of Mathematics and Computer Science, Laurentian University, Sudbury ON P3E 2C6 Canada E-mail: nrobidoux@cs.laurentian.ca.

Stanly Steinberg

Department of Mathematics and Statistics, University of New Mexico, Albuquerque NM 87131-1141 USA E-mail: stanly@wendouree.org.

error lies in the discretization of constitutive laws. Given that constitutive laws (material properties) are generally modeled approximately, this is a distinct advantage of mimetic methods: the truncation error is contained where modeling and experimental errors are found.

The theory is motivated by listing the properties of continuum vector calculus needed to derive additional conservation laws. A *fully mimetic* discrete vector calculus provides the same set of basic identities. We focus on time-independent problems without boundary conditions. In this setting, deriving the additional conservation laws involves showing that the scalar Laplacian is negative (semi-definite) and that the vector Laplacian is positive (semi-definite). This follows from discrete identities satisfied by mimetic methods.

The geometric setting is a grid covering \mathbb{R}^3 . This infinite grid is a tensor product of uniform one-dimensional grids and thus consists of cells with rectangular faces. The theory presented is formal in the sense that important objects such as integrals and inner products are defined as sums over the full unbounded grid. Finite values are ensured by assuming that some fields have compact support.

Discrete scalar and vector fields are associated with nodes, edges, faces, or cells. Staggering field values is key to the discrete gradient, curl (rotation) and divergence mimicking the continuum operators. An alternate way to define discrete scalar and vector Laplacians is by introducing an averaging operator producing field values at locations where they are not directly defined; this unfortunately leads to spurious high-frequency modes in the nullspaces of the Laplacians. In contrast, mimetic methods avoid spurious modes *ab initio* by introducing a *dual grid*. The dual grid is a translated copy of the primal grid with nodes at the centers of the cells of the primal grid. It is then easy to produce Laplacians free of averaging operators. Note however that although the Laplacians are themselves free of averaging, averaging operators do play a role in the analysis of their properties.

2. Contents

§3 discusses the literature. §7 summarizes our views regarding the future of the field.

In §4, we identify the continuum properties used to prove that the scalar Laplacian is negative and the vector Laplacian is positive. The properties of first-order differential operators are summarized through exact sequences, and the properties of second-order differential operators are summarized with double exact sequences. The section ends with a derivation of the sign properties of the Laplacians.

In §5, we define the primal grid and the operator that gives the boundaries of cells, faces, and edges. We then introduce the scalar fields on the nodes, tangential components of vector fields on the edges, normal components of vector fields on the faces, and scalar density fields on the cells. The discrete analogs of the gradient, curl, and divergence are introduced and shown to satisfy analogs of the vanishing of the curl-gradient and divergence-curl compositions. Integrals of fields over regions, surfaces, and curves are discretized with the help of formal sums of geometric objects, namely *chains* [18, 55, 115, 116]. We then prove the fundamental integral-derivative theorems: the Divergence, Stokes', and Potential theorems. The properties of the discrete first order differential operators are summarized using exact sequences of spaces and difference operators. Algorithmic proofs of the existence of scalar and vector potentials are given in Appendix A.

Dual grids and related concepts have been used in several discretization methods [19, 45, 48, 91, 117, 153]. The differential and integral operators on the fields that live on the dual

primal	dual	primal	dual
grid	grid	fields	fields
nodes	cells	scalar	density
edges	faces	tangential	normal
faces	edges	normal	tangential
cells	nodes	density	scalar

Table 2.1. The Primal-Dual Correspondence

grid are briefly described in Appendix B. All results applicable to primal grid objects carry over to dual grid objects; this is emphasized with a simple change of notation. A key point is that there is a one-to-one correspondence between the geometric objects of the primal and dual grids and between primal and dual discrete fields. This duality is shown in Table 2.1. The operator which manifests the correspondence is called a *star* operator. It is an analog of the Hodge star operator from differential geometry. In the present context, it can be understood as a discrete analog of the constitutive laws. The star operator is critical in the definition of the discrete scalar Laplacian (divergence of the gradient), vector Laplacian (curl of the curl), gradient of the divergence [9], and Hodge Laplacian (vector Laplacian minus gradient of the divergence). The key results are summarized with a double exact sequence which involves the primal and dual fields.

The convergence of the discrete solutions to a continuum solution requires the star operator and its inverse to be bounded independent of grid size. This can be difficult to prove, but it is easily confirmed by numerical experiment.

Discrete Laplacians are analyzed in §6. To this end, we introduce the *universal averaging* operator (see Appendix C.2). In the continuum, operations on fields are done by applying the operation to values that are given at the same physical point. Our values are staggered so if a value of a field is needed at some point where it is not defined, then our universal averaging operator averages nearby values to obtain the required values. Note that it is key that averaging is not used to define the second-order discrete operators, only to analyze them.

Next, the wedge product from differential geometry is used to clarify how to define the scalar, dot, and cross products whose formulas are given in Appendix C. Some of these formulas are complicated because of the grid staggering. They are used to produce discrete analogs of the divergence of products of fields. They are used to define discrete integration by parts identities, key tools for deriving additional conservation laws.

Because the fields which are paired through the star operator are defined at the same points in \mathbb{R}^3 , a natural bilinear form can be defined for each row of Table 2.1. The bilinear forms can be written as an integral on either the primal or the dual grid. The bilinear forms combined with the product rules for the divergence yield adjoint relationships that mimic their continuum counterparts. In particular, the bilinear forms and the star operator induce inner products on the primal and dual fields. These inner products are used to determine the signs of the scalar, vector, and Hodge Laplacians.

In Appendix D we introduce projections from continuum fields to discrete fields. Scalar fields are mapped to discrete nodal fields by taking their values at the nodes; continuum vector fields are projected to edge vector fields by taking the average value of their tangential component over edges; continuum vector fields are projected to face vector fields by taking

the average value of their normal component to faces; and scalar fields are projected to discrete cell fields by taking their average value over a cell. These projection operators make the difference and integral operators exact. Consequently, all the discretization error resides in the star operator.

Star operators correspond to constitutive laws and material properties. Such laws and properties are generally based on empirical models and consequently are generally not known accurately. For this reason, concentrating the numerical error in the quantity that describes the material properties is a good idea.

In this article, the material properties are trivial and the grid is uniform. Consequently, the approximation is second-order accurate. For mimetic methods, the Laplacians have an error consisting of a second-order part and a divergence or curl of a second order part. One would think that the second part of the error is not second order; the fact that this is not the case is an important feature of mimetic methods.

When we say that a proof follows by direct computation, we mean that the computation is straightforward or was done using one of several Mathematica notebooks written for this purpose and available for download at the second author's web site. Basic differential forms theory is called in when vector calculus ambiguously specifies discrete properties, and simple concepts from algebraic topology (specifically, elementary cohomology theory) are used to describe the integration of discrete functions.

3. Previous Work

An introduction to mimetic methods accessible to undergraduates conversant with integration by parts is found in [133]. A mimetic one-variable calculus using dual grids is used to discretize general Sturm-Liouville boundary-value problems. Estimates of the truncation error in mimetic methods are derived. How to construct discretizations of arbitrarily high order is explained. In addition, estimates of the error in the solution and its derivative are given. This establishes convergence. (Also see [40].)

The paper [81] extends these ideas to rough logically rectangular grids and proves that solutions of the mimetic discretization of the scalar Laplacian converge to a solution of the continuum Laplacian. The paper [159] provides a proof of convergence that quantifies the dependence on the roughness of the grid (also see [123, 158]). We consider the proofs in these papers mimetic, because these ideas extend to more general, even time dependent, systems. An alternative proof of convergence based on finite element methods is given in [12, 34]. Super-convergence results are given in [13].

Summation by parts formulas are key [105, 106, 107, 113, 121, 123, 134, 136].

The use of mimetic discretizations is motivated in [104, 148]. In general, mimetic methods are free of spurious modes (for example, hourglass modes) [38, 82]. This leads to correct spectra for vector Laplacians [4] and prevents (long-time) instability [150].

Mimetic methods are now used in general logically rectangular grids [83, 84], irregular or unstructured grids [42, 94, 98, 147], triangular grids [14, 83, 58, 99], and polygonal grids [35, 37, 64, 96]. They can be made higher order in 3D [135], and monotone [97]. Mimetic spectral and pseudospectral methods have been derived [31, 59, 60, 114]. They have been implemented in a multiscale setting [1, 95], using interpolation [49]. Iterative solvers have been used to invert the matrices arising from mimetic discretizations [67].

There are now many applications of mimetic methods to continuum problems: geosciences (porous media) [1, 74, 85, 87, 92, 124, 146, 149]; fluid dynamics (Navier-Stokes, shallow water)

[2, 10, 19]; image analysis [65, 155, 156]; general relativity [54], and electromagnetism [79]. Ideas from vector calculus, differential geometry, and algebraic topology have been used to create, understand and analyze discretization methods [8, 51, 52, 53, 86, 100, 101, 103, 102, 104, 120, 121, 122, 123, 140, 153], and to build high-level programming languages for discretization [15, 41, 43, 63, 115, 116]. In [129], the completion to involution of discretizations is studied. Compatible finite element methods [5, 7] are somewhat similar to (generalized) finite difference mimetic schemes. Compatible schemes are commonly derived using ideas from differential geometry and algebraic topology [6, 17, 29, 30, 45, 50, 69, 70, 71, 152]. Researchers in electromagnetics have made extensive use of compatible schemes [3, 16, 20, 21, 22, 23, 24, 25, 26, 27, 28, 32, 61, 62, 72, 73, 75, 88, 89, 112, 138, 137, 139, 141, 143, 144, 145]. Much emphasis is placed on Hodge star operators and Whitney forms [151]. Such convergence of finite difference and finite element methods is also seen, for example, in computational aerodynamics.

Mimetic ideas are not new. For example, the famous Yee grid ([154], published in 1966) for discretizing Maxwell's equations is a prime example of a mimetic finite difference method. Further developments include the Finite Difference Time Domain (FDTD) [90, 126] and Finite Integration Theory (FIT) [28, 46, 47] methods. Rose [125], and Perot and collaborators [117, 118, 119, 157], also developed discretizations based on mimetic ideas. Finite volume methods, such as those used in [93] to study conservation laws, use mimetic ideas to discretize the divergence operator or the integral forms of the conservation laws. Samarskii and collaborators developed methods—known in English as support-operator methods—that enforce integration by parts identities by "brute force" [56, 57, 66, 127, 128, 130]. Support-operator methods have been used to model diffusion [80, 110, 111, 132, 131], electromagnetism [76, 77] and hydrodynamics [39]. The present article owes much to the support-operator literature.

4. Continuum Vector Calculus

In this section, key properties of continuum vector calculus are summarized.

Continuum mechanics modeling is generally done in three dimensional space plus time. We will not discuss time-dependent problems. Consequently, our functions and vector fields are defined on the Euclidean space \mathbb{R}^3 , and differential and integral operators do not involve time. The vector differential operators are

$$\vec{\nabla}f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right), \qquad \text{gradient}$$

$$\vec{\nabla} \times \vec{v} = \left(\frac{\partial v_3}{\partial y} - \frac{\partial v_2}{\partial z}, \frac{\partial v_1}{\partial z} - \frac{\partial v_3}{\partial x}, \frac{\partial v_2}{\partial x} - \frac{\partial v_1}{\partial y}\right), \qquad \text{curl}$$

$$\vec{\nabla} \cdot \vec{v} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z}. \qquad \text{divergence}$$

Let S be the space of smooth scalar fields on \mathbb{R}^3 and V be the space of smooth vector fields on \mathbb{R}^3 . Many of the basic facts about the differential operators of vector calculus can be summarized by saying that the sequence of spaces and operators, shown in the following diagram, is *exact*:

$$\mathbb{R} \longrightarrow S \stackrel{\vec{\nabla}}{\longrightarrow} V \stackrel{\vec{\nabla} \times}{\longrightarrow} V \stackrel{\vec{\nabla} \cdot}{\longrightarrow} S \longrightarrow 0 \tag{4.2}$$

The leftmost arrow means that the real number a is mapped to the constant scalar field with value a, while the second arrow indicates that the gradient $\vec{\nabla}$ maps scalar fields to vector

fields, the third arrow indicates that the curl $\nabla \times$ maps vector fields to vector fields, the fourth arrow indicates that the divergence $\nabla \cdot$ of a vector field is a scalar field, and the last arrow means that all scalar fields are mapped to 0. Exactness means that the nullspace of the gradient consists exactly of the constant fields, the nullspace of the curl consists exactly of the gradients of scalar fields, the nullspace of the divergence consists exactly of the curls of vector fields, and any scalar field can be written as the divergence of a vector field. The exact sequence consequently encapsulates the vector calculus identities

$$\vec{\nabla} \times \vec{\nabla} \equiv 0$$
: $\vec{\nabla} \cdot \vec{\nabla} \times \equiv 0$:

and the existence of scalar and vector potentials in topologically trivial (contractible) regions:

$$\vec{\nabla} f = 0 \implies f = \text{constant}, \qquad \forall f \in S,$$

$$\vec{\nabla} \times \vec{v} = 0 \implies \vec{v} = \vec{\nabla} f, \qquad \forall \vec{v} \in V, \quad \exists f \in S,$$

$$\vec{\nabla} \cdot \vec{v} = 0 \implies \vec{v} = \vec{\nabla} \times \vec{w}, \qquad \forall \vec{v} \in V, \quad \exists \vec{w} \in V$$

$$f = \vec{\nabla} \cdot \vec{v}, \qquad \forall f \in S, \quad \exists \vec{v} \in V.$$

A scalar field $f \in S$ can be integrated over volumes V, surfaces S, curves C and points P:

$$\int_{V} f \, dV, \quad \int_{S} f \, dS, \quad \int_{C} f \, ds, \quad \int_{P} f = f(P), \tag{4.3}$$

where ds is the arclength element, dS is the surface element, and dV is the volume element. In continuum mechanics, the scalar functions f which appear in these integrals are generally interpreted as follows: For integrals over volumes, f is typically a density. For integrals over points (point values), f is typically a potential field. For integrals over curves, f is typically the tangential component of a vector field. For integrals over surfaces, f is typically the normal component of a vector field. These last two types of integral are consequently

$$\int_C \vec{v} \cdot \vec{t} \, ds \text{ and } \int_S \vec{v} \cdot \vec{n} \, dS,$$

where \vec{t} is a unit tangent to the integration curve C and \vec{n} is the unit normal to the integration surface S.

There are three fundamental integration theorems: the Potential, Stokes' and Divergence theorems. If f is a scalar field and \vec{v} is a vector field,

$$\int_{C} \vec{\nabla} f \cdot \vec{t} \, ds = f(P_1) - f(P_0), \qquad \text{Potential theorem}, \tag{4.4}$$

$$\int_{S} \vec{\nabla} \times \vec{v} \cdot \vec{n} \, dS = \int_{\partial S} \vec{v} \cdot \vec{t} \, ds, \qquad \text{Stokes' theorem}, \tag{4.5}$$

$$\int_{V} \vec{\nabla} \cdot \vec{v} \, dV = \int_{\partial V} \vec{v} \cdot \vec{n} \, dS, \qquad \text{Divergence theorem}, \tag{4.6}$$

where C is a curve going from P_0 to P_1 , S is a bounded surface with bounding curve ∂S , and V is a bounded volume with bounding surface ∂V . It is assumed that volumes and points have positive orientation and that the surface is oriented so that the tangent to the boundary of a surface and the normal to the surface satisfy the right-hand rule. In (4.6) the outward normal to the surfaces is used.

The exact sequence (4.2) does not tell the whole story. It is also important to capture the details of the domains and ranges of the differential operators and preserve the integration theorems.

The differential operators change the units by a reciprocal length while the integrals change the units by a length for curve integrals, by a length squared for surface integrals and by a length cubed for volume integrals. If the theory of differential forms was used to describe this situation, we would have four types of forms: zero-, one-, two- and three-forms. Similarly, we introduce point scalar fields (analogs of zero-forms), curve vector fields (analogs of one-forms), surface vector fields (two-forms) and volume scalar fields (three-forms)

- H_P are the scalar fields related to points,
- H_C are the vector fields related to curves,
- \bullet H_S are the vector fields related to surfaces, and
- H_V are the scalar fields related to volumes.

With this notation, the exact sequence (4.2) becomes

$$\mathbb{R} \longrightarrow H_P \stackrel{\vec{\nabla}}{\longrightarrow} H_C \stackrel{\vec{\nabla} \times}{\longrightarrow} H_S \stackrel{\vec{\nabla} \cdot}{\longrightarrow} H_V \longrightarrow 0 \tag{4.7}$$

In the Potential theorem, $f \in H_P$; in Stokes' theorem, $\vec{v} \in H_C$; in the Divergence theorem, $\vec{v} \in H_S$. The basic differential and integral operators along with the primary integration theorems are thus combined into the exact sequence (4.7).

If we try to construct a scalar Laplacian $\Delta = \vec{\nabla} \cdot \vec{\nabla}$ using the diagram we see that the codomain of the gradient is not exactly the same as the domain of the divergence, even though they both correspond to vector fields. This justifies the introduction of an analog of the Hodge star operator from differential geometry to identify these spaces, resulting in the following pair of dual exact sequences:

$$\mathbb{R} \longrightarrow H_P \stackrel{\vec{\nabla}}{\longrightarrow} H_C \stackrel{\vec{\nabla}\times}{\longrightarrow} H_S \stackrel{\vec{\nabla}\cdot}{\longrightarrow} H_V \longrightarrow 0$$

$$\downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow$$

$$0 \longleftarrow H_V \stackrel{\vec{\nabla}\cdot}{\longleftarrow} H_S \stackrel{\vec{\nabla}\times}{\longleftarrow} H_C \stackrel{\vec{\nabla}}{\longleftarrow} H_P \longleftarrow \mathbb{R}$$

$$(4.8)$$

The lower row of (4.2) is simply the upper row in reverse and the \star operators are simple bijections that identify two types of fields: point scalar fields with volume scalar fields, and curve vector fields with surface vector fields. In the differential-geometric setting \star identifies zero-forms with three-forms, and one-forms with two-forms. It is this diagram that we mimic in the discrete setting.

We are now ready to define Laplacians by following arrows around the squares of diagram (4.8). The following formulas show two versions of the most important Laplacians: a first version without star operators explicitly written, and a version with stars inserted according to (4.8). The scalar Laplacian is defined by starting with the H_P in the first row: so $\vec{\nabla}$ maps H_P to H_C , then \star maps the upper H_C to the lower H_S , $\vec{\nabla}$ maps H_S to H_V , and finally, \star maps the lower H_V to the H_S above. Repeating this procedure with the other two squares of (4.8), we obtain the vector Laplacian used in electromagnetics, and another vector operator used in fluid and material modeling [11]:

$$\begin{split} \Delta = & \vec{\nabla} \cdot \vec{\nabla} \equiv \star \vec{\nabla} \cdot \star \vec{\nabla}, & \text{scalar Laplacian,} \\ \Delta = & \vec{\nabla} \times \vec{\nabla} \times \equiv \star \vec{\nabla} \times \star \vec{\nabla} \times, & \text{vector Laplacian,} \\ \mathcal{L} = & \vec{\nabla} \vec{\nabla} \cdot \equiv \star \vec{\nabla} \star \vec{\nabla} \cdot. & \end{split}$$

One can generate other Laplacians by starting at some other space in the dual exact sequence (4.8) and then moving around a square. Because star operators are bijections, \star^2 is an identity map, and thus any other Laplacian is equivalent to one of the above. In differential geometry, linear combinations of some of these Laplacians are studied.

The key point is that once we have a discrete analog of the commuting diagram (4.8), we have natural definitions of the discrete Laplacians that retain the connection between the continuum first and second order differential operators. We can then directly convert continuum results to the discretized setting. For example, energy inequalities (or equalities) play a critical role in the theory of boundary and initial-boundary value problems. Energy inequalities are based on the fundamental theorems (4.4), (4.5) and (4.6), together with product rules for expanding first order differential operators applied to various products of scalar and vector fields. The results are higher-dimensional analogs of integration by parts. As in the derivation of integration by parts, the required identities can be derived by applying the Divergence theorem to products of fields using the identities

$$\vec{\nabla} \cdot (f\vec{v}) = \vec{\nabla} f \cdot \vec{v} + f \vec{\nabla} \cdot \vec{v}, \quad \vec{\nabla} \cdot (\vec{v} \times \vec{w}) = \vec{\nabla} \times \vec{v} \cdot \vec{w} - \vec{v} \cdot \vec{\nabla} \times \vec{w}. \tag{4.9}$$

There is a problem with these identities: they do not take into account the exact sequences. To make the identities in (4.9) fit into the exact sequence (4.8), we use the vector calculus versions of the exterior or wedge product from differential forms:

$$f \in H_{P}, \quad g \in H_{P} \implies f g \in H_{P},$$

$$f \in H_{P}, \quad \vec{w} \in H_{C} \implies f \vec{w} \in H_{C},$$

$$f \in H_{P}, \quad \vec{w} \in H_{S} \implies f \vec{w} \in H_{S},$$

$$f \in H_{P}, \quad g \in H_{V} \implies f g \in H_{V},$$

$$\vec{v} \in H_{C}, \quad \vec{w} \in H_{C} \implies \vec{v} \times \vec{w} \in H_{S},$$

$$\vec{v} \in H_{C}, \quad \vec{w} \in H_{S} \implies \vec{v} \cdot \vec{w} \in H_{V}.$$

$$(4.10)$$

Now, if $f \in H_P$ and $\vec{v} \in H_S$, the first identity in (4.9) makes sense in H_V . Likewise, if $\vec{v} \in H_C$ and $\vec{w} \in H_C$, the second identity in (4.9) makes sense in H_V . These identities can now be used to derive energy inequalities by certain substitutions: In the first part of (4.9), set $\vec{v} = \star \vec{\nabla} f$. In the second part (4.9), set $\vec{w} = \star \vec{\nabla} \times \vec{v}$. Then, use the Divergence theorem (4.6), setting the boundary terms to zero, to obtain

$$-\int_{V} f \, \vec{\nabla} \cdot \star \, \vec{\nabla} f \, dV = \int_{V} \|\vec{\nabla} f\|^{2} \, dV \geqslant 0,$$
$$\int_{V} \vec{v} \cdot \vec{\nabla} \times \star \, \vec{\nabla} \times \vec{v} \, dV = \int_{V} \|\vec{\nabla} \times \vec{v}\| \, dV \geqslant 0,$$
$$-\int_{V} \vec{v} \cdot \vec{\nabla} \star \, \vec{\nabla} \cdot \vec{v} \, dV = \int_{V} |\vec{\nabla} \cdot \vec{v}| \, dV \geqslant 0.$$

Because

$$\int_{V} f \, \vec{\nabla} \cdot \star \, \vec{\nabla} f \, dV = \int_{V} \star f \, \star \, \vec{\nabla} \cdot \star \, \vec{\nabla} f \, dV = \int_{V} \star f \, \Delta f \, dV,$$

$$\int_{V} \vec{v} \cdot \vec{\nabla} \times \star \, \vec{\nabla} \times \vec{v} \, dV = \int_{V} \star \vec{v} \cdot \star \, \vec{\nabla} \times \star \, \vec{\nabla} \times \vec{v} \, dV = \int_{V} \star \vec{v} \cdot \Delta \vec{v} \, dV,$$

$$\int_{V} \vec{v} \cdot (\vec{\nabla} \star \, \vec{\nabla} \cdot \vec{v}) \, dV = \int_{V} \star \vec{v} \cdot \star (\vec{\nabla} \star \, \vec{\nabla} \cdot \vec{v}) \, dV = \int_{V} \star \vec{v} \cdot \mathcal{L} \, dV,$$

we see that the scalar Laplacian is negative while the vector Laplacian is positive. These are the key results for establishing that scalar and vector Laplace equations are solvable or that initial value problems for diffusion equations are well-posed.

Another important result is the Hodge-Helmholtz decomposition of a vector field [78, 89] which allows the rewriting of a vector field as the sum of a conservative and a divergence-free field. So, let $\vec{v} \in H_S$ and assume

$$\vec{v} = \star \vec{\nabla} f + \vec{\nabla} \times \vec{w}$$

for $f \in H_P$ and $\vec{w} \in H_C$. Then

$$\star \vec{\nabla} \cdot \vec{v} = \star \vec{\nabla} \cdot \star \vec{\nabla} f = \Delta f, \quad \star \vec{\nabla} \times \star \vec{v} = \star \vec{\nabla} \times \star \vec{\nabla} \times \vec{w} = \Delta \vec{w}.$$

Thus, if the scalar and vector Laplace equations are solvable, then the scalar and vector potentials exist. Of course, solutions are not unique without appropriate boundary conditions. The potentials are nonetheless orthogonal, as the following demonstrates: For the first identity in (4.9), replace $\vec{v} \in H_S$ by $\nabla \times \vec{w}$ with $\vec{w} \in H_C$ and put this into the Divergence theorem to get

$$\int_{V} \vec{\nabla} f \cdot \vec{\nabla} \times \vec{w} \, dV + \int_{V} f \, \vec{\nabla} \cdot \vec{\nabla} \times \vec{w} \, dV = \int_{\partial V} f \, \vec{\nabla} \times \vec{w} \cdot \vec{n} \, dS.$$

Now, the second term on the left is zero because $\vec{\nabla} \cdot \vec{\nabla} \times \equiv 0$, as is the boundary integral with appropriate boundary conditions.

4.1. Summary of Required Properties

A fully mimetic discretization of vector calculus requires the following:

- a discretization of the differential operators gradient, curl and divergence (4.1).
- a discretization of the three integrals over curves, surfaces and volumes (4.3). (The integral over points is already discrete.)
- a discrete analog of the exact commuting diagram (4.8).
- discrete analogs of the fundamental theorems of vector calculus (4.4), (4.5) and (4.6),
- discrete analogs of the product rules (4.9).

(The Mathematica notebook Continuum.nb contains demonstrations of the properties of the continuum operators.)

5. The Primal Discrete Vector Calculus

In this section, we produce an exact discrete analog of the continuum exact sequence (4.7).

We begin with the description of a simple tensor grid in three-dimensional space. All cell in such grids have rectangular faces. The grid objects are cells, faces, edges, and nodes. As in homology, geometric objects are represented as *chains*, that is, linear combinations of either cells, faces, edges, or nodes. The boundary of a chain plays an important role and is computed using the boundary operator.

Discrete scalar fields are defined on the cells and nodes, while discrete vector fields are defined on the faces and edges. Discrete fields are understood to consist of continuum field averages: cell averages of scalar fields associated with the cells, face averages of the normal

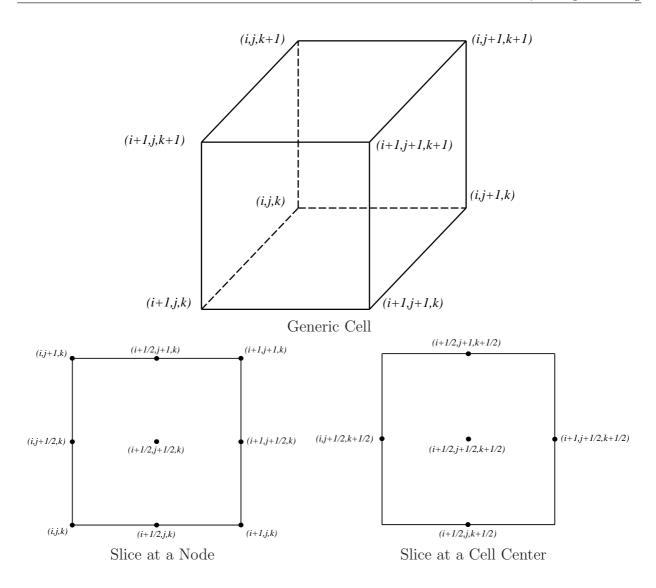


Figure 5.1. Indexing in the Primal Rectangular Grid

components of vector fields associated with the faces, edge averages of the tangential components of vector fields associated with the edges, and point values of scalar fields associated with the nodes. Discrete fields are thus described like chains. The discrete gradient, curl, and divergence are given by simple finite differences. Four integrals are introduced: the integral of a point scalar field over a chain of points, the integral of a edge vector field over a chain of edges, the integral of a face vector field over a chain of faces, and the integral of a cell scalar field over a chain of cells. All of these integrals are simple natural discretizations of Riemann-Stieltjes integrals. These integrals are used to give proofs of the discrete fundamental theorems. The existence of a scalar potential follows the classical argument, but the proof of the existence of a vector potential seems to be novel.

We introduce the star operator that connects the primal and dual grids. This is the key to constructing a double exact sequence analog of the continuum double exact sequence (4.8) and the scalar and vector Laplacians.

name	part	center	orient.
node	$N_{i,j,k} = \{(x_i, y_j, z_k)\}$	(x_i, y_j, z_k)	+
edge	$E_{i+\frac{1}{2},j,k} = \{(x_i + \xi \triangle x, y_j, z_k)\}$	$\left(x_{i+\frac{1}{2}}, y_j, z_k\right)$	(1,0,0)
edge	$E_{i,j+\frac{1}{2},k} = \{(x_i, y_j + \eta \triangle y, z_k)\}$	$\left(x_i, y_{j+\frac{1}{2}}, z_k\right)$	(0,1,0)
edge	$E_{i,j,k+\frac{1}{2}} = \{(x_i, y_j, z_k + \zeta \triangle z)\}$	$\left(x_i, y_j, z_{k+\frac{1}{2}}\right)$	(0,0,1)
face	$F_{i,j+\frac{1}{2},k+\frac{1}{2}} = \{ (x_i, y_j + \eta \triangle y, z_k + \zeta \triangle z) \}$	$\left(x_i, y_{j+\frac{1}{2}}, z_{k+\frac{1}{2}}\right)$	(1,0,0)
face	$F_{i+\frac{1}{2},j,k+\frac{1}{2}} = \{ (x_i + \xi \triangle x, y_j, z_k + \zeta \triangle z) \}$	$\left(x_{i+\frac{1}{2}}, y_j, z_{k+\frac{1}{2}}\right)$	(0,1,0)
face	$F_{i+\frac{1}{2},j+\frac{1}{2},k} = \{ (x_i + \xi \triangle x, y_j + \eta \triangle y, z_k) \}$	$\left(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, z_k\right)$	(0,0,1)
cell	$C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = \{x_i + \xi \triangle x, y_j + \eta \triangle y, z_k + \zeta \triangle z\}$	$(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, z_{k+\frac{1}{2}})$	+

Table 5.1. Geometrical Objects of the Primal Rectangular Grid and their Orientation

5.1. The Tensor Grid

The grid is in 3-dimensional Euclidean space \mathbb{R}^3 and is given by points evenly spaced in each direction, either labeled with an integer or half-integer index. With arbitrary positive real numbers Δx , Δy and Δz , let

$$x_{i} = i \triangle x,$$
 $y_{j} = j \triangle y,$ $z_{k} = k \triangle z,$ $x_{i+\frac{1}{2}} = (i+\frac{1}{2}) \triangle x,$ $y_{j+\frac{1}{2}} = (j+\frac{1}{2}) \triangle y,$ $z_{k+\frac{1}{2}} = (k+\frac{1}{2}) \triangle z,$

where $-\infty < i, j, k < \infty$. The grid is composed of cells \mathcal{C} as shown in Figure 5.1 and the cells are composed of nodes \mathcal{N} , edges \mathcal{E} , and faces \mathcal{F} as described in Table 5.1. The parts of the grids are labeled with their midpoints. The variables ξ , η , and ζ are used to parametrize the edges, faces and cells and satisfy $0 \le \xi \le 1$, $0 \le \eta \le 1$, $0 \le \zeta \le 1$. The nodes \mathcal{N} of the grid have positive orientation, the edges \mathcal{E} are oriented by their unit tangents in the directions of the positive axes, the faces \mathcal{F} are oriented by their unit normals in the directions of the positive axes, and the cells \mathcal{C} have positive orientation.

5.2. Chains

Volume, surface, and line integral play a central role in vector calculus. It is convenient to follow the approach used in algebraic topology and differential geometry and define generalized geometric objects called chains [36, 116]. A chain is simply a sum of geometric objects of the same dimension multiplied by a real number that is the weight for the object. A vanishing weight means that the object not in the chain; weights of ± 1 indicate the two possible orientations. We allow the weights to be in $\mathbb R$ so that the chains are a linear space. However, it is generally assumed that the chains have compact support, that is, that they have only a finite number of nonzero coefficients.

The space of cell chains $C_{\mathcal{C}} = \mathbb{R}^{\mathcal{C}}$ consists of expressions C of the form

$$C = \sum_{i,j,k} a_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}.$$
 (5.1)

The space of face chains $C_{\mathcal{F}} = \mathbb{R}^{\mathcal{F}}$ consists of expressions F of the form

$$F = \sum_{i,j,k} a_{i,j+\frac{1}{2},k+\frac{1}{2}} F_{i,j+\frac{1}{2},k+\frac{1}{2}} + \sum_{i,j,k} a_{i+\frac{1}{2},j,k+\frac{1}{2}} F_{i+\frac{1}{2},j,k+\frac{1}{2}} + \sum_{i,j,k} a_{i+\frac{1}{2},j+\frac{1}{2},k} F_{i+\frac{1}{2},j+\frac{1}{2},k}.$$
(5.2)

The space of edge chains $C_{\mathcal{E}} = \mathbb{R}^{\mathcal{E}}$ consists of expressions E of the form

$$E = \sum_{i,j,k} a_{i+\frac{1}{2},j,k} E_{i+\frac{1}{2},j,k} + \sum_{i,j,k} a_{i,j+\frac{1}{2},k} E_{i,j+\frac{1}{2},k} + \sum_{i,j,k} a_{i,j,k+\frac{1}{2}} E_{i,j,k+\frac{1}{2}}.$$
 (5.3)

The space of node chains $C_{\mathcal{N}} = \mathbb{R}^{\mathcal{N}}$ consists of expressions N of the form

$$N = \sum_{i,j,k} a_{i,j,k} N_{i,j,k}. \tag{5.4}$$

5.3. Boundary Operators for Chains

The operator that computes the boundary is ∂ . For cells, faces, edges, and nodes, the boundaries are

$$\begin{split} \partial C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} &= \\ F_{i+1,j+\frac{1}{2},k+\frac{1}{2}} - F_{i,j+\frac{1}{2},k+\frac{1}{2}} + F_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - F_{i+\frac{1}{2},j,k+\frac{1}{2}} + F_{i+\frac{1}{2},j+\frac{1}{2},k} - F_{i+\frac{1}{2},j+\frac{1}{2},k}, \\ \partial F_{i,j+\frac{1}{2},k+\frac{1}{2}} &= E_{i,j+1,k+\frac{1}{2}} - E_{i,j,k+\frac{1}{2}} - E_{i,j+\frac{1}{2},k+1} + E_{i,j+\frac{1}{2},k}, \\ \partial F_{i+\frac{1}{2},j,k+\frac{1}{2}} &= E_{i+\frac{1}{2},j,k+1} - E_{i+\frac{1}{2},j,k} - E_{i+1,j,k+\frac{1}{2}} + E_{i,j,k+\frac{1}{2}}, \\ \partial F_{i+\frac{1}{2},j+\frac{1}{2},k} &= E_{i+1,j+\frac{1}{2},k} - E_{i,j+\frac{1}{2},k} - E_{i+\frac{1}{2},j+1,k} + E_{i+\frac{1}{2},j,k}, \\ \partial E_{i+\frac{1}{2},j,k} &= N_{i+1,j,k} - N_{i,j,k}, \quad \partial E_{i,j+\frac{1}{2},k} = N_{i,j+1,k} - N_{i,j,k}, \quad \partial E_{i,j,k+\frac{1}{2}} = N_{i,j,k+1} - N_{i,j,k}, \\ \partial N_{i,j,k} &= 0. \end{split}$$

The boundary of a chain is defined by making ∂ linear.

Lemma 5.1.

$$\partial \partial \equiv 0.$$

Proof. A direct calculation shows that the boundary of a boundary is empty for cells, faces, and edges. Linearity extends this result to arbitrary chains. \Box

5.4. Scalar and Vector Fields

Fields have values associated with cells, faces, edges or nodes: scalar fields have values associated with the nodes and cells; vector fields have values associated with edges and faces. Intuitively, the nodal scalar fields $V_{\mathcal{K}}$ correspond to point values of continuum scalar functions, while the cell scalar fields $V_{\mathcal{E}}$ correspond to the averages of a continuum scalar field over cells. The edge vector field $V_{\mathcal{E}}$ corresponds to the average of the tangential component of a continuum vector field over edges, while the face vector field $V_{\mathcal{F}}$ corresponds to the average of the normal component of a vector field over faces.

It is convenient to represent the fields in terms of a basis, and a natural basis to use is points for scalar fields, edges for edge vector fields, faces for face vector fields and cells for cell scalar fields. In this case chains and fields have exactly the same representation. As with chains, a zero component for a vector in an expression is equivalent to leaving the corresponding basis element out of the sum.

Node: If $s \in V_{\mathcal{N}}$ then

$$s = \sum_{i,j,k} s_{i,j,k} N_{i,j,k}. \tag{5.5}$$

Edge: If $\vec{t} \in V_{\mathcal{E}}$, then

$$\vec{t} = \sum_{i,j,k} t_{i+\frac{1}{2},j,k} E_{i+\frac{1}{2},j,k} + t_{i,j+\frac{1}{2},k} E_{i,j+\frac{1}{2},k} + t_{i,j,k+\frac{1}{2}} E_{i,j,k+\frac{1}{2}}.$$
(5.6)

Face: If $\vec{n} \in V_{\mathcal{F}}$, then

$$\vec{n} = \sum_{i,j,k} n_{i,j+\frac{1}{2},k+\frac{1}{2}} F_{i,j+\frac{1}{2},k+\frac{1}{2}} + n_{i+\frac{1}{2},j,k+\frac{1}{2}} F_{i+\frac{1}{2},j,k+\frac{1}{2}} + n_{i+\frac{1}{2},j+\frac{1}{2},k} F_{i+\frac{1}{2},j+\frac{1}{2},k}.$$
(5.7)

Cell: If $m \in V_{\mathcal{C}}$ then

$$m = \sum_{i,j,k} m_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}.$$
 (5.8)

5.5. Difference Operators

The discrete gradient \mathcal{G} , curl \mathcal{R} and divergence \mathcal{D} are defined either by simple differences operating on the coefficients of a field or by their linearity and their values on basis elements. After the definitions, some important analogs of some continuum derivative identities are given.

The Gradient: If $s \in V_{\mathcal{N}}$ is a discrete scalar field, then its gradient $\mathcal{G}s \in V_{\mathcal{E}}$ is an edge vector field. In terms of components

$$(\mathcal{G}s)_{i+\frac{1}{2},j,k} \equiv \frac{s_{i+1,j,k} - s_{i,j,k}}{\triangle x}, \quad (\mathcal{G}s)_{i,j+\frac{1}{2},k} \equiv \frac{s_{i,j+1,k} - s_{i,j,k}}{\triangle y}, \quad (\mathcal{G}s)_{i,j,k+\frac{1}{2}} \equiv \frac{s_{i,j,k+1} - s_{i,j,k}}{\triangle z},$$

while in terms of the basis elements

$$\mathcal{G}N_{i,j,k} = \frac{E_{i-1/2,j,k} - E_{i+1/2,j,k}}{\Delta x} + \frac{E_{i,j-1/2,k} - E_{i,j+1/2,k}}{\Delta y} + \frac{E_{i,j,-1/2k} - E_{i,j,k+1/2}}{\Delta z}.$$

The Curl: If $\vec{t} \in V_{\mathcal{E}}$ is a discrete edge vector field, then its curl $\mathcal{R}\vec{t} \in V_{\mathcal{F}}$ is a discrete face vector field. In terms of components

$$(\mathcal{R}\vec{t})_{i,j+\frac{1}{2},k+\frac{1}{2}} \equiv \frac{t_{i,j+1,k+\frac{1}{2}} - t_{i,j,k+\frac{1}{2}}}{\triangle y} - \frac{t_{i,j+\frac{1}{2},k+1} - t_{i,j+\frac{1}{2},k}}{\triangle z},$$

$$(\mathcal{R}\vec{t})_{i+\frac{1}{2},j,k+\frac{1}{2}} \equiv \frac{t_{i+\frac{1}{2},j,k+1} - t_{i+\frac{1}{2},j,k}}{\triangle z} - \frac{t_{i+1,j,k+\frac{1}{2}} - t_{i,j,k+\frac{1}{2}}}{\triangle x},$$

$$(\mathcal{R}\vec{t})_{i+\frac{1}{2},j+\frac{1}{2},k} \equiv \frac{t_{i+1,j+\frac{1}{2},k} - t_{i,j+\frac{1}{2},k}}{\triangle x} - \frac{t_{i+\frac{1}{2},j+1,k} - t_{i+\frac{1}{2},j,k}}{\triangle y},$$

while in terms of basis elements

$$\begin{split} \mathcal{R}E_{i,j,k+1/2} = & \frac{F_{i+1/2,j,k+1/2} - F_{i-1/2,j,k+1/2}}{\Delta x} + \frac{F_{i,j+1/2,k+1/2} - F_{i,j-1/2,k+1/2}}{\Delta y}, \\ \mathcal{R}E_{i,j+1/2,k} = & \frac{F_{i-1/2,j+1/2,k} - F_{i+1/2,j+1/2,k}}{\Delta x} + \frac{F_{i,j+1/2,k-1/2} - F_{i,j+1/2,k+1/2}}{\Delta z}, \\ \mathcal{R}E_{i+1/2,j,k} = & \frac{F_{i+1/2,j+1/2,k} - F_{i+1/2,j-1/2,k}}{\Delta y} + \frac{F_{i+1/2,j,k-1/2} - F_{i+1/2,j,k+1/2}}{\Delta z}, \end{split}$$

The Divergence: If $\vec{n} \in V_{\mathcal{F}}$ is a discrete face vector field, then its divergence $\mathcal{D}\vec{n} \in V_{\mathcal{C}}$ is a cell scalar field. In terms of components

$$\begin{split} &(\mathcal{D}\vec{n})_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \equiv \\ &\frac{n_{i+1,j+\frac{1}{2},k+\frac{1}{2}} - n_{i,j+\frac{1}{2},k+\frac{1}{2}}}{\triangle x} + \frac{n_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - n_{i+\frac{1}{2},j,k+\frac{1}{2}}}{\triangle y} + \frac{n_{i+\frac{1}{2},j+\frac{1}{2},k+1} - n_{i+\frac{1}{2},j+\frac{1}{2},k}}{\triangle z}, \end{split}$$

while in terms of basis elements

$$\begin{split} \mathcal{D}F_{i,j+1/2,k+1/2} &= \frac{C_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} + C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta x}, \\ \mathcal{D}F_{i+1/2,j,k+1/2} &= \frac{C_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta y}, \\ \mathcal{D}F_{i,j+1/2,k+1/2} &= \frac{C_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} + C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta z}. \end{split}$$

Our first goal is to show that the discrete differential operators form an exact sequence, just as in the continuum. A first step in this direction is the following result, proven by direct computation:

Lemma 5.2.

$$\mathcal{G}c \equiv 0$$
, $\mathcal{R}\mathcal{G} \equiv 0$, $\mathcal{D}\mathcal{R} \equiv 0$.

where c is a constant scalar field.

5.6. Integrals

Integrals that are natural analogs of the Riemann-Stieltjes integral of fields over cells, faces, edges, or nodes are introduced. As noted above, it is assumed that the chain has compact support.

If $m \in V_{\mathcal{C}}$ as in (5.8) and $C \in C_{\mathcal{C}}$ is in (5.1), then the cell integral of m over C is defined by

$$\int_{C} m \, dV = \sum_{i,j,k} a_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \, m_{(i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2})} \triangle x \, \triangle y \, \triangle z. \tag{5.9}$$

If $\vec{n} \in V_{\mathcal{N}}$ as in (5.7) and $F \in C_{\mathcal{F}}$ as in (5.2), then the face integral (of the normal component) of \vec{n} over F is defined by

$$\int_{F} \vec{n} \cdot d\vec{S} = \sum_{i,j,k} a_{i,j+\frac{1}{2},k+\frac{1}{2}} t_{(i,j+\frac{1}{2},k+\frac{1}{2})} \triangle y \triangle z + \sum_{i,j,k} a_{i+\frac{1}{2},j,k+\frac{1}{2}} t_{(i+\frac{1}{2},j,k+\frac{1}{2})} \triangle z \triangle x + \sum_{i,j,k} a_{i+\frac{1}{2},j+\frac{1}{2},k} t_{(i+\frac{1}{2},j+\frac{1}{2},k)} \triangle x \triangle y.$$

If $\vec{t} \in V_{\mathcal{E}}$ as in (5.6) and $E \in C_{\mathcal{E}}$ as in (5.3), then the edge integral (of the tangential component) of \vec{t} over E is defined by

$$\int_{E} \vec{t} \cdot d\vec{L} = \sum_{i,j,k} a_{i+\frac{1}{2},j,k} t_{(i+\frac{1}{2},j,k)} \triangle x + \sum_{i,j,k} a_{i,j+\frac{1}{2},k} t_{(i,j+\frac{1}{2},k)} \triangle y + \sum_{i,j,k} a_{i,j,k+\frac{1}{2}} t_{(i,j,k+\frac{1}{2})} \triangle z.$$

If $f \in V_N$ as in (5.5) and $N \in C_N$ as in (5.4), then the integral of f over N is defined by

$$\int_{N} f = \sum_{i,j,k} a_{i,j,k} f_{i,j,k}.$$

5.7. The Integral-Derivative Theorems

Direct calculations give discrete analogs of the Potential, Stokes', and Divergence theorems for a single cell, face and edge.

Lemma 5.3. If \vec{n} is a face vector field and C is a cell, if \vec{t} is an edge vector field and F is a face, and if f is an nodal scalar field and E is an edge, then

$$\int_C \mathcal{D}\vec{n} \, dV = \int_{\partial C} \vec{n} \cdot d\vec{S}, \quad \int_F \mathcal{R}\vec{t} \cdot d\vec{S} = \int_{\partial F} \vec{t} \cdot d\vec{L}, \quad \int_E \mathcal{G}f \cdot d\vec{L} = \int_{\partial E} f.$$

The next result for general chains follows by linearity:

Theorem 5.1. If $C \in C_C$ is a cell chain and $\vec{n} \in V_N$ is a face vector field then

$$\int_{C} \mathcal{D}\vec{n} \, dV = \int_{\partial C} \vec{n} \cdot d\vec{S}. \tag{5.10}$$

If $F \in C_{\mathcal{F}}$ is a face chain and $\vec{t} \in V_{\mathcal{E}}$ is a edge vector field then

$$\int_{F} \mathcal{R}\vec{t} \cdot d\vec{S} = \int_{\partial F} \vec{t} \cdot d\vec{L}.$$

If $E \in C_{\mathcal{E}}$ is a edge chain and $fV_{\mathcal{N}}$ is a node scalar field then

$$\int_{E} \mathcal{G}f \cdot d\vec{L} = \int_{\partial E} f.$$

5.8. The Existence of Potentials

If C is a chain such that $\partial C = 0$, then the C is said to be *closed*. Similarly, if $\vec{n} \in V_{\mathcal{F}}$ and $\mathcal{D}\vec{n} \equiv 0$, then \vec{n} is said to be *closed*; if $\vec{t} \in V_{\mathcal{E}}$ and $\mathcal{R}\vec{t} \equiv 0$, then \vec{t} is said to be *closed*; likewise for nodal fields.

If a chain is closed, then it is the boundary of a higher dimensional chain. This trivial result plays an important role in the construction and analysis of mimetic discretizations.

Theorem 5.2.

- 1. If $F \in C_{\mathcal{F}}$ has compact support and $\partial F = 0$, then there is a cell chain $C \in C_{\mathcal{C}}$ with compact support such that $\partial C = F$.
- 2. If $E \in C_{\mathcal{E}}$ has compact support and $\partial E = 0$, then there is a face chain $F \in C_{\mathcal{F}}$ with compact support such that $\partial F = E$.

Theorem 5.3.

- 1. If $s \in V_N$ and $\mathcal{G}s \equiv 0$ then s is a constant scalar field.
- 2. If $\vec{t} \in V_{\mathcal{E}}$ and $\mathcal{R}\vec{t} \equiv 0$ then there exists a $f \in V_{\mathcal{N}}$ such that $\vec{t} = \mathcal{G}f$.
- 3. If $\vec{n} \in V_{\mathcal{F}}$ and $\mathcal{D}\vec{n} \equiv 0$ then there exists a $\vec{t} \in V_{\mathcal{E}}$ such that $\vec{n} = \mathcal{R}\vec{t}$.
- 4. For any $m \in V_{\mathcal{C}}$, there exists $\vec{n} \in V_{\mathcal{F}}$ such that $\mathcal{D}\vec{n} = m$.

The proofs of Theorems 5.2 and 5.3 and a discussion of their implementation in computer algebra systems are found in Appendix A.

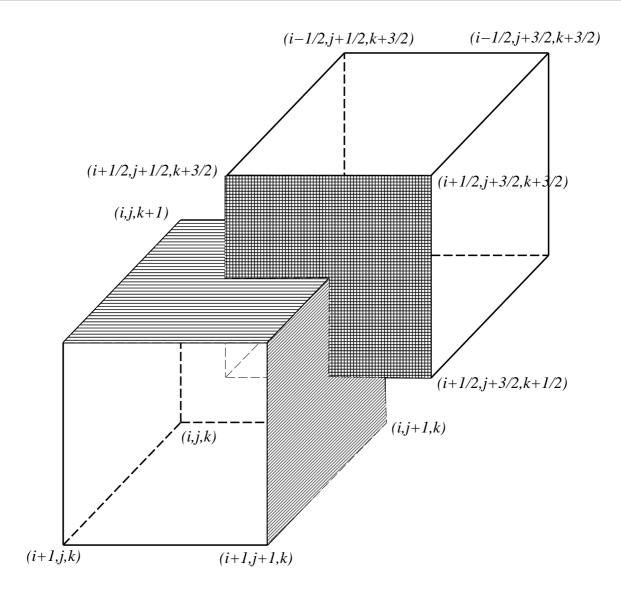


Figure 5.2. The Primal and Dual Grid Cells

5.9. A Mimetic Vector Calculus

The previous results imply that the following sequence is exact, and conversely, the fact that the sequence is exact summarizes the previous results. This defines a mimetic vector calculus (on topologically trivial spaces).

$$\mathbb{R} \longrightarrow V_{\mathcal{N}} \stackrel{\mathcal{G}}{\longrightarrow} V_{\mathcal{E}} \stackrel{\mathcal{R}}{\longrightarrow} V_{\mathcal{F}} \stackrel{\mathcal{D}}{\longrightarrow} V_{\mathcal{C}} \longrightarrow 0.$$

5.10. The Dual Grid

Unlike the continuum, the codomain of \mathcal{G} is not the same space as the domain of \mathcal{D} , so something additional needs to be done to define the scalar Laplacian \mathcal{DG} . In addition, the codomain of \mathcal{R} is not the same as the domain of \mathcal{R} , so something additional is also needed to define the vector Laplacian \mathcal{RR} . A classical solution to this problem is to introduce averaging operators between the spaces $V_{\mathcal{K}}$ and $V_{\mathcal{C}}$, and between the spaces $V_{\mathcal{E}}$ and $V_{\mathcal{F}}$. Unfortunately, averaging operators are generally not invertible. We use another classical way of resolving the mismatch: a dual grid.

All dual grid objects are labeled with a star. As shown in Figure 5.2, the dual grid is obtained by translating the primal grid by $(\Delta x/2, \Delta y/2, \Delta z/2)$ so that nodes correspond to cell centers and edge centers correspond to face centers. The edges in the grid pass perpendicularly through the centers of the dual grid faces and vice versa. Because the dual grid is a translate of the primal grid, all the primal calculus results hold for the dual grid. See Appendix B for details.

5.11. The Star Operator

The geometric \star operator is a bijection that associates the following objects:

$$\star N_{i,j,k} = C_{i,j,k}^{\star}, \quad \star C_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = N_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{\star}$$

$$\star E_{i+\frac{1}{2},j,k} = F_{i+\frac{1}{2},j,k}^{\star}, \quad \cdots, \quad \star F_{i,j+\frac{1}{2},k+\frac{1}{2}} = E_{i,j+\frac{1}{2},k+\frac{1}{2}}^{\star}, \quad \cdots$$

The inverse of this map is also labeled with \star .

Matching indices also defines bijections between primal and dual fields:

$$\star = \star_{(N,C^{\star})} : V_{\mathcal{N}} \to V_{\mathcal{C}^{\star}}, \quad m_{i,j,k}^{\star} = \star f_{i,j,k} = f_{i,j,k},
\star = \star_{(E,F^{\star})} : V_{\mathcal{E}} \to V_{\mathcal{F}^{\star}}, \quad
\begin{cases}
n_{i+\frac{1}{2},j,k}^{\star} = \star t_{i+\frac{1}{2},j,k} = t_{i+\frac{1}{2},j,k},
n_{i,j+\frac{1}{2},k}^{\star} = \star t_{i,j+\frac{1}{2},k} = t_{i,j+\frac{1}{2},k},
n_{i,j,k+\frac{1}{2}}^{\star} = \star t_{i,j,k+\frac{1}{2}} = t_{i,j,k+\frac{1}{2}},
t_{i,j,k+\frac{1}{2}}^{\star} = \star n_{i,j+\frac{1}{2},k+\frac{1}{2}} = n_{i,j+\frac{1}{2},k+\frac{1}{2}},
t_{i+\frac{1}{2},j,k+\frac{1}{2}}^{\star} = \star n_{i+\frac{1}{2},j,k+\frac{1}{2}} = n_{i+\frac{1}{2},j,k+\frac{1}{2}},
t_{i+\frac{1}{2},j+\frac{1}{2},k}^{\star} = \star n_{i+\frac{1}{2},j+\frac{1}{2},k} = n_{i+\frac{1}{2},j+\frac{1}{2},k},
\star = \star_{(C,N^{\star})} : V_{\mathcal{C}} \to V_{\mathcal{N}^{\star}}, \quad f_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{\star} = \star m_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = m_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}, \tag{5.11}$$

with

$$\star_{(C^{\star},N)} = \star_{(N,C^{\star})}^{-1}, \quad \star_{(F^{\star},E)} = \star_{(E,F^{\star})}^{-1}, \quad \star_{(E^{\star},F)} = \star_{(F,E^{\star})}^{-1}, \quad \star_{(N^{\star},C)} = \star_{(C,N^{\star})}^{-1},$$

so that $\star^2 = \star \star$ is the identity.

In the present article, only the simplest star operators—those with "identity matrix" representations with respect to cardinal bases—are considered. In order to get higher order accuracy on non-uniform grids and/or with nontrivial material properties, more complex, generally non-diagonal, star operators must be used.

5.12. The Double Exact Sequence

The operators on the dual grid are like the operators on the primal grid except for a change of notation. So there is both an exact sequence (4.8) and a dual exact sequence. They are related by the \star operator:

$$\mathbb{R} \longrightarrow V_{\mathcal{N}} \xrightarrow{\mathcal{G}} V_{\mathcal{E}} \xrightarrow{\mathcal{R}} V_{\mathcal{F}} \xrightarrow{\mathcal{D}} V_{\mathcal{C}} \longrightarrow 0$$

$$\downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow$$

$$0 \longleftarrow V_{\mathcal{C}^{\star}} \xleftarrow{\mathcal{D}^{\star}} V_{\mathcal{F}^{\star}} \xleftarrow{\mathcal{R}^{\star}} V_{\mathcal{E}^{\star}} \xleftarrow{\mathcal{G}^{\star}} V_{\mathcal{N}^{\star}} \longleftarrow \mathbb{R}$$

$$(5.12)$$

Theorem 5.4. Both sequences in (5.12) are exact and the \star operators are bijective.

5.13. The Laplacians

Each square of the above double exact sequence, traversed in the clockwise direction, defines a discrete Laplacian. Starting with the spaces in the primal exact sequence gives the primal scalar and vector Laplacians, as well as a third operator found in the literature but which does not appear to have a name. When the meaning is clear, the second-order operators are written without explicitly showing star operators:

$$\mathcal{L} = \mathcal{D}^{\star} \mathcal{G} = \star \mathcal{D}^{\star} \star \mathcal{G} \equiv \star_{(C^{\star}, N)} \mathcal{D}^{\star} \star_{(E, F^{\star})} \mathcal{G}, \qquad \text{on } V_{\mathcal{N}}, \qquad (5.13)$$

$$\vec{\mathcal{L}} = \mathcal{R}^* \mathcal{R} = \star \mathcal{R}^* \star \mathcal{R} \equiv \star_{(F^*, E)} \mathcal{R}^* \star_{(F, E^*)} \mathcal{R}, \qquad \text{on } V_{\mathcal{E}},$$
 (5.14)

$$\bar{\mathcal{L}} = \mathcal{G}^* \mathcal{D} = \star \mathcal{G}^* \star \mathcal{D} \equiv \star_{(E^*, F)} \mathcal{G}^* \star_{(C, N^*)} \mathcal{D}, \qquad \text{on } V_{\mathcal{F}}.$$
 (5.15)

Starting with the spaces in the dual exact sequence produces a conjugate set of second-order operators: $\mathcal{D}^* \star \mathcal{G} \star = \star \mathcal{L} \star$ on $V_{\mathcal{C}^*}$, $\mathcal{R}^* \star \mathcal{R} \star = \star \vec{\mathcal{L}} \star$ on $V_{\mathcal{F}^*}$ and $\mathcal{G}^* \star \mathcal{D} \star = \star \vec{\mathcal{L}} \star$ on $V_{\mathcal{E}^*}$.

5.14. Summary

We now have the tools to produce spatial discretizations of the partial differential equations that appear in continuum mechanics. Many of the details in this section were checked in the Mathematica notebooks Discrete.nb and PrimaryGrid.nb.

6. Analysis of the Laplacians

In this section, we show that the scalar Laplacian is negative and the vector Laplacian is positive. These are key results for the analysis boundary value problems involving these operators. It is important to understand that the material in this section is an integral part of mimetic methods; it is only used to analyze them. The analysis depends critically on two of the integration by parts theorems, namely the Stokes' and Divergence theorems. These in turn depend on the definitions of scalar and vector products. Defining these products is straightforward if a bit complicated. The wedge product used in differential geometry (see §C.1) constrains these definitions. We have found that it is only needed to define products between primal and dual fields. Before any of this can be done however, we need to be able to add and multiply discrete fields.

6.1. Universal Averaging and Sums and Products of Fields

In the continuum, scalar fields and vector fields are added by adding their values at the same physical point. The same holds true for scalar, cross and dot products. In addition, summands must have the same units. For example, adding t and n^* is not allowed even though they are defined at the same locations, but t and $*n^*$ can be added.

To compensate for the grid staggering, we introduce the universal averaging operator μ . To obtain the value of a discrete field at a point where it is not defined, the operator μ averages the values of the field at the logically nearest neighbors where the field is defined. In many cases it is not necessary to explicitly write μ . For example, if f is a primal scalar field, then

$$\mu(f)_{i+\frac{1}{2},j,k} = f_{i+\frac{1}{2},j,k} = \frac{f_{i,j,k} + f_{i+1,j,k}}{2},$$

$$\mu(f)_{i+\frac{1}{2},j+\frac{1}{2},k} = f_{i+\frac{1}{2},j+\frac{1}{2},k} = \frac{f_{i,j,k} + f_{i+1,j,k} + f_{i,j+1,k} + f_{i+1,j+1,k}}{2}.$$

1	$f m^* : V_{\mathcal{N}} \times V_{\mathcal{C}^*} \to V_{\mathcal{C}^*},$	$f^{\star} m : V_{\mathcal{N}^{\star}} \times V_{\mathcal{C}} \to V_{\mathcal{C}},$
2	$f \vec{n}^{\star} : V_{\mathcal{N}} \times V_{\mathcal{F}^{\star}} \to V_{\mathcal{F}^{\star}},$	$f^* \vec{n} : V_{\mathcal{N}^*} \times V_{\mathcal{F}} \to V_{\mathcal{F}},$
3	$f \vec{t}^{\star} : V_{\mathcal{N}} \times V_{\mathcal{E}^{\star}} \to V_{\mathcal{E}^{\star}},$	$f^* \vec{t} : V_{\mathcal{N}^*} \times V_{\mathcal{E}} \to V_{\mathcal{E}},$
4	$f f^* : V_{\mathcal{N}} \times V_{\mathcal{N}^*} \to V_{\mathcal{N}^*},$	$f^* f : V_{\mathcal{N}^*} \times V_{\mathcal{N}} \to V_{\mathcal{N}},$
5	$\vec{t} \cdot \vec{n}^* : V_{\mathcal{E}} \times V_{\mathcal{F}^*} \to V_{\mathcal{C}^*},$	$\vec{t}^{\star} \cdot \vec{n} : V_{\mathcal{E}^{\star}} \times V_{\mathcal{F}} \to V_{\mathcal{C}},$
6	$\vec{t} \times \vec{t}^* : V_{\mathcal{E}} \times V_{\mathcal{E}^*} \to V_{\mathcal{F}^*},$	$\vec{t}^{\star} \times \vec{t} : V_{\mathcal{E}^{\star}} \times V_{\mathcal{E}} \to V_{\mathcal{F}},$
7	$\vec{t} f^* : V_{\mathcal{E}} \times V_{\mathcal{N}^*} \to V_{\mathcal{E}^*},$	$\vec{t}^{\star} f : V_{\mathcal{E}^{\star}} \times V_{\mathcal{N}} \to V_{\mathcal{E}},$
8	$\vec{n} \cdot \vec{t}^* : V_{\mathcal{F}} \times V_{\mathcal{E}^*} \to V_{\mathcal{C}^*},$	$\vec{n}^{\star} \cdot \vec{t} : V_{\mathcal{F}^{\star}} \times V_{\mathcal{E}} \to V_{\mathcal{C}},$
9	$\vec{n} f^* : V_{\mathcal{F}} \times V_{\mathcal{N}^*} \to V_{\mathcal{F}^*},$	$\vec{n}^{\star} f : V_{\mathcal{F}^{\star}} \times V_{\mathcal{N}} \to V_{\mathcal{F}},$
10	$m f^* : V_{\mathcal{C}} \times V_{\mathcal{N}^*} \to V_{\mathcal{C}^*},$	$m^{\star} f : V_{\mathcal{C}^{\star}} \times V_{\mathcal{N}} \to V_{\mathcal{C}}.$

Table 6.1. Products of Vectors and Scalars. (Definitions are given in Appendix C.3.)

More formulas are given in Appendix C.2. Again, note that the universal averaging operator is not used to define the key second-order differential operators, only to analyze them.

6.2. Scalar and Vector Products of Fields

We now construct discrete analogs of the continuum scalar and vector products that are listed in (4.10). Defining the discrete products is complicated by the grid staggering, which leads to some large formulas recorded in Appendix C.3.

The discrete star operator is used to reduce the possible products to those between elements of the primal and dual fields. Table 6.1 enumerates the possibilities. Note that the products are defined for objects in different spaces, so that it does not make sense to ask if they commute or anti-commute. Also, there are still two possibilities for the range of a product. We have chosen the convention that the product of a and b ends up in the same space as b. For example, for the formula (6.1), we use the definitions

$$f \, \vec{n}^{\star} : V_{\mathcal{N}} \times V_{\mathcal{F}^{\star}} \to V_{\mathcal{F}^{\star}}, \ (f \, \vec{n}^{\star})_{i+\frac{1}{2},j,k} = \mu(f)_{i+\frac{1}{2},j,k} \, n_{i+\frac{1}{2},j,k}^{\star},$$

$$f \, m^{\star} : V_{\mathcal{N}} \times V_{\mathcal{C}^{\star}} \to V_{\mathcal{C}^{\star}}, \ (f \, m^{\star})_{i,j,k} = f_{i,j,k} \, m_{i,j,k}^{\star},$$

$$\vec{t} \cdot \vec{n}^{\star} : V_{\mathcal{E}} \times V_{\mathcal{F}^{\star}} \to V_{\mathcal{C}^{\star}}, \ (\vec{t} \cdot \vec{n}^{\star})_{i,j,k} = \frac{t_{i-\frac{1}{2},j,k} \, n_{i-\frac{1}{2},j,k}^{\star} + t_{i+\frac{1}{2},j,k} \, n_{i+\frac{1}{2},j,k}^{\star}}{2} + \frac{t_{i,j,k-\frac{1}{2}} \, n_{i,j,k-\frac{1}{2}}^{\star} + t_{i,j,k+\frac{1}{2}} \, n_{i,j,k+\frac{1}{2}}^{\star}}{2}.$$

Dot products are only defined for vectors that are located at the same points in the grid (also see (C.5) and (C.6)), so the dot product is given by multiplying the co-located values and then averaging the result to a cell center in the primal or dual grid.

Cross products are a bit more difficult, but geometrically natural. For example, consider $\vec{t}^* \times \vec{t}$ from the second column of row 9 of Table 6.1, for which the formula is given in (C.7). This is a cell-face quantity in the primary grid of which the x component is

$$(\vec{t}^{\star} \times \vec{t})_{i,j+\frac{1}{2},k+\frac{1}{2}}$$
.

This quantity involves the product of the y component of \vec{t}^* and the z component of \vec{t} minus the product of the z component of \vec{t}^* times the y component of \vec{t} (see C.1). The first of these two terms thus involves the two quantities

$$t_{i+\frac{1}{2},j,k+\frac{1}{2}}^{\star}$$
 and $t_{i,j,k+\frac{1}{2}}$.

To multiply these two terms they have to be at the same point, so we first average t^* to get the quantity

$$Q1_{i,j,k+\frac{1}{2}} = \frac{t_{i-\frac{1}{2},j,k+\frac{1}{2}}^{\star} + t_{i+\frac{1}{2},j,k+\frac{1}{2}}^{\star}}{2} t_{i,j,k+\frac{1}{2}}.$$

However, this quantity is located on an edge of the face on which we are defining $\vec{t}^* \times \vec{t}$, so we average this quantity on the two parallel edges to get

$$Q2_{i,j+\frac{1}{2},k+\frac{1}{2}} = \frac{Q_{i,j,k+\frac{1}{2}} + Q_{i,j+1,k+\frac{1}{2}}}{2}.$$

Q2 is the desired term. The remaining terms in the formula can be computed similarly. Details are found in the Mathematica notebook Conservation.nb.

6.3. Divergence of Products Identities

We are now ready to prove discrete analogs of the continuum divergence identities (4.9).

Theorem 6.1.

$$\mathcal{D}^{\star}(f\,\vec{n}^{\star}) = f\,\mathcal{D}^{\star}(\vec{n}^{\star}) + \mathcal{G}(f)\cdot\vec{n}^{\star}, \qquad in\ V_{\mathcal{C}^{\star}}, \tag{6.1}$$

$$\mathcal{D}(f^* \vec{n}) = f^* \mathcal{D}(\vec{n}) + \mathcal{G}^*(f^*) \cdot \vec{n}, \qquad in V_{\mathcal{C}}, \qquad (6.2)$$

$$\mathcal{D}^{\star}(\vec{t} \times \vec{t}^{\star}) = \mathcal{R}\vec{t} \cdot \vec{t}^{\star} - \vec{t} \cdot \mathcal{R}^{\star}\vec{t}^{\star}, \qquad in V_{\mathcal{C}^{\star}}, \qquad (6.3)$$

$$\mathcal{D}(\vec{t}^* \times \vec{t}) = \mathcal{R}^* \vec{t}^* \cdot \vec{t} - \vec{t}^* \cdot \mathcal{R} \vec{t}, \qquad in V_{\mathcal{C}}.$$
(6.4)

Proof. The Mathematica notebook Conservation.nb provides details of the proofs by direct computation. Because the range of \mathcal{D}^* is $V_{\mathcal{C}^*}$, the first identity means

$$\mathcal{D}^{\star}(f\,\vec{n}^{\star})_{(i,j,k)} = (f\,\mathcal{D}^{\star}(\vec{n}^{\star}))_{(i,j,k)} + (\mathcal{G}(f)\cdot\vec{n}^{\star})_{(i,j,k)}$$

(see (C.3), (C.1) and (C.5)). The second identity must be verified at (i+1/2, j+1/2, k+1/2) because it holds in $V_{\mathcal{C}}$ (see (C.4), (C.2) and (C.6)). The third identity must be verified at (i, j, k) because it holds in $V_{\mathcal{C}^*}$ (see (C.7), (C.9) and (C.5)). Finally, the fourth identity must be verified at (i+1/2, j+1/2, k+1/2) because it holds in $V_{\mathcal{C}}$ (see (C.8), (C.10) and (C.6)).

6.4. Bilinear Forms and Duality

When two spaces in the double exact sequence (5.12) are connected by a vertical arrow, the elements of the spaces have the same indices, that is, they are defined at the same spatial point. Consequently, there are four natural bilinear forms all of which are labeled with \mathcal{B} . The constant area unit $\Delta x \Delta y \Delta z$ is introduced to make it easier to interpret the bilinear forms as integrals. Throughout, we assume that one of the fields in the bilinear form has compact support.

Node-Cell Bilinear Form: If $f \in V_N$ and $m^* \in V_{\mathcal{C}^*}$, then

$$\mathcal{B}(f, m^*) = \sum_{i,j,k} f_{i,j,k} \, m_{i,j,k}^* \, \triangle x \triangle y \triangle z. \tag{6.5}$$

Edge-Face Bilinear Form: If $\vec{t} \in V_{\mathcal{E}}$ and $\vec{n}^* \in V_{\mathcal{F}^*}$, then

$$\mathcal{B}(\vec{t}, \vec{n}^*) = \sum_{i,j,k} \left(t_{i+\frac{1}{2},j,k} \, n_{i+\frac{1}{2},j,k}^* + t_{i,j+\frac{1}{2},k} \, n_{i,j+\frac{1}{2},k}^* + t_{i,j,k+\frac{1}{2}} \, n_{i,j,k+\frac{1}{2}}^* \right) \, \triangle x \triangle y \triangle z. \tag{6.6}$$

Face-Edge Bilinear Form: If $\vec{n} \in V_{\mathcal{F}}$ and $\vec{t}^{\star} \in V_{\mathcal{E}^{\star}}$, then

$$\mathcal{B}(\vec{n}, \vec{t}^*) = \sum_{i,j,k} \begin{pmatrix} n_{i,j+\frac{1}{2},k+\frac{1}{2}} t^*_{i,j+\frac{1}{2},k+\frac{1}{2}} \\ + n_{i+\frac{1}{2},j,k+\frac{1}{2}} t^*_{i+\frac{1}{2},j,k+\frac{1}{2}} \\ + n_{i+\frac{1}{2},j+\frac{1}{2},k} t^*_{i+\frac{1}{2},j+\frac{1}{2},k} \end{pmatrix} \triangle x \triangle y \triangle z.$$
 (6.7)

Cell-Node Bilinear Form: If $m \in V_{\mathcal{C}}$ and $f^* \in V_{\mathcal{N}^*}$, then

$$\mathcal{B}(m, f^*) = \sum_{i,j,k} m_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} f^*_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \triangle x \triangle y \triangle z.$$
 (6.8)

Because the fields in the above definitions are located at the same points,

$$\mathcal{B}(\star m^{\star}, \star f) = \mathcal{B}(f, m^{\star}), \quad \mathcal{B}(\star f^{\star}, \star m) = \mathcal{B}(m, f^{\star}),$$
$$\mathcal{B}(\star \vec{n}^{\star}, \star \vec{t}) = \mathcal{B}(\vec{t}, \vec{n}^{\star}), \quad \mathcal{B}(\star \vec{t}^{\star}, \star \vec{n}) = \mathcal{B}(\vec{n}, \vec{t}^{\star}).$$

Lemma 6.1. The pairs of spaces

$$V_{\mathcal{N}}$$
 and $V_{\mathcal{C}^{\star}}$, $V_{\mathcal{E}}$ and $V_{\mathcal{F}^{\star}}$, $V_{\mathcal{F}}$ and $V_{\mathcal{E}^{\star}}$, $V_{\mathcal{C}}$ and $V_{\mathcal{N}^{\star}}$

are dual under the non-degenerate bilinear form \mathcal{B} . That is, the fields with compact support in one space are non-degenerate linear functionals on arbitrary fields in the dual space.

Under the assumption that one of the fields has compact support, an integral without domain of integration is performed over the full grid. The above bilinear forms can now be written using the following notation:

Lemma 6.2. Each of the four bilinear forms (6.5)–(6.8) has two representations: **Node-Cell Bilinear Form:**

$$\mathcal{B}(f, m^*) = \int m^* f \, dV = \int f \, m^* \, dV^*; \tag{6.9}$$

Cell-Node Bilinear Form:

$$\mathcal{B}(m, f^*) = \int f^* m \, dV = \int m \, f^* \, dV^*; \tag{6.10}$$

Edge-Face Bilinear Form:

$$\mathcal{B}(\vec{t}, \vec{n}^*) = \int \vec{n}^* \cdot \vec{t} \, dV = \int \vec{t} \cdot \vec{n}^* \, dV^*; \tag{6.11}$$

Face-Edge Bilinear Form:

$$\mathcal{B}(\vec{n}, \vec{t}^*) = \int \vec{t}^* \cdot \vec{n} \, dV = \int \vec{n} \cdot \vec{t}^* \, dV^*. \tag{6.12}$$

Proof. The key point is that the sum over the whole grid of the average of a field is the average of the sum, which is just the sum. For the Node-Cell case, $m^* f$ is defined in (C.12) as an average, while $f m^*$ is defined in (C.1) and does not need an average. So

$$\int m^{\star} f \, dV = \sum (m^{\star} f)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \, dx \, dy \, dz$$

$$= \sum \frac{1}{8} \begin{pmatrix} (m^{\star} f)_{i,j,k} + (m^{\star} f)_{i+1,j,k} \\ + (m^{\star} f)_{i,j+1,k} + (m^{\star} f)_{i,j,k+1} \\ + (m^{\star} f)_{i,j+1,k+1} + (m^{\star} f)_{i+1,j,k+1} \end{pmatrix} dx \, dy \, dz$$

$$= \sum (m^{\star} f)_{i,j,k} \, dx \, dy \, dz = \sum (f \, m^{\star})_{i,j,k} \, dx \, dy \, dz = B(f,m^{\star})$$

and

$$\int f \, m^* \, dV^* dV^* = \sum (f \, m^*)_{i,j,k} \, dx \, dy \, dz = B(f, m^*).$$

The remaining cases are similar. For the Cell-Node case, f^*m is defined in (C.2) and does not require an average, while $m f^*$ is defined in (C.11) and needs an average. For the Edge-Face case, $\vec{n}^*\vec{t}$ is defined in (C.10) as an average, and $\vec{t}\,\vec{n}^*$ is defined in (C.5) and also requires an average. For the Face-Edge case $\vec{t}^*\vec{n}$ is defined in (C.6) as an average, and $\vec{n}\,\vec{t}^*$ is defined in (C.9) and also requires an average. (Details are given in the Mathematica notebook Conservation.nb.)

6.5. Duality of the Vector Differential Operators

The next result is critical for understanding the Laplacian operators.

Theorem 6.2. The pairs of operators \mathcal{G} and \mathcal{D}^* , \mathcal{D} and \mathcal{G}^* , and \mathcal{R} and \mathcal{R}^* are \pm duals of each other in the bilinear form B:

$$B(f, \mathcal{D}^{\star}\vec{n}^{\star}) + B(\mathcal{G}f, \vec{n}^{\star}) = 0, \quad B(\mathcal{D}\vec{n}, f^{\star}) + B(\vec{n}, \mathcal{G}^{\star}f^{\star}) = 0, \quad B(\mathcal{R}\vec{t}, \vec{t}^{\star}) - B(\vec{t}, \mathcal{R}^{\star}\vec{t}^{\star}) = 0.$$

$$(6.13)$$

where at least one of the fields in the bilinear form has compact support.

Proof. The proofs consist of integrating product rule identities over the whole grid. For the first identity, integration of (6.1) gives

$$\int \mathcal{D}^{\star}(f\,\vec{n}^{\star})\,dV^{\star} = \int f\,\mathcal{D}^{\star}(\vec{n}^{\star})\,dV^{\star} + \int \mathcal{G}(f)\cdot\vec{n}^{\star}\,dV^{\star}.$$

So the dual of the Divergence theorem (5.10) and the compact support gives that the left-hand side is zero. (6.9) and (6.11) complete the computation.

Integration of (6.2) gives

$$\int \mathcal{D}(f^* \vec{n}) dV = \int f^* \mathcal{D}(\vec{n}) dV + \int \mathcal{G}^*(f^*) \cdot \vec{n} dV,$$

where the integral is given in (5.9). So the Divergence theorem (5.10) and the compact support gives that the left-hand side is zero. Then, (6.10) and (6.12) give the result.

Integration of (6.3) gives

$$\int \mathcal{D}^{\star}(\vec{t} \times \vec{t}^{\star}) \, dV^{\star} = \int \mathcal{R}\vec{t} \cdot \vec{t}^{\star} \, dV^{\star} - \int \vec{t} \cdot \mathcal{R}^{\star} \vec{t}^{\star} \, dV^{\star}.$$

So the dual of the Divergence theorem (5.10), discussed in Appendix B, and the compact support gives that the left-hand side is zero. Then, (6.12) and (6.11) give the result.

6.6. Inner Products and Laplacians

The bilinear forms (6.9), (6.10), (6.11) and (6.12) induce inner products on the compactly supported fields in discrete primal and dual spaces. For the primal case:

$$\langle f_1, f_2 \rangle = B(f_1, \star f_2), \quad \forall f_1, f_2 \in V_{\mathcal{N}},$$

$$\langle \vec{t}_1, \vec{t}_2 \rangle = B(\vec{t}_1, \star \vec{t}_2), \quad \forall \vec{t}_1, \vec{t}_2 \in V_{\mathcal{E}},$$

$$\langle \vec{n}_1, \vec{n}_2 \rangle = B(\vec{n}_1, \star \vec{n}_2), \quad \forall \vec{n}_1, \vec{n}_2 \in V_{\mathcal{F}},$$

$$\langle m_1, m_2 \rangle = B(m_1, \star m_2), \quad \forall m_1, m_2 \in V_{\mathcal{N}}.$$

For the dual case:

$$\langle f_1^{\star}, f_2^{\star} \rangle = B(\star f_1^{\star}, f_2^{\star}), \quad \forall f_1^{\star}, f_2^{\star} \in V_{\mathcal{N}^{\star}},$$

$$\langle \vec{t}_1^{\star}, \vec{t}_2^{\star} \rangle = B(\star \vec{t}_1^{\star}, \vec{t}_2^{\star}), \quad \forall \vec{t}_1^{\star}, \vec{t}_2^{\star} \in V_{\mathcal{E}^{\star}},$$

$$\langle \vec{n}_1^{\star}, \vec{n}_2^{\star} \rangle = B(\star \vec{n}_1^{\star}, \vec{n}_2^{\star}), \quad \forall \vec{n}_1^{\star}, \vec{n}_2^{\star} \in V_{\mathcal{F}^{\star}},$$

$$\langle m_1^{\star}, m_2^{\star} \rangle = B(\star m_1^{\star}, m_2^{\star}), \quad \forall m_1^{\star}, m_2 \in V_{\mathcal{N}^{\star}}.$$

Their related norms are $\|\cdot\|^2 = \langle\cdot,\cdot\rangle$. In fact, these inner products are the standard finite-dimensional mean-square inner products multiplied by the cell area. Note that the symmetry can be seen from, for example,

$$\langle f_1, f_2 \rangle = B(f_1, \star f_2) = B(\star \star f_2, \star f_1) = B(f_2, \star f_1) = \langle f_2, f_1 \rangle.$$

Lemma 6.3. The operators $-\star \mathcal{D}^* \star \mathcal{G}$ (5.13), $-\star \mathcal{G}^* \star \mathcal{D}$ (5.15) and $\star \mathcal{R}^* \star \mathcal{R}$ (5.14) are symmetric and positive.

Proof. The adjoint relationships (6.13) give

$$\langle \star \mathcal{D}^{\star} \star \mathcal{G} f_{1}, f_{2} \rangle = B(\star \mathcal{D}^{\star} \star \mathcal{G} f_{1}, \star f_{2}) = B(f_{2}, \mathcal{D}^{\star} \star \mathcal{G} f_{1}) = -B(\mathcal{G} f_{2}, \star \mathcal{G} f_{1}) = -\langle \mathcal{G} f_{2}, \mathcal{G} f_{1} \rangle;$$

$$\langle \star \mathcal{G}^{\star} \star \mathcal{D} \vec{n}_{1}, \vec{n}_{2} \rangle = B(\star \mathcal{G}^{\star} \star \mathcal{D} \vec{n}_{1}, \star \vec{n}_{2}) = B(\vec{n}_{2}, \mathcal{G}^{\star} \star \mathcal{D} \vec{n}_{1}) = -B(\mathcal{D} \vec{n}_{2}, \star \mathcal{D} \vec{n}_{1}) = -\langle \mathcal{D} \vec{n}_{2}, \mathcal{D} \vec{n}_{1} \rangle;$$

$$\langle \star \mathcal{R}^{\star} \star \mathcal{R} \vec{t}_{1}, \vec{t}_{2} \rangle = B(\star \mathcal{R}^{\star} \star \mathcal{R} \vec{t}_{1}, \star \vec{t}_{2}) = B(\vec{t}_{2}, \mathcal{R}^{\star} \star \mathcal{R} \vec{t}_{1}) = B(\mathcal{R} \vec{t}_{2}, \star \mathcal{R} \vec{t}_{1}) = \langle \mathcal{R} \vec{t}_{2}, \mathcal{R} \vec{t}_{1} \rangle.$$

This implies that

$$\langle -\star \mathcal{D}^{\star} \star \mathcal{G}f, f \rangle = \|\mathcal{G}f\|^{2}; \quad \langle -\star \mathcal{G}^{\star} \star \mathcal{D}\vec{n}, \vec{n}_{\rangle} = \|\mathcal{D}\vec{n}\|^{2}; \quad \langle \star \mathcal{R}^{\star} \star \mathcal{R}\vec{t}, \vec{t} \rangle = \|\mathcal{R}\vec{t}\|^{2}.$$

The Hodge Laplacian $\vec{\nabla} \times \vec{\nabla} \times - \vec{\nabla} \vec{\nabla} \cdot$ plays an important role in differential geometry. A discrete analog of this operator is $\star \mathcal{R}^{\star} \star \mathcal{R} - \mathcal{G} \star \mathcal{D}^{\star} \star$.

Lemma 6.4. The Hodge Laplacian is symmetric and positive.

Proof.

$$\langle \mathcal{G} \star \mathcal{D}^{\star} \star \vec{t_1}, \vec{t_2} \rangle = B(\mathcal{G} \star \mathcal{D}^{\star} \star \vec{t_1}, \star \vec{t_2}) = -B(\star \mathcal{D}^{\star} \star \vec{t_1}, \mathcal{D}^{\star} \star \vec{t_2}) = \langle \mathcal{D}^{\star} \star \vec{t_1}, \mathcal{D}^{\star} \star \vec{t_2} \rangle.$$

Combining this with the second formula in the previous proof gives

$$\langle \vec{\nabla} \times \vec{\nabla} \times \vec{t} - \vec{\nabla} \vec{\nabla} \cdot \vec{t}, \vec{t} \rangle = ||\mathcal{R}\vec{t}|| + ||\mathcal{D}^* \star \vec{t}||^2.$$

7. Future Directions

Mimetic ideas provide a unifying viewpoint for a number of effective (generalized) finite difference, finite volume and finite element methods. In addition, the many ongoing research projects relying on mimetic methods to solve varied applied modeling problems prove that discrete conservation laws/integration identities lead to robust and accurate numerical methods.

What is not so clear is the following: Can mimetic methods solve problems significantly better—more accurately, cheaply, and/or with reduced programming effort—than comparably sophisticated mixed finite element [33] and finite volume methods [44]? An affirmative answer to the first question requires that a mimetic method produce, for an important problem, a numerical solution of a quality unattainable with alternative methods; similarly for the latter two.

Such a "closer" is likely to consist of the successful solution of a problem with one or more of the following features:

- Rough solutions or coefficients, leading to highly non-classical solutions.
- Unusual boundary conditions leading, for example, to non-coercive bilinear forms.
- Unstable problems, or blow up solutions, about which accurate averaged or asymptotic properties are desired.
- Problems better formulated in term of tensors, that is, problems for which vector calculus is insufficiently expressive.

Problems with singular, degenerate, or rapidly varying material properties or solutions may provide problems that non-mimetic methods fail to solve satisfactorily. (General relativity comes to mind.) Somewhat related is the problem of computing effective (averaged) properties for complex materials (homogenization theory), a promising field of application of mimetic principles. In other words, it may be that mimetic methods end up being a preferred method because of their compatibility with the macroscopic modeling of material properties.

To our knowledge, a mimetic "killer application" has yet to be found. For this reason, it is still unclear whether mimetic discretizations will be seen as superior alternatives to finite element and finite volume methods, or whether mimetic properties will eventually come to be seen as important features of high quality methods derived without explicitly using mimetic discretization methods. In other words, the jury is still out regarding whether mimetic discretization methods will survive as a full-fledged derivation, or will eventually be seen as a footnote to the slow convergence of finite element and finite volume methods.

In the remainder of this section, we list a few promising, more theoretical, research directions.

Logically rectangular, but not tensor, grids (grids with "deformed" cells) have received a lot of attention. If the grid is smooth, mapping methods can be used to carry approximations on tensor grids over to the deformed grid without too great an accuracy loss. Mapping methods, however, do not perform well when the grid is not smooth. Furthermore, topological complications arise if the grid is only piecewise logically rectangular. A definitive treatment of rough grids and complex grid topologies is needed.

A promising research avenue concerns the development of (piecewise) spectral and pseudospectral methods that do not lose their rapid convergence when the solution, or the grid, is not smooth everywhere, in other words, the use of mimetic principles to stabilize high order approximations.

Mixed linear or nonlinear boundary conditions in higher dimensions also deserve further study. The linear 1D case was fully treated in [123], but matters are complicated in higher dimensions, especially if the boundary conditions involve field components other than those which appear in the appropriate version of Stokes' Theorem.

Also left out of the present paper is the issue of time discretization. The Finite Difference Time Domain method suggests the use of grids staggered in both time and space [154]. Consider, for example, the scalar wave equation written as a first order system:

$$\frac{\partial f}{\partial t} = \vec{\nabla} \cdot \vec{v}, \quad \frac{\partial \vec{v}}{\partial t} = \vec{\nabla} f.$$

Taking cues from relativity theory, treat time as "just another" spatial variable: Letting

$$f = f(t, x, y, z), \quad \vec{v} = (v_0, v_1, v_2, v_3) \text{ with } v_i = v_i(t, x, y, z),$$

set

$$\Box f = \left(\frac{\partial f}{\partial t}, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right) , \quad \text{and } \Box \cdot \vec{v} = \frac{\partial v_0}{\partial t} + \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z} .$$

Then, if A is the 4×4 diagonal matrix with diagonal equal to (-1,1,1,1),

$$\Box \cdot A \Box f = 0$$

is the wave equation. The space-time divergence \square is the key to fully discrete conservation laws. Following the ideas used in the time-independent case, natural discretizations of \square and \square on staggered grids can be obtained. The question now becomes: How can one construct analogs of the matrix A leading to accurate solutions of the wave equation?

The current paper assumes a rectangular data structure. Triangular/tetrahedral data structures, however, are extremely important. Mimetic methods have been implemented on triangular and tetrahedral grids and these methods work well. With some major changes, the theory presented in the present paper is applicable to this situation: In terms of a master element, a dual grid can be generated by connecting the barycenter of the triangle/tetrahedron to the centers of the sides/faces of the triangle. This leads to auxiliary values on the sides/faces of the triangles. If the side/face is in the interior of the region, the corresponding auxiliary value can be eliminated; If the side/face is on the boundary of the region, the corresponding auxiliary value can be used in the discretization of the boundary conditions. Major complications arise from the fact that the topology of a simplicial grid can be considerably more complex than the topology of a logically rectangular one.

Numerical Hodge-Helmholtz decompositions need refinement and additional flexibility.

The connection between geometric integration and mimetic discretization methods deserves investigation. There has to be a link between the preservation of Lie-Poisson brackets,

generally obtained via integration by parts [109], and mimetic summation-by-parts formulas. Yet, the two fields have evolved without much cross-pollination. This may be because the early development of geometric integration focused on discretizing systems of ordinary differential equations, with special emphasis on the preservation of antisymmetric bilinear forms (and Hamiltonian structures) [108], while the development of many mimetic discretization methods started with the diffusion equation, with an emphasis on preserving symmetric bilinear forms.

Mimetic discretizations based on discrete Hodge star operators constructed with Whitney map reconstruction and deRham projection generally assume one single primal/dual grid pair. A powerful generalization involves the averaging of Hodge star operators over parameterized families of dual grids. For example, if the steady state diffusion equation $-\nabla \cdot (K\nabla u) = 0$ is discretized with a single, fixed primal (cell) grid together with a parameterized family of dual grids obtained by linearly varying the position of the dual nodes within the cells (using, in triangular cells, barycentric coordinates), the Galerkin Hodge star is exactly recovered by averaging when the diffusion coefficient matrix K is constant within each cell. On the other hand, the Galerkin Hodge star is only approximately recovered when K varies within each cell. (In 1D, the averaged and the Galerkin discrete Hodge are the same irregardless of whether or not the diffusion coefficient is constant.) If one could devise a method of constructing the parameterized family of dual grids from the primal, and a matching method of averaging Hodge star operators, which automatically produces the Galerkin discrete Hodge star, this would link the finite element approach toward discretizing material properties (by way of bilinear forms) with the "direct" approach advocated, among others, by Claudio Mattiussi [102, 104], following the work of Enzo Tonti [142, 143]. It would also lead to Whitney-deRham Hodge stars with symmetric matrix representations, a desirable feature from a practical viewpoint. (Note that there is a mild abuse of terminology in the above discussion, since the discrete Hodge star is taken as containing both metric and material property information, a proposition which should not surprise the general relativists in the audience.)

A final note: Currently, there is no user-friendly (Matlab, Scilab or SciPy, for example) general purpose numerical software implementing mimetic methods and their key building blocks. The availability of such software would go a long way toward popularizing the framework, as it would allow researchers to experiment with established and novel mimetic formulations without too high an initial programming investment.

A. The Existence of Potentials

Proof of Theorem 5.2, part 1: Basically, we collapse the face chain toward k = 0, at which point it must be trivial.

Let F be a face chain with compact support and $\partial F = 0$. Without loss of generality, suppose that $F \neq 0$ (otherwise, take C = 0) and that the indices of nonzero coefficients of F are non-negative. Let K be the maximum value of all the third indices (full or half) of the nonzero faces of F. We assert that K must be an integer (not a half-integer). Otherwise, the maximum can be written $K = k + \frac{1}{2}$ with k an integer. There are four possibilities: $F_{i+\frac{1}{2},j,k+\frac{1}{2}}$, $F_{i-\frac{1}{2},j,k+\frac{1}{2}}$, $F_{i,j+\frac{1}{2},k+\frac{1}{2}}$ and $F_{i,j-\frac{1}{2},k+\frac{1}{2}}$ for some integers i and j. Let us consider the first possibility (the other three are similar). The boundary of the face $F_{i+\frac{1}{2},j,k+\frac{1}{2}}$ contains the edge $E_{i+\frac{1}{2},j,k+1}$. This edge is part of only three other faces: $F_{i+\frac{1}{2},j,k+1}$, $F_{i+\frac{1}{2},j-\frac{1}{2},k+1}$, and $F_{i+\frac{1}{2},j,k+\frac{3}{2}}$. For the boundary of the chain to be zero, the chain must contain a face other

than the last, contradicting the assumption that K is maximal.

Now, construct the cell chain C with $\partial C = F$. Start by setting C = 0. Choose any face in F of the form $F_{i\pm\frac{1}{2},j\pm\frac{1}{2},K}$. By linearity, assume that its coefficient is 1. F is in the boundary of the cell $A_{i\pm\frac{1}{2},j\pm\frac{1}{2},K-\frac{1}{2}}$. Now set $C = C + A_{i\pm\frac{1}{2},j\pm\frac{1}{2},K-\frac{1}{2}}$ and $F = F - \partial A_{i\pm\frac{1}{2},j\pm\frac{1}{2},K-\frac{1}{2}}$. Note that the new F still satisfies $\partial F = 0$ (because $\partial^2 = 0$) and that there is only one face with maximal k index in the boundary of $A_{i\pm\frac{1}{2},j\pm\frac{1}{2},K-\frac{1}{2}}$. This is important, because this implies that we have "removed" one face with maximal index and that the only other faces with coefficients affected by this step have smaller third indices. Note also that these affected faces have third index equal to $K - \frac{1}{2}$ or K - 1. For this reason, we can continue until the largest third index is 0, which means that all the third indices of the remaining face are equal to 0. As discussed above, the only way we can get $\partial F = 0$ is by having a face with half-integer third index in the chain. Since there are none, all the coefficients of the final face must be zero, which implies that the initial face is the boundary of the final cell.

The final cell chain C has compact support because at most one cell is added per step, and this algorithm terminates. (This algorithm was implemented in the Mathematica notebook InverseOfBoundary.nb.) \Box

Proof of Theorem 5.2, part 2: The procedure first collapses all third indices toward zero, at which point the remaining edge chain must be trivial.

Let E be an edge chain with compact support and $\partial E = 0$. Without loss of generality, suppose that $E \neq 0$ and that all its nonzero cofficients have non-negative third index. Edges in E have the form $E_{a,b,c}$ where one and only one of a, b and c is a half-integer. Find the maximum value of c over the edges with nonzero coefficients, and choose a corresponding edge $E_{a,b,c}$ with nonzero coefficient. By linearity, assume the coefficient to be 1.

The maximal third index c cannot be a half-integer because otherwise one of its endpoints would have a third index larger than c, which implies that an edge with a larger third index would have to be in E in order for ∂E to vanish. Consequently, $E_{a,b,c} = E_{a,b,K}$ with K an integer. $E_{a,b,K}$ is in the boundary of $F_{a,b,K-\frac{1}{2}}$. Add this face to the chain F being constructed and remove its boundary from E. The new E is still closed. In addition, $E_{a,b,K}$ is the only face with maximal third index which is affected, and the third indices of the other affected edges are $K-\frac{1}{2}$ and K-1. For this reason, we can continue until the maximal third index is 0, which means that the third index of every remaining edge is 0.

Now, consider the maximal second index of the nonzero coefficients of the remaining edge chain. This maximal second index must be an integer. However, the third index is 0. Since edges cannot have two integer indices, we must have that there were no nonzero coefficients. This implies that the boundary of the final face is the initial edge.

The final F has compact support because the algorithm terminates. (This algorithm was implemented in the Mathematica notebook InverseOfBoundary.nb.) \square

Proof of Theorem 5.3, part 1: This is a direct calculation. Its converse was noted earlier.

Proof of Theorem 5.3, part 2: Except for the fact that our integrals and paths are discrete, this is the classical proof based on the fact that the integral of the tangential component of a closed vector field \vec{t} is path independent. \Box

Proof of Theorem 5.3, part 3: As all cells are translates of each other, it is enough to consider $C_{\frac{1}{2},\frac{1}{2},\frac{1}{2}}$. On this cell the divergence condition implies that the given face vector field must satisfy

$$\frac{n_{1,\frac{1}{2},\frac{1}{2}}-n_{0,\frac{1}{2},\frac{1}{2}}}{\triangle x}+\frac{n_{\frac{1}{2},1,\frac{1}{2}}-n_{\frac{1}{2},0,\frac{1}{2}}}{\triangle y}+\frac{n_{\frac{1}{2},\frac{1}{2},1}-n_{\frac{1}{2},\frac{1}{2},0}}{\triangle z}=0,$$

while the desired edge vector field is given by the twelve values $t_{0,0,\frac{1}{2}},\,t_{0,\frac{1}{2},0},\,t_{0,\frac{1}{2},1},\,t_{1,0,\frac{1}{2}},\,t_{1,1,\frac{1}{2}},$

 $t_{1,\frac{1}{2},0}, t_{1,\frac{1}{2},1}, t_{\frac{1}{2},0,0}, t_{\frac{1}{2},0,1}, t_{\frac{1}{2},1,0}$ and $t_{\frac{1}{2},1,1}$. These must satisfy

$$\begin{split} n_{0,\frac{1}{2},\frac{1}{2}} &= +\frac{t_{0,1,\frac{1}{2}} - t_{0,0,\frac{1}{2}}}{\triangle y} - \frac{t_{0,\frac{1}{2},1} - t_{0,\frac{1}{2},0}}{\triangle z}, & n_{1,\frac{1}{2},\frac{1}{2}} &= +\frac{t_{1,1,\frac{1}{2}} - t_{1,0,\frac{1}{2}}}{\triangle y} - \frac{t_{1,\frac{1}{2},1} - t_{1,\frac{1}{2},0}}{\triangle z}, \\ n_{\frac{1}{2},0,\frac{1}{2}} &= +\frac{t_{\frac{1}{2},0,1} - t_{\frac{1}{2},0,0}}{\triangle z} - \frac{t_{1,0,\frac{1}{2}} - t_{0,0,\frac{1}{2}}}{\triangle x}, & n_{\frac{1}{2},1,\frac{1}{2}} &= +\frac{t_{\frac{1}{2},1,1} - t_{\frac{1}{2},1,0}}{\triangle z} - \frac{t_{1,1,\frac{1}{2}} - t_{0,1,\frac{1}{2}}}{\triangle x}, \\ n_{\frac{1}{2},\frac{1}{2},0} &= +\frac{t_{1,\frac{1}{2},0} - t_{0,\frac{1}{2},0}}{\triangle x} - \frac{t_{\frac{1}{2},1,0} - t_{\frac{1}{2},0,0}}{\triangle y}, & n_{\frac{1}{2},\frac{1}{2},1} &= +\frac{t_{1,\frac{1}{2},1} - t_{0,\frac{1}{2},1}}{\triangle x} - \frac{t_{\frac{1}{2},1,1} - t_{\frac{1}{2},0,1}}{\triangle y}. \end{split}$$

This is a system of six equations in 12 unknowns with rank five. Both the right-hand sides and the left-hand sides of these equations have divergence zero, so that the system is consistent. Each unknown appears in exactly two equations. In particular, a solution of any five of the equations determines all of the unknowns and automatically satisfies the sixth.

The constructive proof is an algorithm implemented in the Mathematica notebook Potential.nb. The solution is not unique because if \vec{t} is a solution and f is a scalar then $\vec{t} + \mathcal{G}(f)$ is also a solution. We assume that I_{\max} , J_{\max} and K_{\max} are given numbers larger than three and then we solve the problem on a grid where $0 \le i \le I_{\max}$, $0 \le j \le J_{\max}$ and $0 \le k \le K_{\max}$. We assume we are given all of the $n_{i+\frac{1}{2},j+\frac{1}{2},k}$, $n_{i+\frac{1}{2},j+\frac{1}{2},k}$ and $n_{i+\frac{1}{2},j+\frac{1}{2},k}$. We start by setting the values of all $t_{i+\frac{1}{2},j,k}$ arbitrarily (randomly, even). We also set all $t_{0,j+\frac{1}{2},k}$ values arbitrarily. We then use the equations for $n_{i+\frac{1}{2},j+\frac{1}{2},k}$ marching in the i index to compute the remaining $t_{i,j+\frac{1}{2},k}$. Next we set all $t_{0,0,k+\frac{1}{2}}$ values arbitrarily. We then use the equations for $n_{0,j+\frac{1}{2},k+\frac{1}{2}}$ marching in the j index to compute the remaining $t_{0,i,k+\frac{1}{2}}$. Finally, we use the equation for $n_{i+\frac{1}{2},j,k+\frac{1}{2}}$ marching the i index to compute the remaining $t_{i,j,k+\frac{1}{2}}$. Finally,

This algorithm was tested by generating a random vector field \vec{T} , setting $\vec{n} = \mathcal{R}\vec{T}$, computing t with the above method and then setting $\vec{N} = \mathcal{R}t$. As expected, $t \neq \vec{T}$, but $\vec{n} = \vec{N}$ (within round-off).

Proof of Theorem 5.3, part 4: Set

$$n_{i+\frac{1}{2},j+\frac{1}{2},k} = \sum_{k=0}^{\kappa=k} m_{i+\frac{1}{2},j+\frac{1}{2},\kappa+\frac{1}{2}} \triangle x, \quad n_{i+\frac{1}{2},j,k+\frac{1}{2}} = 0, \quad \text{and } n_{i,j+\frac{1}{2},k+\frac{1}{2}} = 0. \quad \Box$$

B. The Dual Grid

In this section, we introduce the dual grid, boundary operator, scalar and vector fields, difference operators, chains and integrals. All items related to the dual grids are labeled with a " \star ". Because the dual grid is a translate of the primal grid, all results of §5 hold for the dual grid.

B.1. The Dual Grid

The dual grid is obtained by putting the dual nodes at the centers of the primal cells. **Dual Nodes:**

$$N_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{\star} = \left\{ \left(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, z_{k+\frac{1}{2}} \right) \right\}.$$

The remaining geometrical objects follow from this definition.

Dual Edges:

$$\begin{split} E_{i,j+\frac{1}{2},k+\frac{1}{2}}^{\star} &= \left\{ \left(x_{i-\frac{1}{2}} + \xi \bigtriangleup x, y_{j+\frac{1}{2}}, z_{k+\frac{1}{2}} \right) : 0 \leqslant \xi \leqslant 1 \right\}, \\ E_{i+\frac{1}{2},j,k+\frac{1}{2}}^{\star} &= \left\{ \left(x_{i+\frac{1}{2}}, y_{j-\frac{1}{2}} + \eta \bigtriangleup y, z_{k+\frac{1}{2}} \right) : 0 \leqslant \eta \leqslant 1 \right\}, \\ E_{i+\frac{1}{2},j+\frac{1}{2},k}^{\star} &= \left\{ \left(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, z_{k-\frac{1}{2}} + \zeta \bigtriangleup z \right) : 0 \leqslant \zeta \leqslant 1 \right\}. \end{split}$$

Likewise with dual faces and dual cells.

As for the primal grid, the orientations of dual geometric objects are defined consistently with the ordering of the axes, that is, the orientation is consistent with "diagonally" translating the primal grid. The nodes of the primal grid are the centers of the cells of the dual grid, just as the nodes of the dual are the center of the primal. Edges of the primal grid traverse the center of a face of the dual grid perpendicularly and vice versa. For example,

$$E_{i+\frac{1}{2},j,k} \cap F^{\star}_{i+\frac{1}{2},j,k} = \left\{ (x_{i+\frac{1}{2}},y_j,z_k) \right\}, \text{ and } F_{i,j+\frac{1}{2},k+\frac{1}{2}} \cap E^{\star}_{i,j+\frac{1}{2},k+\frac{1}{2}} \quad = \left\{ (x_i,y_{j+\frac{1}{2}},z_{k+\frac{1}{2}}) \right\}.$$

The dual of the dual grid is the grid obtained by putting nodes at dual cell centers; consequently, the dual of the dual grid is the primal grid.

B.2. Dual Scalar and Vector Fields, Dual Difference Operators, Dual Chains, Dual Boundaries, and Dual Integrals

Fields on the dual grid—labeled with a " \star "—are defined by formulas (5.5)–(5.8) with the integers i, j and k replaced by $i + \frac{1}{2}, j + \frac{1}{2}$ and $k + \frac{1}{2}$. The dual grid operators are obtained from their primal counterparts with the same recipe. With the exception of the boundary operator ∂ , dual operators are labeled with a " \star ." Every result applicable to primal objects also applies to the corresponding dual objects. In particular, $\partial \partial \equiv 0$ holds for dual chains.

C. Formulas for the Scalar, Dot, and Cross Products

In this appendix we record the formulas for the universal averaging operator μ and then define various scalar and vector products. We begin with a motivating discussion of differential forms.

C.1. Differential Forms

We associate grid functions with differential forms: Given F, a nodal scalar $(f \text{ or } m^*)$, U, an edge vector $(t \text{ or } n^*)$, W, a face vector $(n \text{ or } t^*)$, and M, a cell scalar $(m \text{ or } f^*)$, let

$\nu_0 = F$	0-form,
$\xi_0 = G$	0-form,
$\nu_1 = U_1 dx + U_2 dy + U_3 dz$	1-form,
$\xi_1 = V_1 dx + V_2 dy + V_3 dz$	1-form,
$\nu_2 = W_1 dy dz + W_2 dz dx + W_3 dx dy$	2-form,
$\nu_3 = M dx dy dz$	3-form.

The non-trivial wedge products are

$$\begin{split} \nu_0 \wedge \xi_0 &= F \, G \\ \nu_0 \wedge \nu_1 &= F \, U_1 \, dx + F \, U_2 \, dy + F \, U_3 \, dz \\ \nu_0 \wedge \nu_2 &= F \, W_1 \, dy \, dz + F \, W_2 \, dz \, dx + F \, W_3 \, dx \, dy \\ \nu_0 \wedge \nu_3 &= F \, M \, dx \, dy \, dz \\ \nu_1 \wedge \xi_1 &= (U_1 \, V_2 - U_2 \, V_1) \, dx \, dy \, (U_3 \, V_1 - U_1 \, V_3) \, dz \, dx \, (U_2 \, V_3 - U_3 \, V_2) \, dy \, dz \\ \nu_1 \wedge \nu_2 &= (U_1 \, W_1 + U_2 \, W_2 + U_3 \, W_3) \, dx \, dy \, dz. \end{split}$$

In the above list there are four formulas that involve a 0-form, three that involve a 1-form, two that involve a 2-form and one that involves a 3-form. This gives rise to the ten cases appearing in Table 6.1. Also, the product of 1-forms give the cross product of two edge vector fields, while the wedge product of a 1-form and a 2-form gives the dot product of an edge vector field with a face vector field. It turns out that the only products needed are those of primary grid fields with dual grid fields (as in Table 6.1).

C.2. The Universal Averaging Operator

For products of fields in spaces connected by the star operator, no averaging is required, that is, the averaging operator is the identity. The other averaging operators are listed here:

$$2 \mu(f)_{i+\frac{1}{2},j,k} = f_{i,j,k} + f_{i+1,j,k},$$

$$4 \mu(f)_{i+\frac{1}{2},j+\frac{1}{2},k} = f_{i,j,k} + f_{i,j+1,k} + f_{i+1,j,k} + f_{i+1,j+1,k},$$

$$8 \mu(f)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = f_{i,j,k} + f_{i+1,j,k} + f_{i,j+1,k} + f_{i,j+1,k}$$

$$+ f_{i,j+1,k+1} + f_{i+1,j,k+1} + f_{i+1,j+1,k} + f_{i+1,j+1,k+1},$$

$$2 \mu(f^{\star})_{i+\frac{1}{2},j+\frac{1}{2},k} = f^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} + f^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}},$$

$$4 \mu(f^{\star})_{i+\frac{1}{2},j,k} = f^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} + f^{\star}_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + f^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} + f^{\star}_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + f^{\star}_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + f^{\star}_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + f^{\star}_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + f^{\star}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + f^{\star}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{$$

C.3. Definitions of the Scalar and Vector Products

Row 1. Products of nodal scalars and cell densities:

$$f m^* : V_{\mathcal{N}} \times V_{\mathcal{C}^*} \to V_{\mathcal{C}^*},$$
 $(f m^*)_{i,j,k} = f_{i,j,k} m^*_{i,j,k}.$ (C.1)

$$f^* m : V_{\mathcal{N}^*} \times V_{\mathcal{C}} \to V_{\mathcal{C}}, \qquad (f^* m)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = f^*_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} m_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}.$$
 (C.2)

Row 2. Products of nodal scalars and face vectors:

$$f \, \vec{n}^* : V_{\mathcal{N}} \times V_{\mathcal{F}^*} \to V_{\mathcal{F}^*}, \qquad (f \, \vec{n}^*)_{i+\frac{1}{2},j,k} = \mu(f)_{i+\frac{1}{2},j,k} \, n_{i+\frac{1}{2},j,k}^*.$$
 (C.3)

$$f^* \vec{n} : V_{\mathcal{N}^*} \times V_{\mathcal{F}} \to V_{\mathcal{F}}, \qquad (f^* \vec{n})_{i+\frac{1}{2},j+\frac{1}{2},k} = \mu(f^*)_{i+\frac{1}{2},j+\frac{1}{2},k} n_{i+\frac{1}{2},j+\frac{1}{2},k}.$$
 (C.4)

Row 3. Products of nodal scalars and edge vectors:

$$\begin{split} f \, \vec{t}^{\star} \, : \, V_{\mathcal{N}} \times V_{\mathcal{E}^{\star}} &\to V_{\mathcal{E}^{\star}}, \\ f^{\star} \, \vec{t} \, : \, V_{\mathcal{N}^{\star}} \times V_{\mathcal{E}} &\to V_{\mathcal{E}^{\star}}, \end{split} \qquad (f \, \vec{t}^{\star})_{i + \frac{1}{2}, j + \frac{1}{2}, k} = \mu(f)_{i + \frac{1}{2}, j + \frac{1}{2}, k} \, t^{\star}_{i + \frac{1}{2}, j + \frac{1}{2}, k}. \\ (f^{\star} \, \vec{t})_{i + \frac{1}{2}, j, k} &= \mu(f^{\star})_{i + \frac{1}{2}, j, k} \, t_{i + \frac{1}{2}, j, k}. \end{split}$$

Row 4. Products of nodal scalars:

$$f f^* : V_{\mathcal{N}} \times V_{\mathcal{N}^*} \to V_{\mathcal{N}^*}, \qquad (f f^*)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = \mu(f)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} f^*_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}.$$

$$f^* f : V_{\mathcal{N}^*} \times V_{\mathcal{N}} \to V_{\mathcal{N}}, \qquad (f^* f)_{i,j,k} = \mu(f^*)_{i,j,k} f_{i,j,k}.$$

 $\vec{t} \cdot \vec{n}^{\star} : V_{\mathcal{E}} \times V_{\mathcal{T}^{\star}} \to V_{\mathcal{C}^{\star}}$

Row 5. Dot products of tangent and normal vectors:

$$(\vec{t} \cdot \vec{n}^{\star})_{i,j,k} = \frac{t_{i-\frac{1}{2},j,k} n_{i-\frac{1}{2},j,k}^{\star} + t_{i+\frac{1}{2},j,k} n_{i+\frac{1}{2},j,k}^{\star}}{2} + \frac{t_{i,j-\frac{1}{2},k} n_{i,j-\frac{1}{2},k}^{\star} + t_{i,j+\frac{1}{2},k} n_{i,j+\frac{1}{2},k}^{\star}}{2} + \frac{t_{i,j,k-\frac{1}{2}} n_{i,j,k-\frac{1}{2}}^{\star} + t_{i,j,k+\frac{1}{2}} n_{i,j,k+\frac{1}{2}}^{\star}}{2}$$
(C.5)

$$\vec{t}^{\star} \cdot \vec{n} : V_{\mathcal{E}^{\star}} \times V_{\mathcal{F}} \to V_{\mathcal{C}},$$

$$(\vec{t}^{*} \cdot \vec{n})_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = \frac{t^{*}_{i+\frac{1}{2},j+\frac{1}{2},k} n_{i+\frac{1}{2},j+\frac{1}{2},k} + t^{*}_{i+\frac{1}{2},j+\frac{1}{2},k+1} n_{i+\frac{1}{2},j+\frac{1}{2},k+1}}{2} + \frac{t^{*}_{i+\frac{1}{2},j,k+\frac{1}{2}} n_{i+\frac{1}{2},j,k+\frac{1}{2}} + t^{*}_{i+\frac{1}{2},j,k+\frac{1}{2}} n_{i+\frac{1}{2},j,k+\frac{1}{2}}}{2} + \frac{t^{*}_{i,j+\frac{1}{2},k+\frac{1}{2}} n_{i,j+\frac{1}{2},k+\frac{1}{2}} + t^{*}_{i+1,j+\frac{1}{2},k+\frac{1}{2}} n_{i+1,j+\frac{1}{2},k+\frac{1}{2}}}{2}.$$
(C.6)

Row 6. Cross products of tangent vectors:

$$\vec{t} \times \vec{t}^* : V_{\mathcal{E}} \times V_{\mathcal{E}^*} \to V_{\mathcal{F}^*},$$

$$4 \left(\vec{t} \times \vec{t}^* \right)_{i+\frac{1}{2},j,k} = + \left(t_{i,j+\frac{1}{2},k} + t_{i+1,j+\frac{1}{2},k} \right) t_{i+\frac{1}{2},j+\frac{1}{2},k}^* + \left(t_{i,j-\frac{1}{2},k} + t_{i+1,j-\frac{1}{2},k} \right) t_{i+\frac{1}{2},j-\frac{1}{2},k}^* \\ - \left(t_{i,j,k+\frac{1}{2}} + t_{i+1,j,k+\frac{1}{2}} \right) t_{i+\frac{1}{2},j,k+\frac{1}{2}}^* - \left(t_{i,j,k-\frac{1}{2}} + t_{i+1,j,k-\frac{1}{2}} \right) t_{i+\frac{1}{2},j,k-\frac{1}{2}}^*,$$

$$4 \left(\vec{t} \times \vec{t}^* \right)_{i,j+\frac{1}{2},k} = + \left(t_{i,j,k+\frac{1}{2}} + t_{i,j+1,k+\frac{1}{2}} \right) t_{i,j+\frac{1}{2},k+\frac{1}{2}}^* + \left(t_{i,j,k-\frac{1}{2}} + t_{i,j+1,k-\frac{1}{2}} \right) t_{i,j+\frac{1}{2},k-\frac{1}{2}}^* - \left(t_{i+\frac{1}{2},j,k} + t_{i+\frac{1}{2},j+1,k} \right) t_{i+\frac{1}{2},j+\frac{1}{2},k}^* - \left(t_{i-\frac{1}{2},j,k} + t_{i-\frac{1}{2},j+1,k} \right) t_{i-\frac{1}{2},j+\frac{1}{2},k}^*$$

$$4 \left(\vec{t} \times \vec{t}^{\star} \right)_{i,j,k+\frac{1}{2}} = + \left(t_{i+\frac{1}{2},j,k} + t_{i+\frac{1}{2},j,k+1} \right) t_{i+\frac{1}{2},j,k+\frac{1}{2}}^{\star} + \left(t_{i-\frac{1}{2},j,k} + t_{i-\frac{1}{2},j,k+1} \right) t_{i-\frac{1}{2},j,k+\frac{1}{2}}^{\star} - \left(t_{i,j+\frac{1}{2},k} + t_{i,j+\frac{1}{2},k+1} \right) t_{i,j+\frac{1}{2},k+\frac{1}{2}}^{\star} - \left(t_{i,j-\frac{1}{2},k} + t_{i,j-\frac{1}{2},k+1} \right) t_{i,j-\frac{1}{2},k+\frac{1}{2}}^{\star}.$$
(C.7)

$$\vec{t}^{\star} \times \vec{t} : V_{\mathcal{E}^{\star}} \times V_{\mathcal{E}} \to V_{\mathcal{F}},$$

$$4 \left(\vec{t}^{*} \times \vec{t} \right)_{i,j+\frac{1}{2},k+\frac{1}{2}} = \\ + \left(t^{*}_{i-\frac{1}{2},j,k+\frac{1}{2}} + t^{*}_{i+\frac{1}{2},j,k+\frac{1}{2}} \right) t_{i,j,k+\frac{1}{2}} + \left(t^{*}_{i-\frac{1}{2},j+1,k+\frac{1}{2}} + t^{*}_{i+\frac{1}{2},j+1,k+\frac{1}{2}} \right) t_{i,j+1,k+\frac{1}{2}} \\ - \left(t^{*}_{i-\frac{1}{2},j+\frac{1}{2},k} + t^{*}_{i+\frac{1}{2},j+\frac{1}{2},k} \right) t_{i,j+\frac{1}{2},k} - \left(t^{*}_{i-\frac{1}{2},j+\frac{1}{2},k+1} + t^{*}_{i+\frac{1}{2},j+\frac{1}{2},k+1} \right) t_{i,j+\frac{1}{2},k+1}, \\ 4 \left(\vec{t}^{*} \times \vec{t} \right)_{i+\frac{1}{2},j,k+\frac{1}{2}} = \\ + \left(t^{*}_{i+\frac{1}{2},j-\frac{1}{2},k+1} + t^{*}_{i+\frac{1}{2},j+\frac{1}{2},k+1} \right) t_{i+\frac{1}{2},j,k+1} + \left(t^{*}_{i+\frac{1}{2},j-\frac{1}{2},k} + t^{*}_{i+\frac{1}{2},j+\frac{1}{2},k} \right) t_{i+\frac{1}{2},j,k} \\ - \left(t^{*}_{i,j-\frac{1}{2},k+\frac{1}{2}} + t^{*}_{i,j+\frac{1}{2},k+\frac{1}{2}} \right) t_{i,j,k+\frac{1}{2}} - \left(t^{*}_{i+1,j-\frac{1}{2},k+\frac{1}{2}} + t^{*}_{i+1,j+\frac{1}{2},k+\frac{1}{2}} \right) t_{i+1,j,k+\frac{1}{2}}, \\ 4 \left(\vec{t}^{*} \times \vec{t} \right)_{i+\frac{1}{2},j+\frac{1}{2},k} = \\ + \left(t^{*}_{i+1,j+\frac{1}{2},k-\frac{1}{2}} + t^{*}_{i+1,j+\frac{1}{2},k+\frac{1}{2}} \right) t_{i+1,j+\frac{1}{2},k} + \left(t^{*}_{i,j+\frac{1}{2},k-\frac{1}{2}} + t^{*}_{i,j+\frac{1}{2},k+\frac{1}{2}} \right) t_{i,j+\frac{1}{2},k} \\ - \left(t^{*}_{i+\frac{1}{2},j+1,k-\frac{1}{2}} + t^{*}_{i+\frac{1}{2},j+1,k+\frac{1}{2}} \right) t_{i+\frac{1}{2},j+1,k} - \left(t^{*}_{i+\frac{1}{2},j,k-\frac{1}{2}} + t^{*}_{i+\frac{1}{2},j,k+\frac{1}{2}} \right) t_{i+\frac{1}{2},j,k}.$$
(C.8)

Row 7. Products of tangent vectors and scalar fields:

$$\vec{t} f^{\star} : V_{\mathcal{E}} \times V_{\mathcal{N}^{\star}} \to V_{\mathcal{F}^{\star}}, \qquad (\vec{t} f^{\star})_{i+\frac{1}{2},j,k} = t_{i+\frac{1}{2},j,k} \mu(f^{\star})_{i+\frac{1}{2},j,k}.$$

$$\vec{t}^{\star} f : V_{\mathcal{E}^{\star}} \times V_{\mathcal{N}} \to V_{\mathcal{F}}, \qquad (\vec{t}^{\star} f)_{i+\frac{1}{2},j+\frac{1}{2},k} = t_{i+\frac{1}{2},j+\frac{1}{2},k}^{\star} \mu(f)_{i+\frac{1}{2},j+\frac{1}{2},k}.$$

Row 8. Dot products of face and tangent vectors:

$$\vec{n} \cdot \vec{t}^{\star} : V_{\mathcal{F}} \times V_{\mathcal{E}^{\star}} \to V_{\mathcal{C}^{\star}},$$

$$4 (\vec{n} \, \vec{t}^{\star})_{i,j,k} = + n_{i+\frac{1}{2},j+\frac{1}{2},k} \, t^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k} + n_{i-\frac{1}{2},j+\frac{1}{2},k} \, t^{\star}_{i-\frac{1}{2},j+\frac{1}{2},k} + n_{i+\frac{1}{2},j-\frac{1}{2},k} \, t^{\star}_{i+\frac{1}{2},j-\frac{1}{2},k} \\
+ n_{i-\frac{1}{2},j-\frac{1}{2},k} \, t^{\star}_{i-\frac{1}{2},j-\frac{1}{2},k} + n_{i+\frac{1}{2},j,k+\frac{1}{2}} \, t^{\star}_{i+\frac{1}{2},j,k+\frac{1}{2}} + n_{i-\frac{1}{2},j,k+\frac{1}{2}} \, t^{\star}_{i-\frac{1}{2},j,k+\frac{1}{2}} \\
+ n_{i+\frac{1}{2},j,k-\frac{1}{2}} \, t^{\star}_{i+\frac{1}{2},j,k-\frac{1}{2}} + n_{i-\frac{1}{2},j,k-\frac{1}{2}} \, t^{\star}_{i,j+\frac{1}{2},k-\frac{1}{2}} + n_{i,j+\frac{1}{2},k+\frac{1}{2}} \, t^{\star}_{i,j+\frac{1}{2},k+\frac{1}{2}} \\
+ n_{i,j-\frac{1}{2},k+\frac{1}{2}} \, t^{\star}_{i,j-\frac{1}{2},k+\frac{1}{2}} + n_{i,j+\frac{1}{2},k-\frac{1}{2}} \, t^{\star}_{i,j+\frac{1}{2},k-\frac{1}{2}} + n_{i,j-\frac{1}{2},k-\frac{1}{2}} \, t^{\star}_{i,j-\frac{1}{2},k-\frac{1}{2}} \\
+ n_{i,j-\frac{1}{2},k+\frac{1}{2}} \, t^{\star}_{i,j-\frac{1}{2},k+\frac{1}{2}} + n_{i,j+\frac{1}{2},k-\frac{1}{2}} \, t^{\star}_{i,j+\frac{1}{2},k-\frac{1}{2}} + n_{i,j-\frac{1}{2},k-\frac{1}{2}} \, t^{\star}_{i,j-\frac{1}{2},k-\frac{1}{2}} \\
+ n_{i,j-\frac{1}{2},k+\frac{1}{2}} \, t^{\star}_{i+\frac{1}{2},j,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \\
+ n^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \, t^{\star}_{i+\frac{1}{2},j,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \\
+ n^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \, t^{\star}_{i+\frac{1}{2},j,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \\
+ n^{\star}_{i+\frac{1}{2},j+\frac{1}{2},k+1} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j,k+1} \, t^{\star}_{i+\frac{1}{2},j+1,k} \, t^{\star}_{i+\frac{1}{2}$$

$$4 \left(\vec{n}^{\star} \cdot t \right)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = + n^{\star}_{i+\frac{1}{2},j,k} t_{i+\frac{1}{2},j,k} + n^{\star}_{i+\frac{1}{2},j+1,k} t_{i+\frac{1}{2},j+1,k} + n^{\star}_{i+\frac{1}{2},j,k+1} t_{i+\frac{1}{2},j,k+1} + n^{\star}_{i+\frac{1}{2},j+1,k+1} t_{i+\frac{1}{2},j+1,k+1} + n^{\star}_{i,j+\frac{1}{2},k} t_{i,j+\frac{1}{2},k} + n^{\star}_{i+1,j+\frac{1}{2},k} t_{i+1,j+\frac{1}{2},k} + n^{\star}_{i,j+\frac{1}{2},k+1} t_{i,j+\frac{1}{2},k+1} + n^{\star}_{i,j+\frac{1}{2},k+1} t_{i+1,j+\frac{1}{2},k+1} + n^{\star}_{i,j,k+\frac{1}{2}} t_{i,j,k+\frac{1}{2}} t_{i,j,k+\frac{1}{2}} + n^{\star}_{i+1,j,k+\frac{1}{2}} t_{i+1,j+1,k+\frac{1}{2}} t_{i+1,j+1,k+\frac{1}{2}}.$$

$$(C.10)$$

Row 9. Products of face vectors and scalar fields:

$$\vec{n} f^{\star} : V_{\mathcal{F}} \times V_{\mathcal{N}^{\star}} \to V_{\mathcal{F}^{\star}}, \qquad (\vec{n} f^{\star})_{i+\frac{1}{2},j,k} = \mu(n)_{i+\frac{1}{2},j,k} \mu(f^{\star})_{i+\frac{1}{2},j,k}.$$

$$\vec{n}^{\star} f : V_{\mathcal{F}^{\star}} \times V_{\mathcal{N}} \to V_{\mathcal{F}}, \qquad (\vec{n}^{\star} f)_{i+\frac{1}{2},j+\frac{1}{2},k} = \mu(n^{\star})_{i+\frac{1}{2},j+\frac{1}{2},k} \mu(f)_{i+\frac{1}{2},j+\frac{1}{2},k}.$$

Row 10. Products of cell and nodal scalars:

$$m f^*: V_{\mathcal{C}} \times V_{\mathcal{N}^*} \to V_{\mathcal{C}^*}, \qquad (m f^*)_{i,j,k} = \mu(m f^*)_{i,j,k}.$$
 (C.11)

$$m^{\star} f: V_{\mathcal{C}^{\star}} \times V_{\mathcal{N}} \to V_{\mathcal{C}}, \qquad (m^{\star} f)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = \mu(m^{\star} f)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}.$$
 (C.12)

D. Accuracy

In this section, the projection of continuum fields onto discrete fields is defined and used to define the truncation error for the difference operators. Because average projections are used, the difference (and the integration operators) are exact. Consequently all the error resides in the star operators which, on uniform tensor grids, are second-order accurate. The truncation errors for the Laplacians contain two terms: one is clearly second order; the other is the divergence of a second-order accurate term, and could in principle be first order. The article [81] relies on such estimates to prove second-order convergence.

D.1. The Projections

If f is a smooth scalar field on \mathbb{R}^3 then its nodal projection is given by

$$\mathcal{P}_N(f)_{(i,j,k)} = f(x_{(i,j,k)}, y_{(i,j,k)}, z_{(i,j,k)}),$$

and its cell projection is given by

$$\mathcal{P}_{C}(f)_{(i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2})} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} f(x_{i+\frac{1}{2}} + \xi \triangle x, y_{j+\frac{1}{2}} + \eta \triangle y, z_{k+\frac{1}{2}} + \zeta \triangle z) \, d\xi \, d\eta \, d\zeta.$$

If $\vec{v} = (v_1, v_2, v_2)$ is a smooth vector field on \mathbb{R}^3 then its edge projection is given by

$$\begin{split} \mathcal{P}_E(\vec{v})_{(i+\frac{1}{2},j,k)} &= \int_{-\frac{1}{2}}^{\frac{1}{2}} v_1(x_{i+\frac{1}{2}} + \xi \triangle x, y_j, z_k) \, d\xi, \\ \mathcal{P}_E(\vec{v})_{(i,j+\frac{1}{2},k)} &= \int_{-\frac{1}{2}}^{\frac{1}{2}} v_2(x_i, y_{j+\frac{1}{2}} + \eta \triangle y, z_k) \, d\eta, \\ \mathcal{P}_E(\vec{v})_{(i,j,k+\frac{1}{2})} &= \int_{-\frac{1}{2}}^{\frac{1}{2}} v_3(x_i, y_j, z_{k+\frac{1}{2}} + \zeta \triangle z) \, d\zeta. \end{split}$$

while its face projection is given by

$$\mathcal{P}_{F}(\vec{v})_{(i,j+\frac{1}{2},k+\frac{1}{2})} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} v_{1}(x_{i}, y_{j+\frac{1}{2}} + \eta \triangle y, z_{k+\frac{1}{2}} + \zeta \triangle z) \, d\eta \, d\zeta,$$

$$\mathcal{P}_{F}(\vec{v})_{(i+\frac{1}{2},j,k+\frac{1}{2})} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} v_{2}(x_{i+\frac{1}{2}} + \xi \triangle x, y_{j}, z_{k+\frac{1}{2}} + \zeta \triangle z) \, d\xi \, d\zeta,$$

$$\mathcal{P}_{F}(\vec{v})_{(i+\frac{1}{2},j+\frac{1}{2},k)} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} v_{3}(x_{i+\frac{1}{2}} + \xi \triangle x, y_{j+\frac{1}{2}} + \eta \triangle y, z_{k}) \, d\xi \, d\eta.$$

The projections onto the dual grids are translates of the projections onto the primal grid.

D.2. Truncation Error for the Difference Operators

Truncation error measures the difference between the projection of a continuum operator and a discrete operator. The truncation errors for the difference operators are

$$\mathcal{T}_{\mathcal{G}}(f) = \mathcal{P}_{E}\vec{\nabla}f - \mathcal{G}\mathcal{P}_{N}f; \qquad \mathcal{T}_{\mathcal{G}^{\star}}(f) = \mathcal{P}_{E^{\star}}\vec{\nabla}f - \mathcal{G}^{\star}\mathcal{P}_{N^{\star}}f;
\mathcal{T}_{\mathcal{R}}(\vec{v}) = \mathcal{P}_{F}\vec{\nabla}\times\vec{v} - \mathcal{R}\mathcal{P}_{E}\vec{v}; \qquad \mathcal{T}_{\mathcal{R}^{\star}}(\vec{v}) = \mathcal{P}_{F^{\star}}\vec{\nabla}\times\vec{v} - \mathcal{R}^{\star}\mathcal{P}_{E^{\star}}\vec{v};
\mathcal{T}_{\mathcal{D}}(\vec{v}) = \mathcal{P}_{C}\vec{\nabla}\cdot\vec{v} - \mathcal{D}\mathcal{P}_{F}\vec{v}; \qquad \mathcal{T}_{\mathcal{D}^{\star}}(\vec{v}) = \mathcal{P}_{C^{\star}}\vec{\nabla}\cdot\vec{v} - \mathcal{D}^{\star}\mathcal{P}_{F^{\star}}\vec{v}.$$

Theorem D.1. The differential operators are exact:

$$\mathcal{T}_{\mathcal{G}} \equiv 0, \quad \mathcal{T}_{\mathcal{G}^{\star}} \equiv 0, \quad \mathcal{T}_{\mathcal{R}} \equiv 0, \quad \mathcal{T}_{\mathcal{R}^{\star}} \equiv 0, \quad \mathcal{T}_{\mathcal{D}} \equiv 0, \quad \mathcal{T}_{\mathcal{D}^{\star}} \equiv 0.$$

Proof. The truncation error for the gradient at $(i + \frac{1}{2}, j, k)$ is

$$\mathcal{T}_{\mathcal{G}}(f)_{(i+\frac{1}{2},j,k)} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\partial f}{\partial x}(x_{i+\frac{1}{2}} + \xi \triangle x, y_j, z_k) d\xi - \frac{f(x_{i+1}, y_j, z_k) - f(x_i, y_j, z_k)}{\triangle x} = 0.$$

The truncation error for the curl at $(i, j + \frac{1}{2}, k + \frac{1}{2})$ is

$$\mathcal{T}_{\mathcal{R}}(\vec{v})_{(i,j+\frac{1}{2},k+\frac{1}{2})} = \left(\mathcal{P}_F \vec{\nabla} \times \vec{v}\right)_{(i,j+\frac{1}{2},k+\frac{1}{2})} - \left(\mathcal{R}\mathcal{P}_E \vec{v}\right)_{(i,j+\frac{1}{2},k+\frac{1}{2})}.$$

The first term is

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(\frac{\partial v_3}{\partial y} (x_i, y_{j+\frac{1}{2}} + \eta \triangle y, z_{k+\frac{1}{2}} + \zeta \triangle z) - \frac{\partial v_2}{\partial z} (x_i, y_{j+\frac{1}{2}} + \eta \triangle y, z_{k+\frac{1}{2}} + \zeta \triangle z) \right) d\eta d\zeta.$$

The first part of the integrand is

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\partial v_3}{\partial y}(x_i, y_{j+\frac{1}{2}} + \eta \triangle y, z_{k+\frac{1}{2}} + \zeta \triangle z) \, d\eta \, d\zeta =$$

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{v_3(x_i, y_{j+1}, z_{k+\frac{1}{2}} + \zeta \triangle z) - v_3(x_i, y_j, z_{k+\frac{1}{2}} + \zeta \triangle z)}{\triangle y} \, d\zeta$$

which is exactly the first part of

$$(\mathcal{R}\mathcal{P}_{E}\vec{v})_{(i,j+\frac{1}{2},k+\frac{1}{2})} = \frac{(\mathcal{P}_{E}\vec{v})_{(i,j+1,k+\frac{1}{2})} - (\mathcal{P}_{E}\vec{v})_{(i,j,k+\frac{1}{2})}}{\triangle y} - \frac{(\mathcal{P}_{E}\vec{v})_{(i,j+\frac{1}{2},k+1)} - (\mathcal{P}_{E}\vec{v})_{(i,j+\frac{1}{2},k)}}{\triangle z}.$$

Doing likewise with the second part gives the curl result.

The truncation error for the divergence is equal to $\mathcal{P}_C \vec{\nabla} \cdot \vec{v} - \mathcal{D} \mathcal{P}_F \vec{v}$. Evaluating the first term at $(i + \frac{1}{2}, j + \frac{1}{2}, k + \frac{1}{2})$ gives

$$\begin{split} \mathcal{P}_{C}\vec{\nabla}\cdot\vec{v}_{(i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2})} &= \\ \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(\begin{array}{c} \frac{\partial v_{1}}{\partial x} \left(x_{i+\frac{1}{2}} + \xi \bigtriangleup x, y_{j+\frac{1}{2}} + \eta \bigtriangleup y, z_{k+\frac{1}{2}} + \zeta \bigtriangleup z \right) + \\ \frac{\partial v_{3}}{\partial y} \left(x_{i+\frac{1}{2}} + \xi \bigtriangleup x, y_{j+\frac{1}{2}} + \eta \bigtriangleup y, z_{k+\frac{1}{2}} + \zeta \bigtriangleup z \right) + \\ \frac{\partial v_{3}}{\partial z} \left(x_{i+\frac{1}{2}} + \xi \bigtriangleup x, y_{j+\frac{1}{2}} + \eta \bigtriangleup y, z_{k+\frac{1}{2}} + \zeta \bigtriangleup z \right) + \\ \end{array} \right) \, d\xi \, d\eta \, d\zeta. \end{split}$$

The first term of this triple integral is equal to

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(\frac{v_1 \left(x_{i+1}, y_{j+\frac{1}{2}} + \eta \bigtriangleup y, z_{k+\frac{1}{2}} + \zeta \bigtriangleup z \right)}{\triangle x} - \frac{v_1 \left(x_i y_{j+\frac{1}{2}} + \eta \bigtriangleup y, z_{k+\frac{1}{2}} + \zeta \bigtriangleup z \right)}{\triangle x} \right) d\eta \, d\zeta,$$

On the other hand, the second term of the truncation error for the divergence at $(i + \frac{1}{2}, j + \frac{1}{2}, k + \frac{1}{2})$ is

$$\mathcal{DP}_{F}\vec{v}_{(i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2})} = \frac{1}{\triangle x} \left(\int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} v_{1}(x_{i+1},y_{j+\frac{1}{2}} + \eta \triangle y,z_{k+\frac{1}{2}} + \zeta \triangle z) \, d\eta \, d\zeta \right) - \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} v_{1}(x_{i},y_{j+\frac{1}{2}} + \eta \triangle y,z_{k+\frac{1}{2}} + \zeta \triangle z) \, d\eta \, d\zeta + \cdots$$

Cancelling matching terms leads to the divergence result.

The proofs for $\mathcal{T}_{\mathcal{G}^*}$, $\mathcal{T}_{\mathcal{R}^*}$, and $\mathcal{T}_{\mathcal{D}^*}$ are similar.

D.3. Truncation Error for the Star Operators

In the continuum, if f is a smooth scalar field then $\star f = f$, while if \vec{v} is a smooth vector field then $\star \vec{v} = \vec{v}$. So the truncation errors for the star operators (5.11) are

$$\mathcal{T}_{\star_{(C,N^{\star})}}(f) = \mathcal{P}_{N^{\star}}(\star f) - \star \mathcal{P}_{C}f = \mathcal{P}_{N^{\star}}(\star f) - \star_{(C,N^{\star})}\mathcal{P}_{C}f;$$

$$\mathcal{T}_{\star_{(F,E^{\star})}}(\vec{v}) = \mathcal{P}_{E^{\star}}(\star \vec{v}) - \star \mathcal{P}_{F}\vec{v} = \mathcal{P}_{E^{\star}}(\star \vec{v}) - \star_{(F,E^{\star})}\mathcal{P}_{F}\vec{v};$$

$$\mathcal{T}_{\star_{(E,F^{\star})}}(\vec{v}) = \mathcal{P}_{F^{\star}}(\star \vec{v}) - \star \mathcal{P}_{E}\vec{v} = \mathcal{P}_{F^{\star}}(\star \vec{v}) - \star_{(E,F^{\star})}\mathcal{P}_{E}\vec{v};$$

$$\mathcal{T}_{\star_{(N,C^{\star})}}(f) = \mathcal{P}_{C^{\star}}(\star f) - \star \mathcal{P}_{N}f = \mathcal{P}_{C^{\star}}(\star f) - \star_{(N,C^{\star})}\mathcal{P}_{N}f;$$

$$\mathcal{T}_{\star_{(C^{\star},N)}}(f) = \mathcal{P}_{N}(\star f) - \star \mathcal{P}_{C^{\star}}f = \mathcal{P}_{N}(\star f) - \star_{(C^{\star},N)}\mathcal{P}_{C^{\star}}f;$$

$$\mathcal{T}_{\star_{(F^{\star},E)}}(\vec{v}) = \mathcal{P}_{E}(\star \vec{v}) - \star \mathcal{P}_{F^{\star}}\vec{v} = \mathcal{P}_{E}(\star \vec{v}) - \star_{(F^{\star},E)}\mathcal{P}_{F^{\star}}\vec{v};$$

$$\mathcal{T}_{\star_{(E^{\star},F)}}(\vec{v}) = \mathcal{P}_{F}(\star \vec{v}) - \star \mathcal{P}_{E^{\star}}\vec{v} = \mathcal{P}_{F}(\star \vec{v}) - \star_{(E^{\star},F)}\mathcal{P}_{E^{\star}}\vec{v};$$

$$\mathcal{T}_{\star_{(N^{\star},C)}}(f) = \mathcal{P}_{C}(\star f) - \star \mathcal{P}_{N^{\star}}f = \mathcal{P}_{C}(\star f) - \star_{(N^{\star},C)}\mathcal{P}_{N^{\star}}f.$$

Simple identities relate these quantities:

$$\mathcal{T}_{\star_{(C,N^{\star})}}(f) = -\star_{(N^{\star},C)}\mathcal{T}_{\star_{(N^{\star},C)}}(f); \qquad \mathcal{T}_{\star_{(F,E^{\star})}}(\vec{v}) = -\star_{(E^{\star},F)}\mathcal{T}_{\star_{(E^{\star},F)}}(\vec{v}); \\ \mathcal{T}_{\star_{(E,F^{\star})}}(\vec{v}) = -\star_{(F^{\star},E)}\mathcal{T}_{\star_{(F^{\star},E)}}(\vec{v}); \qquad \mathcal{T}_{\star_{(N,C^{\star})}}(f) = -\star_{(C^{\star},N)}\mathcal{T}_{\star_{(C^{\star},N)}}(f).$$

Theorem D.2. The star operators are second-order accurate. That is, $\mathcal{T}_{\star_{(C^{\star},N)}}$, $\mathcal{T}_{\star_{(C,N^{\star})}}$, $\mathcal{T}_{\star_{(F^{\star},E)}}$, $\mathcal{T}_{\star_{(F^{\star},E)}}$, $\mathcal{T}_{\star_{(E^{\star},F)}}$, $\mathcal{T}_{\star_{(E,F^{\star})}}$, $\mathcal{T}_{\star_{(N^{\star},C)}}$ and $\mathcal{T}_{\star_{(N,C^{\star})}}$ are O ($\triangle x^2 + \triangle y^2 + \triangle z^2$). *Proof.*

$$(\mathcal{P}_{N}f)_{(i,j,k)} = f(x_{i}, y_{j}, z_{k}), \text{ and}$$

$$(\star \mathcal{P}_{C^{\star}}f)_{(i,j,k)} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} f(x_{i} + \xi \triangle x, y_{j} + \eta \triangle y, z_{k} + \zeta \triangle z) d\xi d\eta d\zeta$$

$$= f(x_{i}, y_{j}, z_{k}) + O\left(\triangle x^{2} + \triangle y^{2} + \triangle z^{2}\right).$$

Consequently, $(\mathcal{T}_{\star_{(C^{\star},N)}}(f))_{(i,j,k)}$ is $O(\triangle x^2 + \triangle y^2 + \triangle z^2)$.

$$(\mathcal{P}_{E}\vec{v})_{(i+\frac{1}{2},j,k)} = \int_{-\frac{1}{2}}^{\frac{1}{2}} v_{1}(x_{i+\frac{1}{2}+\xi\triangle x}, y_{j}, z_{k}) d\xi = v_{1}(x_{i+\frac{1}{2}}, y_{j}, z_{k}) + \mathcal{O}\left(\triangle x^{2}\right), \text{ and}$$

$$(\star \mathcal{P}_{F^{\star}}\vec{v})_{(i+\frac{1}{2},j,k)} = \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} v_{1}(x_{i+\frac{1}{2}}, y_{j} + \eta\triangle y, z_{k} + \zeta\triangle z) d\eta d\zeta$$

$$= v_{1}(x_{i+\frac{1}{2}}, y_{j}, z_{k}) + \mathcal{O}\left(\triangle y^{2} + \triangle z^{2}\right)$$

Consequently,
$$\mathcal{T}_{\star(F^{\star},E)}(\vec{v})_{(i+\frac{1}{2},j,k)}$$
 is O $(\triangle x^2 + \triangle y^2 + \triangle z^2)$.
The remaining cases are similar.

D.4. Truncation Error for the Laplacians

The truncation error for the scalar Laplacian \mathcal{L} (see (5.13)) is

$$\mathcal{T}_{\mathcal{L}}(f) = \mathcal{P}_{N}(\Delta f) - \mathcal{L}\mathcal{P}_{N}(f),$$

where f is a smooth scalar field. The truncation error for the vector Laplacian $\vec{\mathcal{L}}$ (see (5.14)) is

$$\mathcal{T}_{\vec{\mathcal{L}}}(\vec{v}) = \mathcal{P}_E(\Delta \vec{v}) - \vec{\mathcal{L}} \mathcal{P}_E(\vec{v}),$$

where \vec{v} is a smooth vector field. Because the truncation error for the first-order difference operators is zero, the truncation errors for the scalar and vector Laplacians depend only on the truncation errors of the star operators. However, the Laplacian truncation errors contain the divergence of a truncation error which, in general, can only be expected to be of first-order.

Theorem D.3. The truncation error for the scalar Laplacian satisfies

$$\mathcal{T}_{\mathcal{L}}(f) = \mathcal{T}_{\star_{(C^{\star}N)}}(\Delta f) + \star_{(C^{\star},N)} \mathcal{D}^{\star} \mathcal{T}_{\star_{(E,F^{\star})}}(\vec{\nabla} f).$$

Proof. The following identity implies the result.

$$\mathcal{T}_{\mathcal{L}}(f) = \mathcal{P}_{N}(\Delta f) - \star_{(C^{\star},N)} \mathcal{D}^{\star} \star_{(E,F^{\star})} \mathcal{G} \mathcal{P}_{N}(f)$$

$$= \mathcal{P}_{N}(\star \Delta f) - \star_{(C^{\star},N)} \mathcal{P}_{C^{\star}}(\Delta f) + \star_{(C^{\star},N)} \mathcal{P}_{C^{\star}}(\vec{\nabla} \cdot \vec{\nabla} f) - \star_{(C^{\star},N)} \mathcal{D}^{\star} \star_{(E,F^{\star})} \mathcal{G} \mathcal{P}_{N}(f)$$

$$= \mathcal{T}_{\star_{(C^{\star},N)}}(\Delta f) + \star_{(C^{\star},N)} \left(\mathcal{P}_{C^{\star}}(\vec{\nabla} \cdot \vec{\nabla} f) - \mathcal{D}^{\star} \mathcal{P}_{F^{\star}} \vec{\nabla} f + \mathcal{D}^{\star} \mathcal{P}_{F^{\star}} \vec{\nabla} f - \mathcal{D}^{\star} \star_{(E,F^{\star})} \mathcal{G} \mathcal{P}_{N}(f) \right)$$

$$= \mathcal{T}_{\star_{(C^{\star},N)}}(\Delta f) + \star_{(C^{\star},N)} \left(\mathcal{T}_{\mathcal{D}^{\star}}(\vec{\nabla} f) + \mathcal{D}^{\star} \left(\mathcal{P}_{F^{\star}} \star \vec{\nabla} f - \star_{(E,F^{\star})} \mathcal{G} \mathcal{P}_{N}(f) \right) \right)$$

$$= \mathcal{T}_{\star_{(C^{\star},N)}}(\Delta f) + \star_{(C^{\star},N)} \left(\mathcal{T}_{\mathcal{D}^{\star}}(\vec{\nabla} f) + \mathcal{D}^{\star} \left(\mathcal{T}_{\star_{(E,F^{\star})}}(\vec{\nabla} f) + \star_{(E,F^{\star})} \mathcal{T}_{\mathcal{G}}(f) \right) \right).$$

Theorem D.4. The truncation error for the vector Laplacian satisfies

$$\mathcal{T}_{\vec{\mathcal{L}}}(\vec{v}) = \mathcal{T}_{\star_{(F^{\star},E)}}(\Delta \vec{v}) + \star_{(F^{\star},E)} \mathcal{R}^{\star} \mathcal{T}_{\star_{(F,E^{\star})}}(\vec{\nabla} \times \vec{v}).$$

Proof. This follows from

$$\begin{split} & \mathcal{T}_{\vec{\mathcal{L}}}(\vec{v}) = \mathcal{P}_{E}(\Delta \vec{v}) - \star_{(F^{\star},E)} \mathcal{R}^{\star} \star_{(F,E^{\star})} \mathcal{R} \mathcal{P}_{E}(\vec{v}) \\ & = \mathcal{P}_{E}(\star \Delta \vec{v}) - \star_{(F^{\star},E)} \mathcal{P}_{F^{\star}}(\Delta \vec{v}) + \star_{(F^{\star},E)} \mathcal{P}_{F^{\star}}(\Delta \vec{v}) - \star_{(F^{\star},E)} \mathcal{R}^{\star} \star_{(F,E^{\star})} \mathcal{R} \mathcal{P}_{E}(\vec{v}) \\ & = \mathcal{T}_{\star_{(F^{\star},E)}}(\Delta \vec{v}) + \star_{(F^{\star},E)} \left(\mathcal{P}_{F^{\star}}(\vec{\nabla} \times \vec{\nabla} \times \vec{v}) - \mathcal{R}^{\star} \star_{(F,E^{\star})} \mathcal{R} \mathcal{P}_{E}(\vec{v}) \right) \\ & = \mathcal{T}_{\star_{(F^{\star},E)}}(\Delta \vec{v}) + \star_{(F^{\star},E)} \left(\mathcal{T}_{\mathcal{R}^{\star}}(\vec{\nabla} \times \vec{v}) + \mathcal{R}^{\star} \left(\mathcal{P}_{E^{\star}}(\vec{\nabla} \times \vec{v}) - \star_{(F,E^{\star})} \mathcal{R} \mathcal{P}_{E}(\vec{v}) \right) \right) \\ & = \mathcal{T}_{\star_{(F^{\star},E)}}(\Delta \vec{v}) + \star_{(F^{\star},E)} \left(\mathcal{T}_{\mathcal{R}^{\star}}(\vec{\nabla} \times \vec{v}) + \mathcal{R}^{\star} \left(\mathcal{T}_{\star_{(F,E^{\star})}}(\vec{\nabla} \times \vec{v}) + \star_{(F,E^{\star})} \mathcal{T}_{\mathcal{R}}(\vec{v}) \right) \right). \end{split}$$

D.5. Summary

The integral operators are exact by additivity of integration. The first order mimetic difference operators are exact. The truncation errors for the scalar and vector Laplacian only depend on the truncation error of the star operators; they are second order on uniform grids.

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