Adjoint Operators for the Natural Discretizations of the Divergence, Gradient, and Curl on Logically Rectangular Grids

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Abstract

We use the support-operator method to derive new discrete approximations of the divergence, gradient, and curl using discrete analogs of the integral identities satisfied by the differential operators. These new discrete operators are adjoint to the previously derived natural discrete operators defined using 'natural' coordinate-invariant definitions, such as Gauss' theorem for the divergence. The natural operators cannot be combined to construct discrete analogs of the second-order operators **div grad**, **grad div**, and **curl curl** because of incompatibilities in domains and in the ranges of values for the operators. The same is true for the adjoint operators. However, the adjoint operators have complementary domains and ranges of values and the combined set of natural and adjoint operators allow a consistent formulation for all the compound discrete operators. We also prove that the operators satisfy discrete analogs of the major theorems of vector analysis relating the differential operators, including $\mathbf{div}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{curl}\,\vec{B}$; $\mathbf{curl}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{grad}\varphi$.

Keywords: Finite-difference; Logically-rectangular grids; Discrete vector analysis.

1 Introduction

Discrete models that preserve the fundamental properties of their original continuum model for the underlying physical problem can be derived based on solid mathematical theory. These properties include conservation laws, symmetries in the solution, and the nondivergence of particular vector fields (i.e., they are divergence free).

We have developed a discrete analog of vector and tensor calculus that can be used to accurately approximate continuum models for a wide range of physical processes. This is the second in a series of papers that create the *discrete analog of vector analysis on logically rectangular, nonorthogonal, nonsmooth grids.*

In the first paper [6], we introduced the natural spaces of discrete scalar and vector functions. Discrete analogs of the divergence, gradient, and curl were constructed based on coordinate-invariant definitions. Discrete analogs of line, surface, and volume integrals were described. The first paper included proofs of the discrete theorems of vector analysis including Gauss' theorem; the theorem that $\mathbf{div}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{curl}\,\vec{B}$; $\mathbf{curl}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{grad}\varphi$; the theorem that if $\vec{A} = \mathbf{grad}\,\varphi$, then the line integral does not depend on path; and the theorem that if the line integral of a vector function is equal to zero for any closed path, then this vector is the gradient of a scalar function. We also introduced the primitive forward and backward difference operators and the primitive metric operators (related to multiplications of discrete functions by the lengths of edges, the areas of surfaces, and the volumes of 3-D cells).

The domains and ranges of the natural discrete operators defined in [6] arise "naturally" from discrete analogs of Stokes' theorem. To form second-order nontrivial combinations of these operators, which are discrete analogs of **div grad**, **grad div**, and **curl curl**, the range of the first operator must be equal to the domain of the second operator. The domains and ranges of the natural operators alone are not sufficient to form these compound operators. By constructing the adjoints to the natural discrete operators, we create additional discrete first-order operators with complementary domains and ranges. This extended set of discrete operators allows all possible combinations of the first-order operators to be formed in a consistent way. Furthermore, the new operators are defined to be compatible with their original discrete operators, so that discrete versions of the integral identities between the gradient, divergence, and curl are satisfied by construction.

We use *support-operator method* (SOM) [14, 15, 18, 16], to construct discrete operators with compatible domains and ranges on the basis of discrete analogs of the integral identities:

$$\int_V u \,\mathbf{div}\, \vec{W}\, dV + \int_V (\vec{W}, \mathbf{grad}\, u)\, dV = \oint_{\partial V} u\, (\vec{W}, \vec{n})\, dS\,, \tag{1.1}$$

$$\int_V (\vec{A}, \mathbf{curl}\vec{B})\, dV - \int_V (\vec{B}, \mathbf{curl}\vec{A})\, dV = \oint_{\partial V} (\vec{n}, \vec{A} \times \vec{B})\, dS\,, \tag{1.2}$$

where u is an arbitrary scalar function, $\vec{W}$, $\vec{A}$, and $\vec{B}$ are arbitrary vector functions defined on domain V with boundary ∂V, and $\vec{n}$ is the unit outward normal to ∂V. In the simplest case, when boundary integrals vanish, the above identities imply that $\mathbf{div} = -\mathbf{grad}^*$ and $\mathbf{curl} = \mathbf{curl}^*$, if we define inner products in spaces of scalar and vector functions as

$$(u, v)_H = \int_V u\, v\, dV\,, \quad \text{and} \quad (\vec{A}, \vec{B})_{\mathcal{H}} = \int_V (\vec{A}, \vec{B})\, dV\,.$$

The SOM uses the discrete versions of integral identities as the basis to construct discrete operators with compatible domains and ranges. In [6], the natural discrete divergence was defined as a discrete operator with domain $\mathcal{HS}$ and range HC,

$$\mathbf{DIV} : \mathcal{HS} \to HC\,,$$

where $\mathcal{HS}$ is the space of discrete vector functions defined by their orthogonal projections onto directions perpendicular to face of the cell, and HC is the space of discrete scalar functions given by their values in the cell (see [6] for details).

Following the SOM approach, to construct a new discrete gradient

$$\overline{\mathbf{GRAD}} : HC \to \mathcal{HS}\,,$$

we use the discrete analog of the identity 1.1 and operator **DIV** as the *prime operator*. The discrete gradient, *derived operator*, by construction is negative adjoint to **DIV**:

$$\overline{\mathbf{GRAD}} = -\mathbf{DIV}^*\,. \tag{1.3}$$

We indicate derived adjoint operators by the over-bar.

The natural discrete gradient **GRAD** was defined as a discrete operator with domain HN and range $\mathcal{HL}$,

$$\mathbf{GRAD} : HN \to \mathcal{HL}\,,$$

where $\mathcal{HL}$ is the space of discrete vector functions defined by their orthogonal projections onto directions of the edges of the cell, and HN is the space of discrete scalar functions given by their values in the nodes (see [6] for details).

To construct a new discrete divergence, we again use the discrete analog of the identity 1.1, but in this case **GRAD** is used as the prime operator; then

$$\overline{\mathbf{DIV}} : \mathcal{HL} \to HN$$

and

$$\overline{\mathbf{DIV}} = -\mathbf{GRAD}^*\,. \tag{1.4}$$

In a similar way, the natural **CURL** : $\mathcal{HL} \to \mathcal{HS}$ is used to construct another discrete curl, $\overline{\mathbf{CURL}} : \mathcal{HS} \to \mathcal{HL}$, and

$$\overline{\mathbf{CURL}} = \mathbf{CURL}^*\,. \tag{1.5}$$

We then prove that these adjoint operators satisfy the same discrete theorems of vector analysis as natural operators [6]. The proofs are reduced to theorems for simple differences by representing the derived adjoint operators in terms of primitive difference operators and metric operators.

Natural operators can be combined to construct only the *trivial* operators:

$$\mathbf{DIV}\,\mathbf{CURL} : \mathcal{HL} \to HC\,, \qquad \mathbf{DIV}\,\mathbf{CURL} \equiv 0\,, \tag{1.6}$$

$$\mathbf{CURL}\,\mathbf{GRAD} : HN \to \mathcal{HS}\,, \qquad \mathbf{CURL}\,\mathbf{GRAD} \equiv 0\,. \tag{1.7}$$

We cannot apply **DIV** to **GRAD** because the range of values for **GRAD** does not coincide with the domain of operator **DIV**, and so on.

Adjoint operators can also be combined to construct the *trivial* operators:

$$\overline{\mathbf{DIV}}\,\overline{\mathbf{CURL}} : \mathcal{HS} \to HN\,, \qquad \overline{\mathbf{DIV}}\,\overline{\mathbf{CURL}} \equiv 0\,, \tag{1.8}$$

$$\overline{\mathbf{CURL}}\,\overline{\mathbf{GRAD}} : HC \to \mathcal{HL}\,, \qquad \overline{\mathbf{CURL}}\,\overline{\mathbf{GRAD}} \equiv 0\,. \tag{1.9}$$

Natural operators and adjoints to them can be combined to form the *nontrivial* second-order operators:

$$\mathbf{DIV}\,\overline{\mathbf{GRAD}} : HC \to HC\,, \qquad \overline{\mathbf{DIV}}\,\mathbf{GRAD} : HN \to HN\,, \tag{1.10}$$

$$\mathbf{CURL}\,\overline{\mathbf{CURL}} : \mathcal{HS} \to \mathcal{HS}\,, \qquad \overline{\mathbf{CURL}}\,\mathbf{CURL} : \mathcal{HL} \to \mathcal{HL}\,, \tag{1.11}$$

$$\mathbf{GRAD}\,\overline{\mathbf{DIV}} : \mathcal{HL} \to \mathcal{HL}\,, \qquad \overline{\mathbf{GRAD}}\,\mathbf{DIV} : \mathcal{HS} \to \mathcal{HS}\,. \tag{1.12}$$

Using constructed first- and second-order discrete operators we can construct mimetic finite-difference methods for most of the partial differential equations arising in mathematical physics [1, 2, 3, 4, 5, 9, 8, 18, 17]. The resulting formulas for all first-order discrete operators on tensor product, rectangular grids are listed in Appendix.

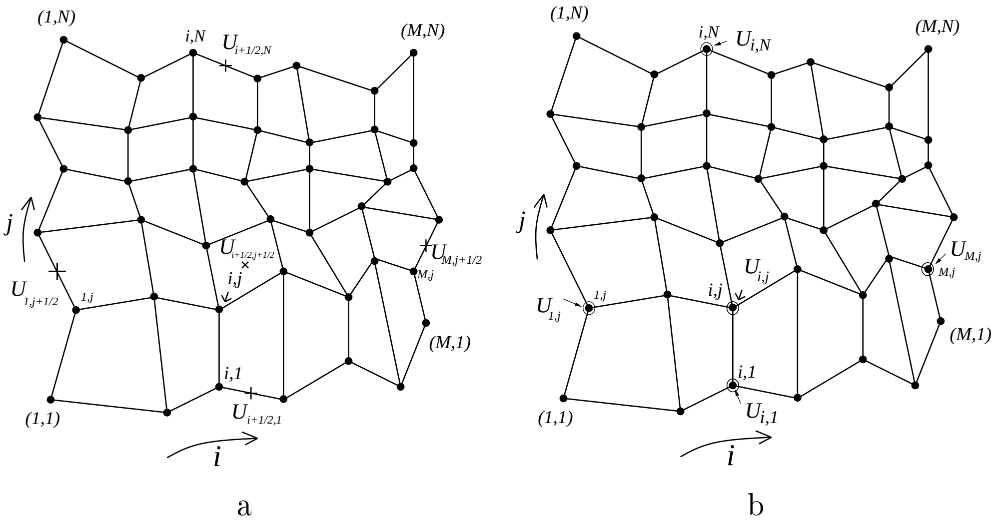


Figure 2.1: On a logically rectangular grid, the scalar function values can be either cell-centered (HC), as in (a), or defined at the nodes (HN), as in (b).

2 Grids and Discrete Functions

2.1 Grid

We index the nodes of a logically rectangular grid using (i, j), where $1 \leq i \leq M$ and $1 \leq j \leq N$ (see Figure 2.1). The quadrilateral defined by the nodes (i, j), $(i + 1, j)$, $(i + 1, j + 1)$, and $(i, j + 1)$ is called the $(i + 1/2, j + 1/2)$ cell [see Figure 2.2 a)]. The area of the $(i+1/2, j+1/2)$ cell is denoted by $VC_{i+1/2,j+1/2}$, the length of the side that connects the vertices (i, j) and $(i, j + 1)$ is denoted $S\xi_{i,j+1/2}$, and the length of the side that connects the vertices (i, j) and $(i + 1, j)$ is denoted $S\eta_{i+1/2,j}$. The angle between any two adjacent sides of cell $(i + 1/2, j + 1/2)$ that meet at node (k, l) is denoted $\varphi_{k,l}^{i+1/2,j+1/2}$.

When we determine discrete differential operators, such as **CURL**, it is useful to consider a 2-D grid as a projection of a 3-D grid. This approach makes it is easier to later generalize finite-difference method to three dimensions and simplifies the notation. In this paper we consider functions of the coordinates x and y and extend the grid into a third dimension, z, when convenient. The extended 3-D mesh is constructed by extending a grid line of unit length into the z direction to form a prism with unit height and with a 2-D quadrilateral cell as its base [see Figure 2.2 b)].

Sometimes it is useful to interpret the grid as being formed by intersections of broken lines that approximate the coordinate curves of some underlying curvilinear coordinate system (ξ, η, ζ). The ξ coordinate corresponds to the grid line where the index i is changing, the η coordinate corresponds to the grid line where the index j is changing, and the ζ coordinate

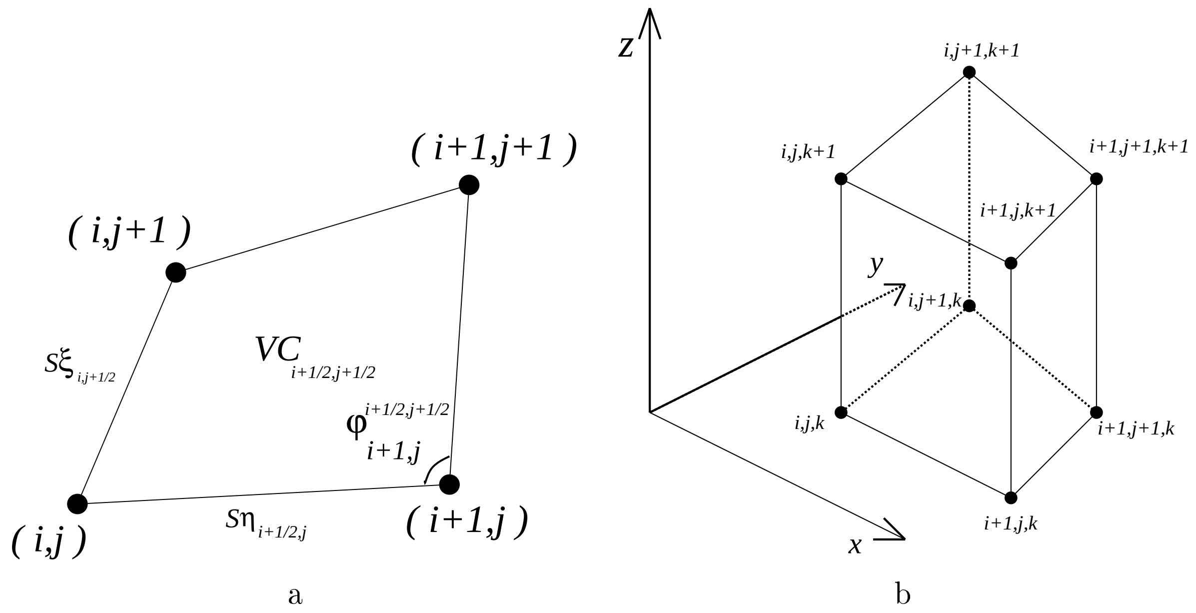


Figure 2.2: (a) The $(i+1/2, j+1/2)$ cell in a logically rectangular grid has area $VC_{i+1/2,j+1/2}$ and sides $S\xi_{i,j+1/2}$, $S\eta_{i+1/2,j}$, $S\xi_{i+1,j+1/2}$, and $S\eta_{i+1/2,j+1}$. The interior angle between $S\eta_{i+1/2,j}$ and $S\xi_{i+1,j+1/2}$ is $\varphi_{i+1,j}^{i+1/2,j+1/2}$. (b) The 2-D $(i+1/2, j+1/2)$ cell ($z = 0$) is interpreted as the base of a 3-D logically cuboid $(i+1/2, j+1/2, k+1/2)$ cell (a prism) with unit height.

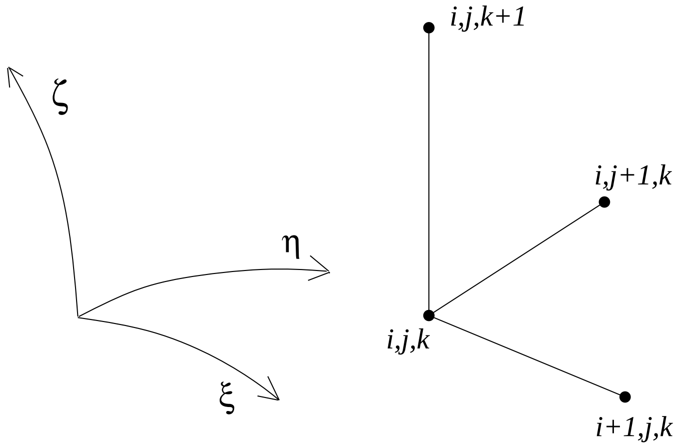


Figure 2.3: The (ξ, η, ζ) curvilinear coordinate system is approximated by the i, j, and k piecewise linear grid lines.

corresponds to the grid line where the index k is changing (i.e., height of the prism; see Figure 2.3).

We denote the length of the edge $(i,j,k)-(i+1,j,k)$ by $l\xi_{i+1/2,j,k}$, the length of the edge $(i,j,k)-(i,j+1,k)$ by $l\eta_{i,j+1/2,k}$, and the length of the edge $(i,j,k)-(i,j,k+1)$ by $l\zeta_{i,j,k+1/2}$ (which we have chosen to be equal to 1). The area of the surface $(i,j,k)-(i,j+1,k)-(i,j,k+1)-(i,j+1,k+1)$ is denoted by $S\xi_{i,j+1/2,k+1/2}$ because it is the analog of the element of the coordinate surface $dS\xi$. Similarly, the area of surface $(i,j,k)-(i+1,j,k)-(i,j,k+1)-(i+1,j,k+1)$ is denoted by $S\eta_{i+1/2,j,k+1/2}$. We use the notation $S\zeta_{i+1/2,j+1/2,k}$ for the area of the 2-D cell $(i+1/2, j+1/2)$, that is, $S\zeta_{i+1/2,j+1/2,k} = VC_{i+1/2,j+1/2}$. Because the artificially constructed 3-D cell is a right prism with unit height, we have

$$S\xi_{i,j+1/2,k+1/2} = l\eta_{i,j+1/2,k} \cdot l\zeta_{i,j,k+1/2} = l\eta_{i,j+1/2,k} \tag{2.1}$$

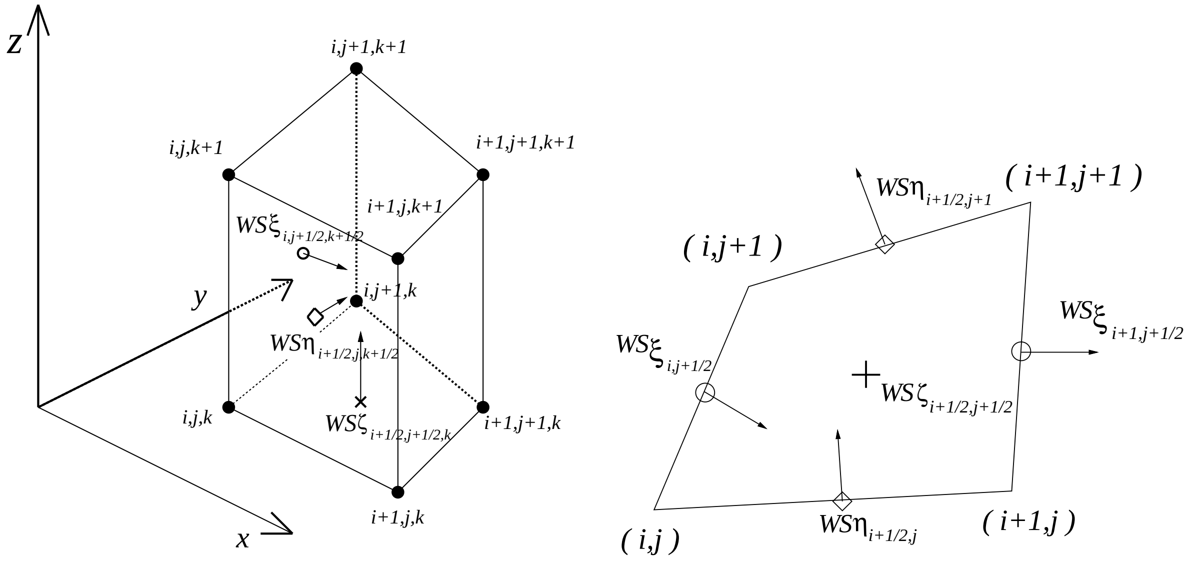
and

$$S\eta_{i+1/2,j,k+1/2} = l\xi_{i+1/2,j,k} \cdot l\zeta_{i,j,k+1/2} = l\xi_{i+1/2,j,k}\,. \tag{2.2}$$

With this 3-D interpretation, the 2-D notations $S\xi_{i,j+1/2}$ and $S\eta_{i+1/2,j}$ are not ambiguous because the 3-D surface $(i,j,k),(i,j+1,k),(i,j,k+1),(i,j+1,k+1)$ corresponds to an element of the coordinate surface $S\xi$; and, since the prism has unit height, the length of the side $(i,j)-(i,j+1)$ is equal to the area of the element of this coordinate surface.

2.2 Discrete Scalar Functions

In a cell-centered discretization, the discrete scalar function $U_{i+1/2,j+1/2}$ is defined in the space HC and is given by its values in the cells [see Figure 2.1 (a)], except at the boundary cells. The treatment of the boundary conditions requires introducing scalar function values



a b

Figure 2.4: (a) $\mathcal{HS}$ discretization of a vector in three dimensions; (b) 2-D interpretation of the $\mathcal{HS}$ discretization of a vector.

at the centers of the boundary segments: $U_{(1,j+1/2)}$, $U_{(M,j+1/2)}$, where $j = 1, \ldots, N-1$, and $U_{(i+1/2,0)}$, $U_{(i+1/2,N)}$, where $i = 1, \ldots, M-1$. In three dimensions, the cell-centered scalar functions are defined in the centers of the 3-D prisms, except in the boundary cells where they are defined on the boundary faces. The 2-D case can be considered a projection of these values onto the 2-D cells and midpoints of the boundary segments.

In a nodal discretization, the discrete scalar function $U_{i,j}$ is defined in the space HN and is given by its values in the nodes [see Figure 2.1 (b)]. The indices vary in the same range as for coordinates $x_{i,j}$, $y_{i,j}$.

2.3 Discrete Vector Functions

We assume that vectors may have three components, but in our 2-D analysis, the components depend on only two spatial coordinates, x and y. We consider two different spaces of discrete vector functions for our 3-D coordinate system. The $\mathcal{HS}$ space [see Figure 2.4 (a)], where the vector components are defined perpendicular to the cell faces, is the natural space when the approximations are based on Gauss' divergence theorem. The $\mathcal{HL}$ space [see Figure 2.5 (a)], where the vectors are defined tangential to the cell edges, is natural for approximations based on Stokes' circulation theorem.

The projection of the 3-D $\mathcal{HS}$ vector discretization space into two dimensions results in the vectors being defined perpendicular to the quadrilateral cell sides and in a vertical vector

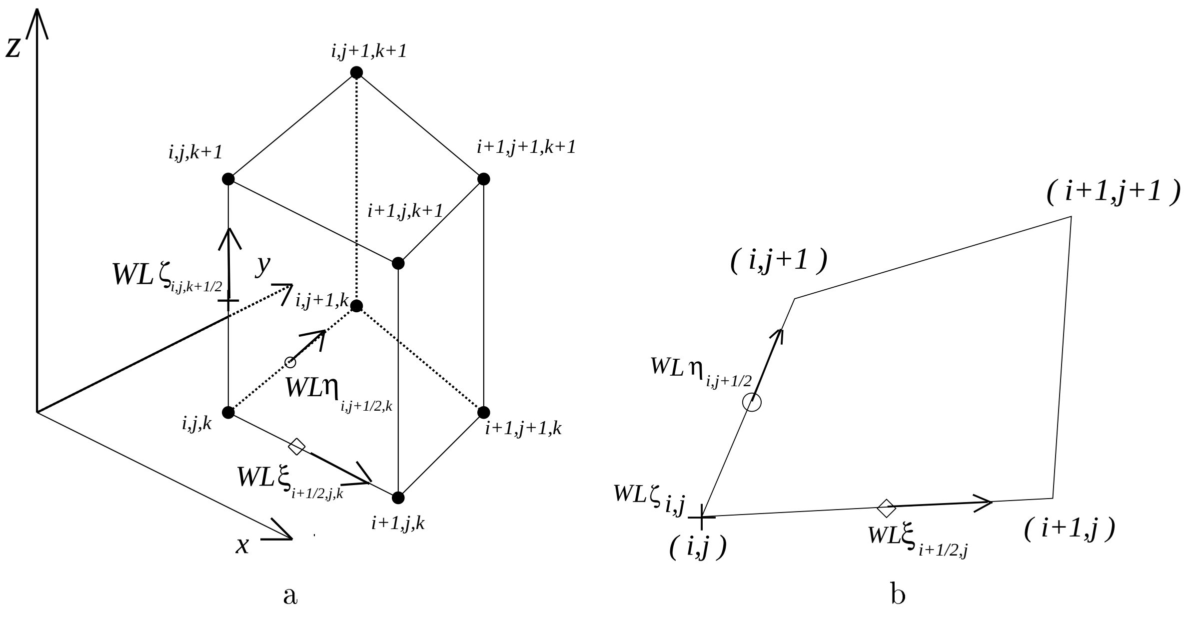


Figure 2.5: (a) $\mathcal{HL}$ discretization of a vector in three dimensions (b) 2-D interpretation of the $\mathcal{HL}$ discretization of a vector.

in the cell center [see Figure 2.4 (b)]. We use the notation

$$WS\xi_{(i,j+1/2)} \; : i = 1, \ldots, M \, ; \, j = 1, \ldots, N-1$$

for the vector component at the center of face $S\xi_{(i,j+1/2)}$ (side $l\eta_{(i,j+1/2)}$); the notation

$$WS\eta_{(i+1/2,j)} \; : i = 1, \ldots, M-1 \, ; \, j = 1, \ldots, N$$

for the vector component at the center of face $S\eta_{(i+1/2,j)}$ (side $l\xi_{(i+1/2,j)}$); and the notation

$$WS\zeta_{(i+1/2,j+1/2)} \; : i = 1, \ldots, M-1 \, ; \, j = 1, \ldots, N-1$$

for the component at the center of face $S\zeta_{(i+1/2,j+1/2)}$ (2-D cell $V_{i+1/2,j+1/2}$).

The projection of the 3-D $\mathcal{HL}$ vector discretization space into two dimensions results in the vectors being defined as tangential to the quadrilateral cell sides and in a vertical vector at the nodes [see Figure 2.5 (b)]. We use the notation

$$WL\xi_{(i+1/2,j)} \; : i = 1, \ldots, M-1 \, ; \, j = 1, \ldots, N$$

for the component at the center of edge $l\xi_{(i+1/2,j)}$ [in 2-D, the same position as for $WS\eta_{(i+1/2,j)}$]; the notation

$$WL\eta_{(i,j+1/2)} \; : i = 1, \ldots, M \, ; \, j = 1, \ldots, N-1$$

for the component at the center of edge $l\eta_{(i,j+1/2)}$ [in 2-D, the same position as for $WS\xi_{(i,j+1/2)}$]; and the notation

$$WL\zeta_{(i,j)} \,:\, i = 1, \ldots, M \,;\; j = 1, \ldots, N$$

for the component at the center of edge $l\zeta_{(i,j)}$ [in 2-D the position that corresponds to node (i,j)].

From here on, there will not be any dependence on the k index, and it is dropped from the notations.

3 Support-Operator Method

We use the SOM [16] to derive operators $\overline{\mathbf{DIV}}$, $\overline{\mathbf{GRAD}}$, and $\overline{\mathbf{CURL}}$ from discrete analogs of the integral identities 1.1 and 1.2. These identities connect the differential operators **div**, **grad**, and **curl** and allow us to obtain their discrete analogs with consistent domains and ranges of values.

In the SOM, first a discrete approximation is defined for a first-order differential operator, such as the divergence or gradient, that satisfies the appropriate discrete analog of an integral identity, such as Stokes' theorem. This initial discrete operator, called the *prime* operator, then *supports* the construction of other discrete operators, using discrete formulations of the integral identities 1.1 or 1.2 . For example, if the initial discretization is defined for the divergence (*prime operator*), it should satisfy a discrete form of Gauss' theorem. This prime discrete divergence, **DIV** is then used to *support* the *derived* discrete operator $\overline{\mathbf{GRAD}}$ satisfying a discrete version of the integral identity 1.1. The derived operator $\overline{\mathbf{GRAD}}$ would then also be the negative adjoint of **DIV**.

We first consider identity 1.1 and introduce the space of scalar functions H with the inner product:

$$(u,\, v)_H = \int_V u\, v\, dV + \oint_{\partial V} u\, v\, dS\,, \quad u, v \in H\,. \tag{3.1}$$

We also introduce the space of vector functions $\mathbf{H}$ so that if two vector functions $\vec{A}, \vec{B} \in \mathbf{H}$, their inner product is defined as

$$(\vec{A},\, \vec{B})_{\mathbf{H}} = \int_V (\vec{A},\, \vec{B})\, dV\,. \tag{3.2}$$

To extend the operator **div** to the boundary, we define the extended divergence operator

$$\mathbf{d} : \mathbf{H} \rightarrow H$$

as

$$\mathbf{d}\vec{w} = \begin{cases} +\mathbf{div}\, \vec{w}\,, & (x,y) \in V \\ -(\vec{w}, \vec{n})\,, & (x,y) \in \partial V \end{cases}\,. \tag{3.3}$$

Identity 1.1 can be used to prove

$$\mathbf{d} = -\mathbf{grad}^*\,; \tag{3.4}$$

namely,

$$
\begin{aligned}
(\mathbf{d}\,\vec{w},\,u)_H &= \int_V u\,\mathbf{div}\,\vec{w}\,dV - \oint_{\partial V} u\,(\vec{w},\,\vec{n})\,dS \\
&= -\int_V (\vec{w},\,\mathbf{grad} u)\,dV \\
&= (\vec{w},\,-\mathbf{grad}\,u)_{\mathbf{H}}\,.
\end{aligned}
\tag{3.5}
$$

We will establish a similar relationship for operator **curl** when we consider construction of operator $\overline{\mathbf{CURL}}$.

4 Derived Adjoint Operators

4.1 Operator $\overline{\mathbf{GRAD}}$

To derive the discrete operator

$$
\overline{\mathbf{GRAD}} : HC \rightarrow \mathcal{HS}\,,
\tag{4.1}
$$

we must first define the inner products in spaces HC and $\mathcal{HS}$ and extend the operator **DIV** to the boundary.

4.1.1 Extension of Operator DIV to the Boundary: Operator D

To determine the discrete analog of operator **d**, we note that in the interior of the region, the prime operator **D**, which is the analog of the divergence, is given in [6] as

$$
\begin{aligned}
&(\mathbf{D}\,\vec{W})_{(i+1/2,j+1/2)} = (\mathbf{DIV}\,\vec{W})_{(i+1/2,j+1/2)} = \\
&\quad \Big\{ \Big(WS\xi_{(i+1,j+1/2)}\,S\xi_{(i+1,j+1/2)} - WS\xi_{(i,j+1/2)}\,S\xi_{(i,j+1/2)} \Big) + \\
&\quad \Big(WS\eta_{(i+1/2,j+1)}\,S\eta_{(i+1/2,j+1)} - WS\eta_{(i+1/2,j)}\,S\eta_{(i+1/2,j)} \Big) \Big\} \Big/ VC_{(i+1/2,j+1/2)}\,.
\end{aligned}
\tag{4.2}
$$

On the boundary, where, in correspondence with definition 3.3, the operator **d** gives the normal component of the vector, we define the operator **D** as

$$
\begin{aligned}
(\mathbf{D}\,\vec{W})_{(i+1/2,1)} &= -WS\eta_{(i+1/2,1)}\,, \quad i = 1, \cdots, M-1\,, \\
(\mathbf{D}\,\vec{W})_{(i+1/2,N)} &= +WS\eta_{(i+1/2,N)}\,, \quad i = 1, \cdots, M-1\,, \\
(\mathbf{D}\,\vec{W})_{(1,j+1/2)} &= -WS\xi_{(1,j+1/2)}\,, \quad j = 1, \cdots, N-1\,, \\
(\mathbf{D}\,\vec{W})_{(M,j+1/2)} &= +WS\xi_{(M,j+1/2)}\,, \quad j = 1, \cdots, N-1\,.
\end{aligned}
\tag{4.3}
$$

If we introduce generalized operators of central differencing as

$$
(\delta_\xi\, U)_{\alpha,\beta} = U_{\alpha+1/2,\beta} - U_{\alpha-1/2,\beta}\,, \quad (\delta_\eta\, U)_{\alpha,\beta} = U_{\alpha,\beta+1/2} - U_{\alpha,\beta-1/2}\,,
\tag{4.4}
$$

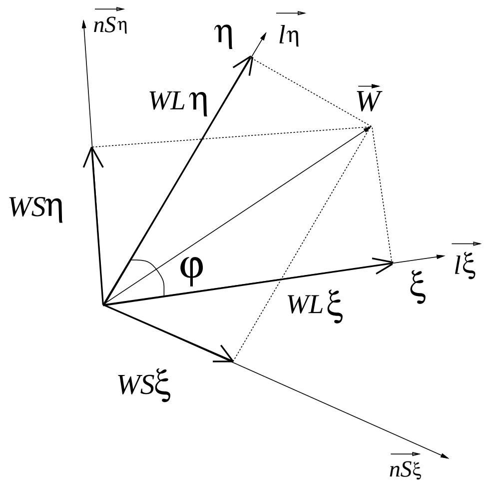


Figure 4.1: The grid lines (ξ, η) form a local nonorthogonal coordinate system with unit vectors $\vec{l\xi}$, $\vec{l\eta}$ and corresponding unit normals to these directions, $n\vec{S}\xi$ and $n\vec{S}\eta$. In this basis, the components ($WL\xi$, $WL\eta$) of vector $\vec{W}$ are the orthogonal projections onto grid lines, and components ($WS\xi$, $WS\eta$) are orthogonal projections to normal directions.

where α and β can be integer or half indicies, then equation 4.2 can be presented in compact form

$$
\begin{aligned}
&(\mathbf{D}\,\vec{W})_{(i+1/2,j+1/2)} = (\mathbf{DIV}\,\vec{W})_{(i+1/2,j+1/2)} = \\
&\quad \frac{[\delta_\xi\,(WS\xi\,S\xi)]_{(i+1/2,j+1/2)} + [\delta_\eta\,(WS\eta\,S\eta)]_{(i+1/2,j+1/2)}}{VC_{(i+1/2,j+1/2)}}\,.
\end{aligned} \tag{4.5}
$$

4.1.2 Spaces of Discrete Functions

In the space of discrete scalar functions, HC, (functions defined in the cell centers), the *natural* inner product corresponding to the continuous inner product 3.1 is

$$
\begin{aligned}
(U,V)_{HC} &= \sum_{i=1}^{M-1}\sum_{j=1}^{N-1} U_{(i+1/2,j+1/2)}\,V_{(i+1/2,j+1/2)}\,VC_{(i+1/2,j+1/2)} \\
&+ \sum_{i=1}^{M-1} U_{(i+1/2,1)}\,V_{(i+1/2,1)}\,S\eta_{(i+1/2,1)} + \sum_{j=1}^{N-1} U_{(M,j+1/2)}\,V_{(M,j+1/2)}\,S\xi_{(M,j+1/2)} \\
&+ \sum_{i=1}^{M-1} U_{(i+1/2,N)}\,V_{(i+1/2,N)}\,S\eta_{(i+1/2,N)} + \sum_{j=1}^{N-1} U_{(1,j+1/2)}\,V_{(1,j+1/2)}\,S\xi_{(1,j+1/2)}\,.
\end{aligned} \tag{4.6}
$$

In the space of vector functions $\mathcal{HS}$, the *natural* inner product corresponding to the continuous inner product 3.2 is

$$(\vec{A},\vec{B})_{\mathcal{HS}} = \sum_{i=1}^{M-1}\sum_{j=1}^{N-1}(\vec{A},\vec{B})_{(i+1/2,j+1/2)}\,VC_{(i+1/2,j+1/2)}\,, \tag{4.7}$$

where $(\vec{A},\vec{B})$ is the dot product of two vectors. Next, we define this dot product in terms of the components of the vectors perpendicular to the cell sides (see Figure 4.1). Suppose that the axes ξ and η form a nonorthogonal basis and that φ is the angle between these axes. If the unit normals to the axes are $n\vec{S}\xi$ and $n\vec{S}\eta$, then the components of the vector $\vec{W}$ in this basis are the orthogonal projections $WS\xi$ and $WS\eta$ of $\vec{W}$ onto the normal vectors (see the discussion in Chapter 2 of [10] for more details). The expression for the dot product of $\vec{A}=(AS\xi, AS\eta)$ and $\vec{B}=(BS\xi, BS\eta)$, is

$$(\vec{A},\vec{B}) = \frac{AS\xi\,BS\xi + AS\eta\,BS\eta + (AS\xi\,BS\eta + AS\eta\,BS\xi)\,\cos\varphi}{\sin^2\varphi}\,. \tag{4.8}$$

From this expression, the dot product in the cell is approximated by

$$\begin{aligned}
&(\vec{A},\vec{B})_{(i+1/2,j+1/2)} = \\
&\quad\sum_{k,l=0}^{1}\frac{V_{(i+k,j+l)}^{(i+1/2,j+1/2)}}{\sin^2\varphi_{(i+k,j+l)}^{(i+1/2,j+1/2)}} \\
&\quad\cdot\Big[AS\xi_{(i+k,j+1/2)}\,BS\xi_{(i+k,j+1/2)} + AS\eta_{(i+1/2,j+l)}\,BS\eta_{(i+1/2,j+l)} \\
&\quad+(-1)^{k+l}\,\Big(AS\xi_{(i+k,j+1/2)}\,BS\eta_{(i+1/2,j+l)}+ \\
&\quad AS\eta_{(i+1/2,j+l)}\,BS\xi_{(i+k,j+1/2)}\Big)\cos\varphi_{(i+k,j+l)}^{(i+1/2,j+1/2)}\Big]\,,
\end{aligned} \tag{4.9}$$

where $V_{(i+k,j+l)}^{(i+1/2,j+1/2)}$ are some weights that satisfy

$$V_{(i+k,j+l)}^{(i+1/2,j+1/2)} \geq 0\,, \qquad \sum_{k,l=0}^{1} V_{(i+k,j+l)}^{(i+1/2,j+1/2)} = 1\,. \tag{4.10}$$

In this formula, each index (k,l) corresponds to one of the vertices of the $(i+1/2, j+1/2)$ cell, and notations for weights are the same as for angles of cell.

When computing the adjoint relationships between the discrete operators, it is helpful to introduce the *formal* inner products, (to denote which we will use square brackets $[\cdot,\cdot]$), in the spaces of scalar and vector functions. In HC, the formal inner product is

$$\begin{aligned}
[U,V]_{HC} &= \sum_{i=1}^{M-1}\sum_{j=1}^{N-1} U_{(i+1/2,j+1/2)}\,V_{(i+1/2,j+1/2)} + \sum_{i=1}^{M-1} U_{(i+1/2,1)}\,V_{(i+1/2,1)} \\
&+ \sum_{j=1}^{N-1} U_{(M,j+1/2)}\,V_{(M,j+1/2)} + \sum_{i=1}^{M-1} U_{(i+1/2,N)}\,V_{(i+1/2,N)} + \sum_{j=1}^{N-1} U_{(1,j+1/2)}\,V_{(1,j+1/2)}\,;
\end{aligned} \tag{4.11}$$

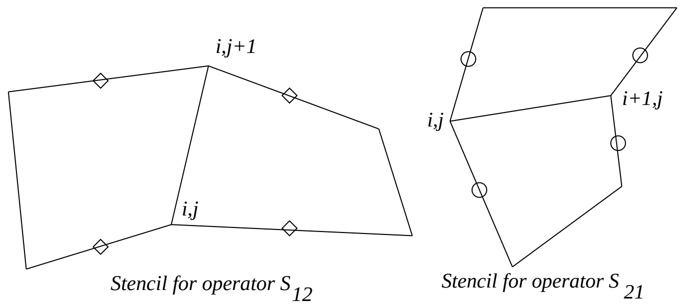


Figure 4.2: The stencils of the components S_{12} and S_{21} of the symmetric positive operator $\mathcal{S}$ that connects the natural and formal inner products $(\vec{A}, \vec{B})_{\mathcal{HS}} = [\mathcal{S}\,\vec{A}, \vec{B}]_{\mathcal{HS}}$.

in $\mathcal{HS}$, the formal inner product is

$$[\vec{A}, \vec{B}]_{\mathcal{HS}} = \sum_{i=1}^{M} \sum_{j=1}^{N-1} AS\xi_{(i,j+1/2)}\, BS\xi_{(i,j+1/2)} + \sum_{i=1}^{M-1} \sum_{j=1}^{N} AS\eta_{(i+1/2,j)}\, BS\eta_{(i+1/2,j)}\,. \tag{4.12}$$

The natural and formal inner products satisfy the relationships

$$(U, V)_{HC} = [\mathcal{C}\,U,\, V]_{HC}\,, \quad \text{and} \quad (\vec{A}, \vec{B})_{\mathcal{HS}} = [\mathcal{S}\,\vec{A},\, \vec{B}]_{\mathcal{HS}}\,, \tag{4.13}$$

where $\mathcal{C}$ and $\mathcal{S}$ are symmetric positive operators in the formal inner products. For operator $\mathcal{C}$ we have

$$[\mathcal{C}\,U, V]_{HC} = [U, \mathcal{C}\,V]_{HC}\,, \quad \text{and} \quad [\mathcal{C}\,U, U]_{HC} > 0\,. \tag{4.14}$$

A comparison of the natural and formal inner products gives

$$\begin{aligned}
(\mathcal{C}\,U)_{(i+1/2,j+1/2)} &= VC_{(i+1/2,j+1/2)}\, U_{(i+1/2,j+1/2)}\,, \quad i = 1, \cdots, M-1\,; \quad j = 1, \cdots, N-1\,, \\
(\mathcal{C}\,U)_{(i,j+1/2)} &= S\xi_{(i,j+1/2)}\, U_{(i,j+1/2)}\,, \quad i = 1 \text{ and } i = M\,; \quad j = 1, \cdots, N-1\,, \\
(\mathcal{C}\,U)_{(i+1/2,j)} &= S\eta_{(i+1/2,j)}\, U_{(i+1/2,j)}\,, \quad i = 1, \cdots, M-1\,; \quad j = 1 \text{ and } j = N\,.
\end{aligned} \tag{4.15}$$

The operator $\mathcal{S}$ can be written in block form:

$$\mathcal{S}\,\vec{A} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} AS\xi \\ AS\eta \end{pmatrix} = \begin{pmatrix} S_{11}\, AS\xi + S_{12}\, AS\eta \\ S_{21}\, AS\xi + S_{22}\, AS\eta \end{pmatrix}. \tag{4.16}$$

This operator is symmetric and positive in the formal inner product:

$$[\mathcal{S}\,\vec{A}, \vec{B}]_{\mathcal{HS}} = [\vec{A}, \mathcal{S}\,\vec{B}]_{\mathcal{HS}}\,, \quad [\mathcal{S}\,\vec{A}, \vec{A}]_{\mathcal{HS}} > 0\,. \tag{4.17}$$

By comparing the formal and natural inner products,

$$\begin{aligned}
(\vec{A}, \vec{B})_{\mathcal{HS}} &= [\mathcal{S}\,\vec{A}, \vec{B}]_{\mathcal{HS}} = \sum_{i=1}^{M} \sum_{j=1}^{N-1} [(S_{11}\, AS\xi)_{(i,j+1/2)} + (S_{12}\, AS\eta)_{(i,j+1/2)}]\, BS\xi_{(i,j+1/2)} \\
&+ \sum_{i=1}^{M-1} \sum_{j=1}^{N} [(S_{21}\, AS\xi)_{(i+1/2,j)} + (S_{22}\, AS\eta)_{(i+1/2,j)}]\, BS\eta_{(i+1/2,j)}\,,
\end{aligned} \tag{4.18}$$

we can derive the formulas for operator $\mathcal{S}$:

$$
\begin{aligned}
(S_{11}\,AS\xi)_{(i,j+1/2)} &= \left(\sum_{k,l=0}^{1} \frac{V_{(i,j+l)}^{(i-k/2,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i-k/2,j+1/2)}}\right) AS\xi_{(i,j+1/2)}\,, \\
(S_{12}\,AS\eta)_{(i,j+1/2)} &= \sum_{k,l=0}^{1} (-1)^{k+l}\, \frac{V_{(i,j+l)}^{(i-k/2,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i-k/2,j+1/2)}}\, \cos\varphi_{(i,j+l)}^{(i-k/2,j+1/2)}\; AS\eta_{(i-k/2,j+l)}\,, \\
(S_{21}\,AS\xi)_{(i+1/2,j)} &= \sum_{k,l=0}^{1} (-1)^{k+l}\, \frac{V_{(i+l,j)}^{(i+1/2,j-k/2)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j-k/2)}}\, \cos\varphi_{(i+l,j)}^{(i+1/2,j-k/2)}\, AS\xi_{(i+l,j-k/2)}\,, \\
(S_{22}\,AS\eta)_{(i+1/2,j)} &= \left(\sum_{k,l=0}^{1} \frac{V_{(i+l,j)}^{(i+1/2,j-k/2)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j-k/2)}}\right) AS\eta_{(i+1/2,j)}\,.
\end{aligned}
\tag{4.19}
$$

These formulas are valid only for sides of the grid cells interior to the domain; however, they can be extended to the boundary sides if the grid and discrete functions are first extended to a row of points outside the domain by using the appropriate boundary conditions. The operators S_{11} and S_{22} are diagonal, and the stencils for the operators S_{12} and S_{21} are shown on Figure 4.2.

4.1.3 Construction of Operator $\overline{\mathbf{GRAD}}$

The derived gradient operator is defined by $\overline{\mathbf{GRAD}} \stackrel{def}{=} -\mathbf{D}^*$, where the adjoint is taken in the natural inner products (from here on, we will use notation $\stackrel{def}{=}$, when we define a new object). Recall that $\mathbf{D} : \mathcal{HS} \to HC$. The definition of the adjoint gives

$$
(\mathbf{D}\,\vec{W}, U)_{HC} = (\vec{W}, \mathbf{D}^* U)_{\mathcal{HS}}\,, \tag{4.20}
$$

which can be translated to the formal inner products as

$$
[\mathbf{D}\,\vec{W}, \mathcal{C}\,U]_{HC} = [\vec{W}, \mathcal{S}\,\mathbf{D}^* U]_{\mathcal{HS}}\,. \tag{4.21}
$$

The formal adjoint $\mathbf{D}^\dagger$ of $\mathbf{D}$ is defined to be the adjoint in the formal inner product,

$$
[\vec{W}, \mathbf{D}^\dagger\,\mathcal{C}\,U]_{\mathcal{HS}} = [\vec{W}, \mathcal{S}\,\mathbf{D}^* U]_{\mathcal{HS}}\,. \tag{4.22}
$$

This relationship must be true for all $\vec{W}$ and U, so $\mathbf{D}^\dagger\,\mathcal{C} = \mathcal{S}\,\mathbf{D}^*$ or $\mathbf{D}^* = \mathcal{S}^{-1}\,\mathbf{D}^\dagger\,\mathcal{C}$, and the discrete analog of operator **grad** is given by

$$
\overline{\mathbf{GRAD}} = -\mathbf{D}^* = -\mathcal{S}^{-1}\,\mathbf{D}^\dagger\,\mathcal{C}\,. \tag{4.23}
$$

Therefore for a general nonorthogonal, logically rectangular grid, it is not possible to write explicit formulas for the components of the operator $\overline{\mathbf{GRAD}}$ because the operator $\mathcal{S}$ is banded and consequently $\mathcal{S}^{-1}$ is full, that is, $\overline{\mathbf{GRAD}}$ has a *nonlocal* stencil.

The discrete flux,

$$\vec{W} = -\overline{\mathbf{GRAD}}\, U = \mathcal{S}^{-1}\, \mathbf{D}^{\dagger}\, \mathcal{C}\, U\,,$$

is obtained by solving the banded linear system (recall that $\mathcal{C}$, $\mathcal{S}$, and $\mathbf{D}$ are local operators)

$$\mathcal{S}\,\vec{W} = \mathbf{D}^{\dagger}\, \mathcal{C}\, U\,, \tag{4.24}$$

where the right-hand side is defined by $\mathbf{D}^{\dagger}\, \mathcal{C}$, which is

$$-\begin{pmatrix} S\xi_{i,j+1/2}\ (\delta_\xi\, U)_{i,j+1/2} \\ S\eta_{i+1/2,j}\ (\delta_\eta\, U)_{i+1/2,j} \end{pmatrix}. \tag{4.25}$$

Similar systems arise in defining the flux in finite element methods, HODIE (High Order Differences with Identity Expansion) methods [13], and other *compact* finite-difference schemes [11, 12]. The discrete operator $\mathcal{S}$ is symmetric positive definite, which matrix has five nonzero elements in each row (see, equation 4.19 and Figure 4.2).

4.2 Operator $\overline{\mathbf{DIV}}$

The operator $\overline{\mathbf{DIV}}$ is defined as the negative adjoint to the natural operator **GRAD**. The **div** and **grad** satisfy the integral identity 1.1:

$$\int_V (\vec{W}, \mathbf{grad}\ u)\, dV = -\int_V u\, \mathbf{div}\, \vec{W}\, dV + \oint_{\partial V} u\, (\vec{W}, \vec{n})\, dS\,. \tag{4.26}$$

In the subspace of scalar functions, $\overset{0}{H}$, where $u(x,y) = 0\,, (x,y) \in \partial V$, the boundary term is zero, and therefore

$$\int_V (\vec{W}, \mathbf{grad}\ u)\, dV = -\int_V u\, \mathbf{div}\, \vec{W}\, dV\,, \tag{4.27}$$

(use of the notation of "zero" above the name of the space indicates that values of corresponding functions are equal to zero on the boundary). That is, in this subspace **div** is the negative adjoint of **grad** in the sense of

$$(u, v)_{\overset{0}{H}} = \int_V u\, v\, dV\,, \quad \text{and} \quad (\vec{A}, \vec{B})_{\mathcal{H}} = \int_V (\vec{A}, \vec{B})\, dV\,. \tag{4.28}$$

To mimic the continuous case, we define the space of discrete scalar functions $\overset{0}{HN}$ as

$$\overset{0}{HN} \overset{def}{=} \{U \in HN, U_{i,j} = 0 \text{ on the boundary}\}$$

with the inner product defined as

$$(U, V)_{\overset{0}{HN}} \overset{def}{=} \sum_{i=2}^{M-1} \sum_{j=2}^{N-1} U_{(i,j)}\, V_{(i,j)}\, VN_{(i,j)}\,, \tag{4.29}$$

where $VN_{(i,j)}$ is the nodal volume. The relationship between the natural and formal inner products in $\overset{0}{HN}$ is

$$(U,V)_{\overset{0}{HN}} = [\mathcal{N}\,U,\,V]_{\overset{0}{HN}}\,, \tag{4.30}$$

where $\mathcal{N}$ is the symmetric positive operator in the formal inner product,

$$[\mathcal{N}\,U,V]_{HN} = [U,\mathcal{N}\,V]_{HN}\,, \quad [\mathcal{N}\,U,U]_{HN} > 0\,, \tag{4.31}$$

and

$$(\mathcal{N}\,U)_{(i,j)} = VN_{(i,j)}\,U_{(i,j)}\,, \quad i=2,\cdots,M-1\,; \quad j=2,\cdots,N-1. \tag{4.32}$$

The inner product in $\mathcal{HL}$ is similar to the inner product for space $\mathcal{HS}$:

$$(\vec{A},\vec{B})_{\mathcal{HL}} = \sum_{i=1}^{M-1}\sum_{j=1}^{N-1}(\vec{A},\vec{B})_{(i,j)}\,VC_{(i+1/2,j+1/2)}\,, \tag{4.33}$$

where $(\vec{A},\vec{B})_{i+1/2,j+1/2}$ approximates the dot product of two vectors at the cell $(i+1/2,j+1/2)$. In $\mathcal{HL}$, the vectors are represented by orthogonal projections to the directions of the edges of the 3-D cells (see Figure 4.1). If the axes ξ and η form a nonorthogonal basis, the components of the vector $\vec{W}$ in this basis are the orthogonal projections $WL\xi$ and $WL\eta$ of $\vec{W}$ onto the directions of coordinate axes. If $\vec{A}=(AL\xi,AL\eta)$ and $\vec{B}=(BL\xi,BL\eta)$, then the dot product is

$$(\vec{A},\vec{B}) = \frac{AL\xi\,BL\xi + AL\eta\,BL\eta - (AL\xi\,BL\eta + AL\eta\,BL\xi)\,\cos\varphi}{\sin^2\varphi}\,, \tag{4.34}$$

where φ is the angle between these axes (see Figure 4.1). From a formal point of view, the only difference between this formula and the one for the surface components, (see equation4.8), is the minus sign before the third term. This difference can be easily understood if we take into account that basis vectors of one nonorthogonal local system are perpendicular to another.

Formula 4.34 is used to approximate the dot product in a cell:

$$\begin{aligned}(\vec{A},\vec{B})_{(i+1/2,j+1/2)} \quad = \quad & \sum_{k,l=0}^{1}\frac{V_{(i+k,j+l)}^{(i+1/2,j+1/2)}}{\sin^2\varphi_{(i+k,j+l)}^{(i+1/2,j+1/2)}} \\ & \cdot\Big[AL\xi_{(i+1/2,j+l)}\,BL\xi_{(i+1/2,j+l)} + AL\eta_{(i+k,j+1/2)}\,BL\eta_{(i+k,j+1/2)} \\ & -(-1)^{k+l}\,\Big(AL\xi_{(i+1/2,j+l)}\,BL\eta_{(i+k,j+1/2)}+ \\ & AL\eta_{(i+k,j+1/2)}\,BL\xi_{(i+1/2,j+l)}\Big)\cos\varphi_{(i+k,j+l)}^{(i+1/2,j+1/2)}\Big]\,,\end{aligned} \tag{4.35}$$

where $V_{(i+k,j+l)}^{(i+1/2,j+1/2)}$ represents the same weights as for space $\mathcal{HS}$.

The operator $\mathcal{L}$, which connects the formal and natural inner products in $\mathcal{HL}$ (similar to operator $\mathcal{S}$ for space $\mathcal{HS}$), can be written in block form as

$$\mathcal{L}\,\vec{A} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} AL\xi \\ AL\eta \end{pmatrix} = \begin{pmatrix} L_{11}\,AL\xi + L_{12}\,AL\eta \\ L_{21}\,AL\xi + L_{22}\,AL\eta \end{pmatrix}. \tag{4.36}$$

This operator is symmetric and positive in the formal inner product:

$$[\mathcal{L}\,\vec{A}, \vec{B}]_{\mathcal{HL}} = [\vec{A}, \mathcal{L}\,\vec{B}]_{\mathcal{HL}}\,, \quad [\mathcal{L}\,\vec{A}, \vec{A}]_{\mathcal{HL}} > 0\,. \tag{4.37}$$

A comparison of formal and natural inner products gives the following:

$$\begin{aligned}
(L_{11}\,AL\xi)_{(i+1/2,j)} &= \left(\sum_{k,l=0}^{1} \frac{V_{(i,j+l)}^{(i-k/2,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i-k/2,j+1/2)}} \right) AL\xi_{(i+1/2,j)}\,, \\
(L_{12}\,AL\eta)_{(i+1/2,j)} &= -\sum_{k,l=0}^{1} (-1)^{k+l}\, \frac{V_{(i,j+l)}^{(i-k/2,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i-k/2,j+1/2)}}\, \cos\varphi_{(i,j+l)}^{(i-k/2,j+1/2)}\; AL\eta_{(i-k,j+l/2)}\,, \\
(L_{21}\,AL\eta)_{(i,j+1/2)} &= -\sum_{k,l=0}^{1} (-1)^{k+l}\, \frac{V_{(i+l,j)}^{(i+1/2,j-k/2)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j-k/2)}}\, \cos\varphi_{(i+l,j)}^{(i+1/2,j-k/2)}\; AL\eta_{(i+l,j-k/2)}\,, \\
(L_{22}\,AL\eta)_{(i,j+1/2)} &= \left(\sum_{k,l=0}^{1} \frac{V_{(i+l,j)}^{(i+1/2,j-k/2)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j-k/2)}} \right) AL\eta_{(i,j+1/2)}\,.
\end{aligned} \tag{4.38}$$

The operators L_{11} and L_{22} are diagonal, and the stencils for the operators L_{12} and L_{21} (in 2-D) are the same as for the operators S_{12} and S_{21} (see Figure 4.2).

4.2.1 Construction of Operator $\overline{\mathbf{DIV}}$

The $\overline{\mathbf{DIV}} : \mathcal{HL} \to HN$ operator is defined as the negative adjoint of $\mathbf{GRAD} : HN \to \mathcal{HL}$,

$$\overline{\mathbf{DIV}} \stackrel{def}{=} -\mathbf{GRAD}^*\,. \tag{4.39}$$

Using the connections between formal and natural inner products,

$$\overline{\mathbf{DIV}} = -\mathcal{N}^{-1} \cdot \mathbf{GRAD}^\dagger \cdot \mathcal{L}\,, \tag{4.40}$$

we see that $\overline{\mathbf{DIV}}$ is local because $\mathcal{N}$ is diagonal and that both $\mathbf{GRAD}^\dagger$ and $\mathcal{L}$ are local. It is easy to see that

$$-\mathbf{GRAD}^\dagger\,\vec{A} = (\delta_\xi\,AL\xi)_{i,j} + (\delta_\eta\,AL\eta)_{i,j} \tag{4.41}$$

The stencil for $\overline{\mathbf{DIV}}$ at the interior nodes is obtained by combining this formula with the stencil for operators L_{11}, L_{12}, L_{21}, and L_{22} (shown in Figure 4.3).

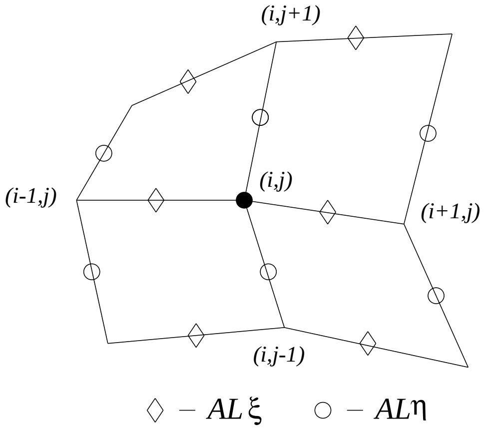


Figure 4.3: Stencil for the operator $\overline{\mathbf{DIV}} = -\mathbf{GRAD}^* : \mathcal{HL} \to HN$.

4.3 Operator $\overline{\mathbf{CURL}}$

Operator **curl** satisfies the integral identity 1.2:

$$\int_V (\mathbf{curl}\vec{A}, \vec{B})\, dV = \int_V (\vec{A}, \mathbf{curl}\,\vec{B})\, dV - \oint_{\partial V} (\vec{A}, \vec{n} \times \vec{B})\, dS\,. \tag{4.42}$$

In the subspace of vectors $\vec{A}$, where the surface integral on the right-hand side vanishes, **curl** is self-adjoint,

$$\mathbf{curl} = \mathbf{curl}^*\,, \tag{4.43}$$

in the inner product

$$(\vec{A}, \vec{B})_{\mathcal{H}} = \int_V (\vec{A}, \vec{B})\, dV\,. \tag{4.44}$$

In the discrete case, for $\vec{A} \in \mathcal{HL}$, vector $\mathbf{CURL}\,\vec{A} \in \mathcal{HS}$, and we define $\overline{\mathbf{CURL}} : \mathcal{HS} \to \mathcal{HL}$ as adjoint to $\mathbf{CURL} : \mathcal{HL} \to \mathcal{HS}$ by

$$\overline{\mathbf{CURL}} \stackrel{def}{=} \mathbf{CURL}^*\,. \tag{4.45}$$

That is,

$$(\mathbf{CURL}\,\vec{A}, \vec{B})_{\mathcal{HS}} - (\vec{A}, \overline{\mathbf{CURL}}\,\vec{B})_{\mathcal{HL}} = 0\,. \tag{4.46}$$

We can express $\overline{\mathbf{CURL}}$ as

$$\overline{\mathbf{CURL}} = \mathcal{L}^{-1} \cdot \mathbf{CURL}^{\dagger} \cdot \mathcal{S} \tag{4.47}$$

and see that, although **CURL** is a local operator, the operator $\overline{\mathbf{CURL}}$ is *nonlocal*.

We can determine $\vec{C} = \overline{\mathbf{CURL}}\,\vec{B}$ by solving the system of linear equations

$$\mathcal{L}\,\vec{C} = \mathbf{CURL}^{\dagger} \cdot \mathcal{S}\,\vec{B}\,, \tag{4.48}$$

with local operators $\mathcal{L}$ and $\mathbf{CURL}^{\dagger} \cdot \mathcal{S}$.

5 Structure of Discrete Operators

In this section we introduce primitive differencing and metric operators and present expressions for **GRAD**, **DIV**, **CURL**; $\overline{\mathbf{GRAD}}$, $\overline{\mathbf{DIV}}$, and $\overline{\mathbf{CURL}}$ in terms of these primitive operators. This representation is useful for investigating the properties of discrete divergence, gradient, and curl, and, in particular, for proving the discrete analogs of the differential operator theorems of vector analysis.

The *primitive metric operators* correspond to the multiplication of scalars by length, area, or volume and can be defined as the following diagonal operators:

$$\begin{aligned}
&(L\xi\, U)_{i+1/2,j} = l\xi_{i+1/2,j}\, U_{i+1/2,j}\ , (L\eta\, U)_{i,j+1/2} = l\eta_{i,j+1/2}\, U_{i,j+1/2}\ , (L\zeta\, U)_{i,j} = l\zeta_{i,j}\, U_{i,j}\ , \\
&(S\xi\, U)_{i,j+1/2} = S\xi_{i,j+1/2}\, U_{i,j+1/2}\ , (S\eta\, U)_{i+1/2,j} = S\eta_{i+1/2,j}\, U_{i+1/2,j}\ , \qquad (5.1)\\
&(S\zeta\, U)_{i+1/2,j+1/2} = S\zeta_{i+1/2,j+1/2}\, U_{i+1/2,j+1/2}\ , \\
&(V^C(U))_{i+1/2,j+1/2} = VC_{i+1/2,j+1/2}\, U_{i+1/2,j+1/2}\ ,
\end{aligned}$$

and

$$(V^N(U))_{i,j} = VN_{i,j}\, U_{i,j}\ . \qquad (5.2)$$

The formal discrete gradient, $\mathcal{GRAD} : \mathrm{HN} \to \mathcal{HL}$, is

$$\mathcal{GRAD} = \begin{pmatrix} \delta_\xi \\ \delta_\eta \end{pmatrix} . \qquad (5.3)$$

The natural discrete gradient, **GRAD** : $HN \to \mathcal{HL}$, is

$$\mathbf{GRAD} = \begin{pmatrix} L\xi^{-1} & 0 \\ 0 & L\eta^{-1} \end{pmatrix} \cdot \mathcal{GRAD}\, . \qquad (5.4)$$

The formal discrete divergence, $\mathcal{DIV} : \mathcal{HS} \to \mathrm{HC}$, is

$$\mathcal{DIV} = (\delta_\xi\, ,\, \delta_\eta)\ . \qquad (5.5)$$

The natural discrete divergence, **DIV** : $\mathcal{HS} \to HC$, is

$$\mathbf{DIV} = \left(V^C\right)^{-1} \cdot \mathcal{DIV} \cdot \begin{pmatrix} S\xi & 0 \\ 0 & S\eta \end{pmatrix} . \qquad (5.6)$$

The formal discrete curl, $\mathcal{CURL} : \mathcal{HL} \to \mathcal{HS}$, is

$$\mathcal{CURL} = \begin{pmatrix} 0 & 0 & \delta_\eta \\ 0 & 0 & -\delta_\xi \\ -\delta_\eta & \delta_\xi & 0 \end{pmatrix} . \qquad (5.7)$$

The natural discrete curl, **CURL** : $\mathcal{HL} \to \mathcal{HS}$, is

$$\mathbf{CURL} = \begin{pmatrix} S\xi^{-1} & 0 & 0 \\ 0 & S\eta^{-1} & 0 \\ 0 & 0 & S\zeta^{-1} \end{pmatrix} \cdot \mathcal{CURL} \cdot \begin{pmatrix} L\xi & 0 & 0 \\ 0 & L\eta & 0 \\ 0 & 0 & L\zeta \end{pmatrix} . \qquad (5.8)$$

The formal adjoint to the formal discrete divergence, $\overline{\mathcal{GRAD}} = -\mathcal{DIV}^{\dagger} : \mathrm{HC} \to \mathcal{HS}$, is

$$\overline{\mathcal{GRAD}} = \begin{pmatrix} \delta_\xi \\ \delta_\eta \end{pmatrix} . \tag{5.9}$$

The adjoint to the natural discrete divergence, $\overline{\mathbf{GRAD}} = -\mathbf{DIV}^* : HC \to \mathcal{HS}$, is

$$\overline{\mathbf{GRAD}} = \mathcal{S}^{-1} \cdot \begin{pmatrix} S\xi & 0 \\ 0 & S\eta \end{pmatrix} \cdot \overline{\mathcal{GRAD}} . \tag{5.10}$$

The formal adjoint to the formal discrete gradient, $\overline{\mathcal{DIV}} = -\mathcal{GRAD}^{\dagger} : \mathcal{HL} \to \mathrm{HN}$, is

$$\overline{\mathcal{DIV}} = \begin{pmatrix} \delta_\xi & \delta_\eta \end{pmatrix} , \tag{5.11}$$

The adjoint to the natural discrete gradient, $\overline{\mathbf{DIV}} = -\mathbf{GRAD}^* : \mathcal{HL} \to HN$, is

$$\overline{\mathbf{DIV}} = \left(V^N\right)^{-1} \cdot \overline{\mathcal{DIV}} \cdot \begin{pmatrix} L\xi^{-1} & 0 \\ 0 & L\eta^{-1} \end{pmatrix} \cdot \mathcal{L} . \tag{5.12}$$

The formal adjoint to the formal discrete curl, $\overline{\mathcal{CURL}} = \mathcal{CURL}^{\dagger} : \mathcal{HS} \to \mathcal{HL}$, is

$$\overline{\mathcal{CURL}} = \begin{pmatrix} 0 & 0 & -\delta_\eta \\ 0 & 0 & \delta_\xi \\ \delta_\eta & -\delta_\xi & 0 \end{pmatrix} . \tag{5.13}$$

The adjoint to the natural discrete curl, $\overline{\mathbf{CURL}} = \mathbf{CURL}^* : \mathcal{HS} \to \mathcal{HS}$, is

$$\overline{\mathbf{CURL}} = \mathcal{L}^{-1} \cdot \begin{pmatrix} L\xi & 0 & 0 \\ 0 & L\eta & 0 \\ 0 & 0 & L\zeta \end{pmatrix} \cdot \overline{\mathcal{CURL}} \cdot \begin{pmatrix} S\xi^{-1} & 0 & 0 \\ 0 & S\eta^{-1} & 0 \\ 0 & 0 & S\zeta^{-1} \end{pmatrix} \cdot \mathcal{S} . \tag{5.14}$$

6 Discrete Operator Theorems

6.1 Theorems for Formal Operators

We define the formal discrete volume, surface, and line integrals, to be the same as given in [6] if the volumes, areas, and lengths are set equal to one.

In HC, the formal volume integral is

$$\mathcal{I}_{\tilde{V}}^{V}(U) = \sum_{cells} U_{i,j} , \tag{6.1}$$

where $\tilde{V}$ is the union of the primitive (i,j) cells (in the case of formal integrals, this volume is defined by set of indices (i,j) over which summation is made).

In $\mathcal{HS}$, the formal surface integral is

$$\mathcal{I}_{\tilde{S}}^{S}(\vec{A}) = \sum_{\xi-\text{faces}} WS\xi_{i,j+1/2} + \sum_{\eta-\text{faces}} WS\eta_{i+1/2,j} + \sum_{\zeta-\text{faces}} WS\zeta_{i+1/2,j+1/2}\,, \tag{6.2}$$

where $\tilde{S}$ is the union of primitive cell faces.

We define the formal discrete line integral for $\vec{A} \in \mathcal{HL}$ as

$$\mathcal{I}_{\tilde{L}}^{L}(\vec{A}) = \sum_{\xi-\text{edges}} AL\xi_{i+1/2,j} + \sum_{\eta-\text{edges}} AL\eta_{i,j+1/2}\,, \tag{6.3}$$

where $\tilde{L}$ is the set of edges that determine the discrete path.

The formal operators $\mathcal{GRAD}$, $\mathcal{DIV}$, and $\mathcal{CURL}$ coincide with operators **GRAD**, **DIV**, and **CURL**, respectively, for the special grid in which all volumes of the cells, areas of the faces, and lengths of the edges are equal to one, and therefore all matrices relating to geometry are the identity. Therefore all theorems proved in [6] are valid for formal operators and formal integrals. In particular, we will use the theorems

$\mathcal{DIV}\,\vec{\mathrm{A}} = 0$, if and only $\vec{A} = \mathcal{CURL}\,\vec{\mathrm{B}}$,

and

$\mathcal{CURL}\,\vec{\mathrm{A}} = 0$ **if and only if** $\vec{A} = \mathcal{GRAD}\,\varphi$.

We will now prove the corresponding theorems for the adjoint operators:

$\overline{\mathcal{DIV}}\,\vec{A} = 0$, if and only if $\vec{A} = \overline{\mathcal{CURL}}\,\vec{B}$, where $\vec{A} \in \mathcal{HL}$ and $\vec{B} \in \mathcal{HS}$,

and

$\overline{\mathcal{CURL}}\,\vec{A} = 0$ **if and only if** $\vec{A} = \overline{\mathcal{GRAD}}\,\varphi$, where $\vec{A} \in \mathcal{HS}$ and $\varphi \in \overset{0}{HC}$.

The proofs are simplified by noting that for the formal operators we need only consider a grid with unit mesh size. To make the proof more descriptive, we will introduce the *dual grid* by shifting a unit grid by a half mesh cell (see Figure 6.1). The nodes of the original grid are the centers of cells of dual grid, and vice versa. That is, $HC^o \sim HN^d$, where superscript "o" refers to the original grid, and superscript "d" refers to the dual grid. Note that, the normal components of vectors on the original grid are tangential to the dual grid and vice versa.

The relationships between these two grids and the simplified geometry reduce the proof for the adjoint operators to a simple modification of the proof for the formal operators (with an obvious change in the range of indices).

6.2 $\overline{\mathbf{CURL}}\,\overline{\mathbf{GRAD}} = 0$

To prove that the analog of the identity $\mathbf{curl}\,\mathbf{grad}\,u = 0$ holds for the adjoint discrete operators, we note that for any vector $\vec{A}$, the definition of $\overline{\mathbf{GRAD}}$ implies

$$(\overline{\mathbf{GRAD}}\,U, \vec{A})_{\mathcal{HS}} + (U, \mathbf{DIV}\vec{A})_{HC} = 0. \tag{6.4}$$

If we take $\vec{A} = \mathbf{CURL}\,\vec{B}$, then

$$(\overline{\mathbf{GRAD}}\,U, \mathbf{CURL}\,\vec{B})_{\mathcal{HS}} + (U, \mathbf{DIV}\,\mathbf{CURL}\,\vec{B})_{HC} = 0\,. \tag{6.5}$$

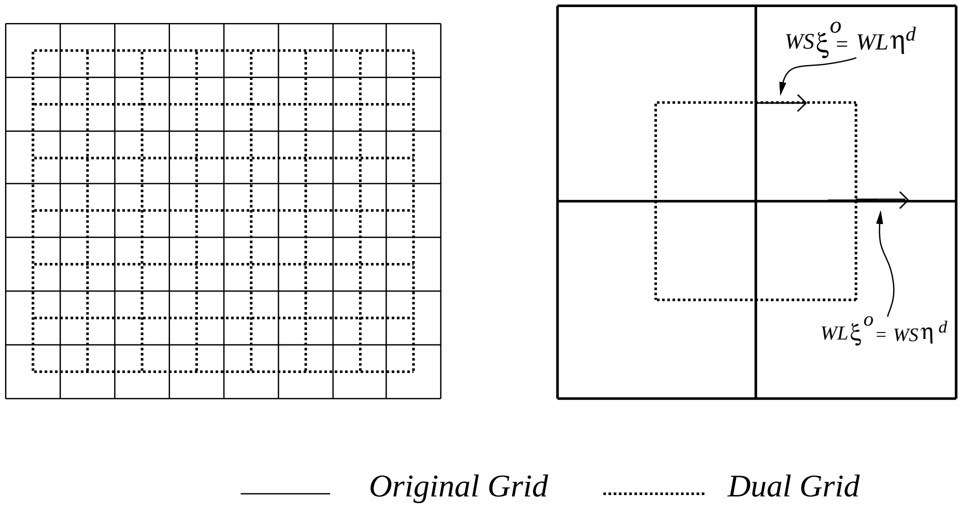


Figure 6.1: The original unit grid (solid lines) is shifted by half a mesh to create the dual grid (dotted lines). Centers of the cells of the original grid are nodes of the dual grid and vice versa. Vectors that are normal to faces of the original grid are tangential to the edges of the dual grid and vice versa.

Because $\mathbf{DIV}\,\mathbf{CURL}\,\vec{B} = 0$ (see [6]) for any vector $\vec{B}$, the second term in equation 6.5 is zero, and $(\overline{\mathbf{GRAD}}\,U, \mathbf{CURL}\,\vec{B})_{\mathcal{HS}} = 0$ for any U and $\vec{B}$. Using the definition of the adjoint operator, we can rewrite equation 6.5 as

$$(\overline{\mathbf{CURL}}\,\overline{\mathbf{GRAD}}\,U, \vec{B})_{\mathcal{HL}} = 0\,. \tag{6.6}$$

This equation holds for any $\vec{B} \in \mathcal{HL}$; hence,

$$\overline{\mathbf{CURL}}\,\overline{\mathbf{GRAD}}\,U = 0\,. \tag{6.7}$$

6.3 $\overline{\mathbf{DIV}}\,\overline{\mathbf{CURL}} = 0$

Similarly, using the identity

$$(\mathbf{CURL}\,\vec{A}, \vec{B})_{\mathcal{HS}} - (\vec{A}, \overline{\mathbf{CURL}}\,\vec{B})_{\mathcal{HL}} = 0 \tag{6.8}$$

and taking $\vec{A} = \mathbf{GRAD}\,\varphi$, where $\varphi \in HN$, it follows that

$$\overline{\mathbf{DIV}}\,\overline{\mathbf{CURL}}\,\vec{B} = 0\,. \tag{6.9}$$

6.4 If $\overline{\mathbf{DIV}}\,\vec{A} = 0$, then $\vec{A} = \overline{\mathbf{CURL}}$

The condition $\overline{\mathbf{DIV}}\,\vec{A} = 0$, where $\vec{A} \in \mathcal{HL}$, can be written as

$$\left(V^N\right)^{-1} \cdot \overline{\mathcal{DIV}} \cdot \begin{pmatrix} L\xi^{-1} & 0 \\ 0 & L\eta^{-1} \end{pmatrix} \cdot \mathcal{L}\,\vec{A} = 0\,. \tag{6.10}$$

This equation is equivalent to

$$\overline{\mathcal{DIV}}\,\vec{A}' = 0\,, \tag{6.11}$$

where

$$\vec{A}' = \begin{pmatrix} L\xi^{-1} & 0 \\ 0 & L\eta^{-1} \end{pmatrix} \cdot \mathcal{L}\,\vec{A}\,. \tag{6.12}$$

Using the theorem about the formal operator $\overline{\mathcal{DIV}}$ (proved at the beginning of this section), it follows that

$$\vec{A}' = \overline{\mathcal{CURL}}\,\vec{B}'\,, \quad \text{where} \quad \vec{B}' \in \mathcal{HS}\,, \tag{6.13}$$

and therefore

$$\vec{A} = \mathcal{L}^{-1} \cdot \begin{pmatrix} L\xi & 0 \\ 0 & L\eta \end{pmatrix} \overline{\mathcal{CURL}}\,\vec{B}'\,. \tag{6.14}$$

If we define the vector $\vec{B}$ as

$$\vec{B} = \begin{pmatrix} S\xi^{-1} & 0 & 0 \\ 0 & S\eta^{-1} & 0 \\ 0 & 0 & S\zeta^{-1} \end{pmatrix} \cdot \mathcal{S}\,\vec{B}'\,, \tag{6.15}$$

then

$$\vec{A} = \mathcal{L}^{-1} \cdot \begin{pmatrix} L\xi & 0 & 0 \\ 0 & L\eta & 0 \\ 0 & 0 & L\zeta \end{pmatrix} \cdot \overline{\mathcal{CURL}} \cdot \begin{pmatrix} S\xi^{-1} & 0 & 0 \\ 0 & S\eta^{-1} & 0 \\ 0 & 0 & S\zeta^{-1} \end{pmatrix} \cdot \mathcal{S}\,\vec{B} = \overline{\mathbf{CURL}}\,\vec{B}\,, \tag{6.16}$$

and the theorem follows. Note that the transformation between vector $\vec{B}$ and $\vec{B}'$ is one-to-one because matrix $\mathcal{S}$ and the area matrix are positive definite.

6.5 If $\overline{\mathbf{CURL}}\,\vec{A} = 0$, then $\vec{A} = \overline{\mathbf{GRAD}}$

The condition $\overline{\mathbf{CURL}}\,\vec{A} = 0$, where $\vec{A} \in \mathcal{HS}$, can be written as

$$\mathcal{L}^{-1} \cdot \begin{pmatrix} L\xi & 0 & 0 \\ 0 & L\eta & 0 \\ 0 & 0 & L\zeta \end{pmatrix} \cdot \overline{\mathcal{CURL}} \cdot \begin{pmatrix} S\xi^{-1} & 0 & 0 \\ 0 & S\eta^{-1} & 0 \\ 0 & 0 & S\zeta^{-1} \end{pmatrix} \cdot \mathcal{S}\,\vec{A} = 0\,. \tag{6.17}$$

Because matrix $\mathcal{L}$ and the length matrix are positive definite, the previous equation is equivalent to

$$\overline{\mathcal{CURL}} \cdot \begin{pmatrix} S\xi^{-1} & 0 & 0 \\ 0 & S\eta^{-1} & 0 \\ 0 & 0 & S\zeta^{-1} \end{pmatrix} \cdot \mathcal{S}\,\vec{A} = 0\,. \tag{6.18}$$

We define vector $\vec{A}'$ as

$$\vec{A}' = \begin{pmatrix} S\xi^{-1} & 0 & 0 \\ 0 & S\eta^{-1} & 0 \\ 0 & 0 & S\zeta^{-1} \end{pmatrix} \cdot \mathcal{S}\,\vec{A}\,, \tag{6.19}$$

and rewrite equation 6.18 in the form

$$\overline{\mathcal{CURL}}\,\vec{A}' = 0\,. \tag{6.20}$$

Using the theorem for formal operators and equation 6.20, we can conclude that

$$\vec{A}' = \overline{\mathcal{GRAD}}\,\varphi\,, \quad \text{where} \quad \varphi \in \overset{0}{HC}\,, \tag{6.21}$$

and the result below follows directly from equations 6.19 and 5.4:

$$\vec{A} = \mathcal{S}^{-1} \cdot \begin{pmatrix} S\xi & 0 & 0 \\ 0 & S\eta & 0 \\ 0 & 0 & S\zeta \end{pmatrix} \overline{\mathcal{GRAD}}\,\varphi = \overline{\mathbf{GRAD}}\,\varphi\,. \tag{6.22}$$

7 Conclusion and Discussion

The natural discrete operators constructed in [6],

$$\mathbf{DIV} : \mathcal{HS} \to HC\,, \ \ \mathbf{GRAD} : HN \to \mathcal{HL}\,, \ \text{ and } \ \mathbf{CURL} : \mathcal{HL} \to \mathcal{HS}\,. \tag{7.1}$$

can be combined only to construct the *trivial* operators:

$$\mathbf{DIV}\,\mathbf{CURL} : \mathcal{HL} \to HC\,, \qquad \mathbf{DIV}\,\mathbf{CURL} \equiv 0\,, \tag{7.2}$$

$$\mathbf{CURL}\,\mathbf{GRAD} : HN \to \mathcal{HS}\,, \qquad \mathbf{CURL}\,\mathbf{GRAD} \equiv 0\,. \tag{7.3}$$

In this paper we used SOM to construct the operators

$$\overline{\mathbf{DIV}} : \mathcal{HL} \to HN\,, \ \ \overline{\mathbf{GRAD}} : HC \to \mathcal{HS}\,, \ \text{ and } \ \overline{\mathbf{CURL}} : \mathcal{HS} \to \mathcal{HL}\,. \tag{7.4}$$

By construction

$$\overline{\mathbf{DIV}} = -\mathbf{GRAD}^*\,, \ \ \overline{\mathbf{GRAD}} = -\mathbf{DIV}^*\,, \ \text{ and } \ \overline{\mathbf{CURL}} = \mathbf{CURL}^*\,. \tag{7.5}$$

We then proved that discrete versions of the differential operator theorems hold for these derived adjoint operators as well as for the natural operators **DIV**, **GRAD**, and **CURL**.

Namely, we have proved the discrete theorems of vector analysis including Gauss' theorem; the theorem that $\mathbf{div}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{curl}\,\vec{B}$; and the theorem that $\mathbf{curl}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{grad}\varphi$.

The adjoint operators have different domains and ranges and can combined with natural operators to form the *nontrivial* second-order operators:

$$\mathbf{DIV}\,\overline{\mathbf{GRAD}} : HC \to HC\,, \qquad \overline{\mathbf{DIV}}\,\mathbf{GRAD} : HN \to HN\,, \tag{7.6}$$

$$\mathbf{CURL}\,\overline{\mathbf{CURL}} : \mathcal{HS} \to \mathcal{HS}\,, \qquad \overline{\mathbf{CURL}}\,\mathbf{CURL} : \mathcal{HL} \to \mathcal{HL}\,, \tag{7.7}$$

$$\mathbf{GRAD}\,\overline{\mathbf{DIV}} : \mathcal{HL} \to \mathcal{HL}\,, \qquad \overline{\mathbf{GRAD}}\,\mathbf{DIV} : \mathcal{HS} \to \mathcal{HS}\,. \tag{7.8}$$

We also can construct two discrete analogs of the vector-Laplacian

$$\Delta\,\vec{A} = \mathbf{grad\,div}\,\vec{A} - \mathbf{curl\,curl}\,\vec{A} :$$

$$\Delta_h^{\mathcal{L}} : \mathcal{HL} \to \mathcal{HL}\,, \quad \Delta_h^{\mathcal{L}} = \mathbf{GRAD}\,\overline{\mathbf{DIV}} - \overline{\mathbf{CURL}}\,\mathbf{CURL}$$

and

$$\Delta_h^{\mathcal{S}} : \mathcal{HS} \to \mathcal{HS}\,, \quad \Delta_h^{\mathcal{S}} = \overline{\mathbf{GRAD}}\,\mathbf{DIV} - \mathbf{CURL}\,\overline{\mathbf{CURL}}$$

One of the most important theorems of vector analysis is the theorem of orthogonal decomposition of the vector field; that is, any vector can be represented in the following form:

$$\vec{A} = \mathbf{grad}\,\varphi + \mathbf{curl}\,\vec{B}\,. \tag{7.9}$$

This theorem plays a very important role in many theoretical considerations in continuous case. The main goal of our next paper [7] is to prove discrete analogs of the theorem for vectors from spaces $\mathcal{HL}$ and $\mathcal{HS}$. Namely, we will prove that any vector $\vec{A} \in \mathcal{HS}$ can be presented as

$$\vec{A} = \overline{\mathbf{GRAD}}\,\varphi + \mathbf{CURL}\,\vec{B}\,, \tag{7.10}$$

where $\varphi \in HC$ and $\vec{B} \in \mathcal{HL}$, and similarly that any vector $\vec{A} \in \mathcal{HL}$ can be presented as

$$\vec{A} = \mathbf{GRAD}\,\varphi + \overline{\mathbf{CURL}}\,\vec{B}\,, \tag{7.11}$$

where $\varphi \in HN$ and $\vec{B} \in \mathcal{HS}$.

Acknowledgment

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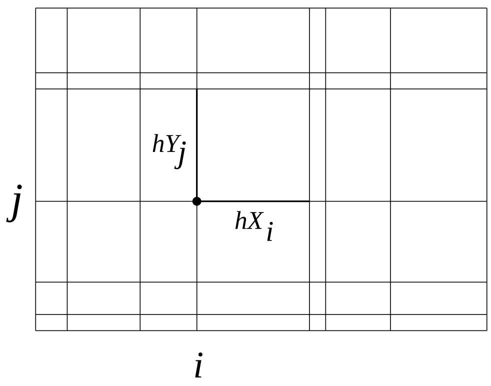

Figure 7.1: Rectangular Grid

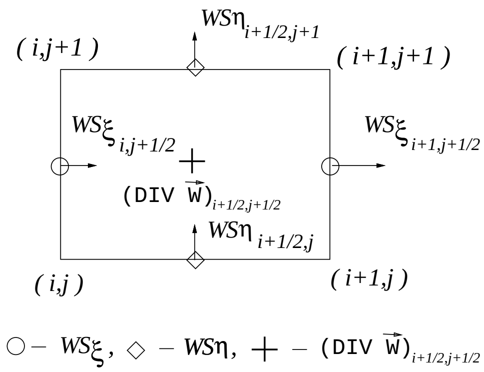

Figure 7.2: Stencil for operator **DIV**

Appendix. Formulas for Discrete Operators on a Rectangular Grid

In this appendix we present formulas for operators **DIV**, **GRAD**, and **CURL** on a nonuniform rectangular grid with spatial steps hX_i and hY_j (see Figure 7.1).

Operator **DIV**

For all cells $(i+1/2, j+1/2)$, where $i = 1, \dots, M-1$ and $j = 1, \dots, N-1$, formulas for operator **DIV** are

$$\left(\mathbf{DIV}\,\vec{W}\right)_{i+1/2,j+1/2} = \frac{(\delta_\xi\, WS\xi)_{i+1/2,j+1/2}}{hX_i} + \frac{(\delta_\eta\, WS\eta)_{i+1/2,j+1/2}}{hY_j}\,. \tag{7.1}$$

The stencil for operator **DIV** is shown in Figure 7.2

Operator **GRAD**

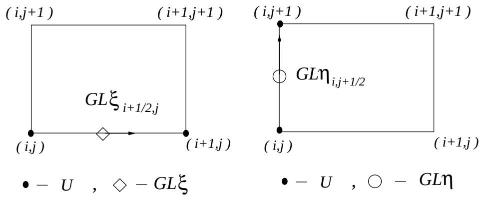

Figure 7.3: Stencil for operator **GRAD**

Vector $\vec{G} = \mathbf{GRAD}\, U$ has two components, $\vec{G} = (GL\xi, GL\eta)$, which are defined on the corresponding edges.

For $l\xi_{(i+1/2,j)}$ edges, where $i = 1, \ldots, M-1$ and $j = 1, \ldots, N$, formulas for $GL\xi_{i+1/2,j}$ are

$$GL\xi_{i+1/2,j} = \frac{(\delta_\xi\, U)_{i+1/2,j}}{hX_i}\,. \tag{7.2}$$

For $l\eta_{(i,j+1/2)}$ edges, where $i = 1, \ldots, M$ and $j = 1, \ldots, N-1$, formulas for $GL\eta_{i,j+1/2}$ are

$$GL\eta_{i,j+1/2} = \frac{(\delta_\eta\, U)_{i,j+1/2}}{hY_j}\,. \tag{7.3}$$

The stencil for operator **GRAD** is shown in Figure 7.3

Operator **CURL**

Vector $\vec{R} = \mathbf{CURL}\, B$ has three components, $\vec{R} = (RS\xi, RS\eta, RS\zeta)$, which are defined on corresponding surfaces.

For faces $S\xi_{(i,j+1/2)}$, where $i = 1, \ldots, M$ and $j = 1, \ldots, N-1$, formulas for operator $RS\xi_{i,j+1/2}$ are

$$RS\xi_{i,j+1/2} = \frac{(\delta_\eta\, BL\zeta)_{i,j+1/2}}{hY_j}\,. \tag{7.4}$$

For faces $S\eta_{(i+1/2,j)}$, where $i = 1, \ldots, M-1$ and $j = 1, \ldots, N$, formulas for operator $RS\eta_{i+1/2,j}$ are

$$RS\eta_{i+1/2,j} = -\frac{(\delta_\xi\, BL\zeta)_{i+1/2,j}}{hX_i}\,. \tag{7.5}$$

For faces $S\zeta_{(i+1/2,j+1/2)}$, where $i = 1, \ldots, M-1$ and $j = 1, \ldots, N-1$, formulas for operator $RS\zeta_{i+1/2,j+1/2}$ are

$$RS\zeta_{i+1/2,j+1/2} = \frac{(\delta_\xi\, BL\eta)_{i+1/2,j+1/2}}{hX_i} - \frac{(\delta_\eta\, BL\xi)_{i+1/2,j+1/2}}{hY_j}\,. \tag{7.6}$$

The stencil for operator **CURL** is shown in Figure 7.4

Operator $\overline{\mathbf{GRAD}}$

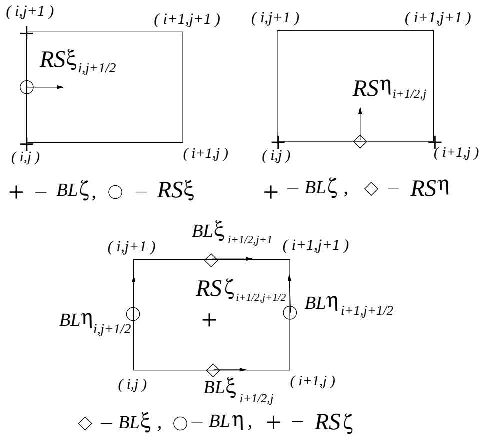

Figure 7.4: Stencil for operator **CURL**

Vector $\overline{\mathbf{GRAD}}\,U$ has two components, $(GS\xi, GS\eta)$, which are defined on corresponding faces.

For internal faces $S\xi_{(i,j+1/2)}$, where $i = 2, \dots, M-1$ and $j = 1, \dots, N-1$, formulas are

$$GS\xi_{i,j+1/2} = \frac{(\delta_\xi\, U)_{i,j+1/2}}{0.5\,(hX_{i-1} + hX_i)}\,. \tag{7.7}$$

For internal faces $S\eta_{(i+1/2,j)}$, where $i = 1, \dots, M-1$ and $j = 2, \dots, N-1$, formulas are

$$GS\eta_{i+1/2,j} = \frac{(\delta_\eta\, U)_{i+1/2,j}}{0.5\,(hY_{j-1} + hY_j)}\,. \tag{7.8}$$

On the boundary faces, components of discrete gradient are defined by one-sides differences, for example for $i = 1$ and $j = 1, \dots, N-1$ formulas are:

$$GS\xi_{1,j+1/2} = \frac{U_{3/2,j+1/2} - U_{1,j+1/2}}{0.5\,hX_1}\,, \tag{7.9}$$

similar, for $j = 1$ and $i = 1, \dots, M-1$ formulas are:

$$GS\eta_{i+1/2,1} = \frac{U_{i+1/2,3/2} - U_{i+1/2,1}}{0.5\,hY_1}\,. \tag{7.10}$$

On other boundaries formulas are similar.

The stencil for operator $\overline{\mathbf{GRAD}}$ is shown in Figure 7.5.

<u>Operator $\overline{\mathbf{DIV}}$</u>

For nodes (i,j), where $i = 2, \dots, M-1$ and $j = 2, \dots, N-1$, formulas for $\overline{\mathbf{DIV}}$ are

$$(\overline{\mathbf{DIV}}\,\vec{W})_{i,j} = \frac{(\delta_\xi\, WL\xi)_{i,j}}{0.5\,(hX_i + hX_{i-1})} + \frac{(\delta_\eta\, WL\eta)_{i,j}}{0.5\,(hY_j + hY_{j-1})}\,. \tag{7.11}$$

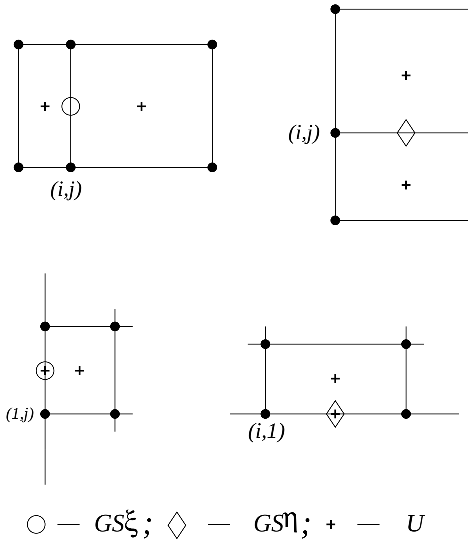

Figure 7.5: Stencil for operator $\overline{\mathbf{GRAD}}$

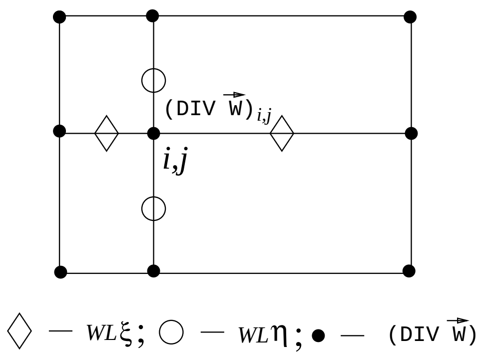

Figure 7.6: Stencil for operator $\overline{\mathbf{DIV}}$

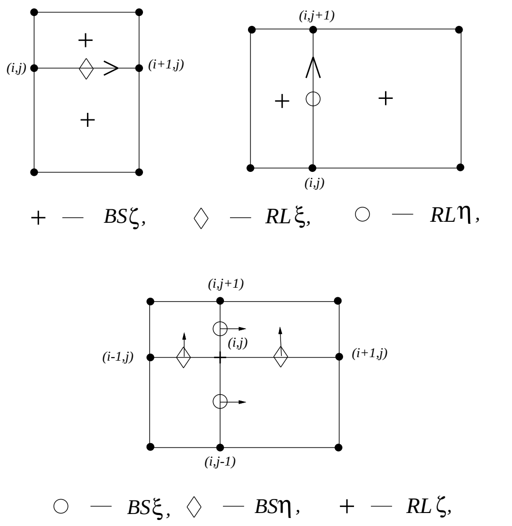

Figure 7.7: Stencil for operator $\overline{\mathbf{CURL}}$

The stencil for operator $\overline{\mathbf{DIV}}$ is shown on Figure 7.6.

Operator $\overline{\mathbf{CURL}}$

Vector $\vec{R} = \overline{\mathbf{CURL}}\, B$ has three components – $\vec{R} = (RL\xi, RL\eta, RL\zeta)$, which are defined on corresponding surfaces.

For edges $l\xi_{(i+1/2,j)}$, where $i = 1, \ldots, M-1$ and $j = 1, \ldots, N$, formulas for operator $RL\xi_{i+1/2,j}$ are

$$RL\xi_{i+1/2,j} = \frac{(\delta_\eta\, BS\zeta)_{i+1/2,j}}{0.5\,(hY_{j-1} + hY_j)}\,. \tag{7.12}$$

For edges $l\eta_{(i,j+1/2)}$, where $i = 1, \ldots, M$ and $j = 1, \ldots, N-1$, formulas for operator $RL\eta_{i,j+1/2}$ are

$$RL\eta_{i,j+1/2} = -\frac{(\delta_\xi\, BS\zeta)_{i,j+1/2}}{0.5\,(hX_{i-1} + hX_i)}\,. \tag{7.13}$$

For edges $l\zeta_{(i,j)}$, where $i = 1, \ldots, M-1$ and $j = 1, \ldots, N-1$, formulas for operator $RL\zeta_{i,j}$ are

$$RL\zeta_{i,j} = \frac{(\delta_\xi\, BS\eta)_{i,j}}{0.5\,(hX_{i-1} + hX_i)} - \frac{(\delta_\eta\, BS\xi)_{i,j}}{0.5\,(hY_{j-1} + hY_j)}\,. \tag{7.14}$$

The stencil for operator $\overline{\mathbf{CURL}}$ is shown in Figure 7.7.

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