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

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Abstract—This is the first in series of papers creating a *discrete analog of vector analysis on logically rectangular, nonorthogonal, nonsmooth grids*. We introduce notations for 2-D logically rectangular grids, describe both cell-valued and nodal discretizations for scalar functions, and construct the natural discretizations of vector fields, using the vector components normal and tangential to the cell boundaries. We then define natural discrete analogs of the divergence, gradient, and curl operators based on coordinate invariant definitions and interpret these formulas in terms of curvilinear coordinates, such as length of elements of coordinate lines, areas of elements of coordinate surfaces, and elementary volumes.

We introduce the discrete volume integral of scalar functions, the discrete surface integral, and a discrete analog of the line integral and prove discrete versions of the main theorems relating these objects. These theorems include the following: the discrete analog of relationship $\mathbf{div}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{curl}\,\vec{B}$; $\mathbf{curl}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{grad}\varphi$; if $\vec{A} = \mathbf{grad}\,\varphi$, then the line integral does not depend on path; and 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.

Last, we define the discrete operators **DIV**, **GRAD**, and **CURL** in terms of primitive differencing operators (based on forward and backward differences) and primitive metric operators (related to multiplications of discrete functions by length of edges, areas of surfaces, and volumes of 3-D cells). These formulations elucidate the structure of the discrete operators and are useful when investigating the relationships between operators and their adjoints.

Keywords—Finite-difference, Logically-rectangular grids, Discrete vector analysis.

NOMENCLATURE

x,y,z	Cartesian coordinates in 3-D physical space
ξ,η,ζ	Curvilinear coordinates in 3-D logical space
$X(\xi,\eta,\zeta), Y(\xi,\eta,\zeta), Z(\xi,\eta,\zeta)$	Functions mapping between logica and physical space
V, Ω	3-D and 2-D domains
$\partial V, S$	Boundaries of 3-D and 2-D domains
$\vec{n}$	Outward normal unit vector
div	Differential divergence operator

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grad	Differential gradient operator
curl	Differential curl operator
H	Space of continuous scalar functions
$\overset{0}{H}$	Subspace of space H, where $u \in \overset{0}{H}$ if $u(x,y,z) \in H$ and $u(x,y,z) = 0$, for $(x,y,z) \in \partial V$
$(u,v)_H$	Inner product of u and v in H
$\mathcal{H}$	Space of continuous vector functions
$\vec{A}$	Vector function
AX, AY	Cartesian components of the vector $\vec{A}$
h	Characteristic size of the spatial grid
$\Delta\xi, \Delta\eta, \Delta\zeta$	Spacing of a uniform grid in logical space
$x_{i,j,k}, y_{i,j,k}, z_{i,j,k}$	Coordinates of the grid nodes in 3-D physical space
$\xi_{i,j,k}, \eta_{i,j,k}, \zeta_{i,j,k}$	Coordinates of the grid nodes in 3-D logical space
$VC_{i,j,k}, VC_{i,j}$	Volume of a grid cell in 3-D and area of a cell in 2-D
$S\xi_{i,j,k}, S\eta_{i,j,k}, S\zeta_{i,j,k}$	Areas of the faces of a 3-D cell and lengths of the sides in 2-D
$l\xi_{i,j,k}, l\eta_{i,j,k}, l\zeta_{i,j,k}$	Lengths of the edges of a 3-D cell
$\varphi_{i,j}^{k,l}$	Internal angle in cell (i,j) with vertex (k,l)
$C_1, C_2,$ $C_{\min}, C_{\max} \cdots,$	Different constants in inequalities
$U_{i,j,k}, U_{i,j}$	Discrete scalar functions
$WS\xi_{i,j,k}, WS\eta_{i,j,k}, WS\zeta_{i,j,k}$	Components of a discrete vector functions described by its orthogonal projections onto directions normal to the faces
$WL\xi_{i,j,k}, WL\eta_{i,j,k}, WL\zeta_{i,j,k}$	Components of a discrete vector function, described by its orthogonal projections onto directions of the edges of the cell
HN	Space of a discrete scalar function given by its values in nodes
HC	Space of a discrete scalar function given by its values in cells
$\mathcal{H}S$	Space of discrete vector functions given by components $WS\xi, WS\eta,$ and $WS\zeta$
$\mathcal{H}L$	Space of discrete vector functions given by components $WL\xi, WL\eta,$ and $WL\zeta$
$D\xi, D\eta$	Primitive difference operators; forward differences with respect to indices i and j, respectively
$\overline{D\xi}, \overline{D\eta}$	Primitive difference operators; backward differences with respect to indices i and j, respectively
$L\xi, L\eta, L\zeta$	Primitive metric operators, multiplication by length
$S\xi, S\eta, S\zeta$	Primitive metric operators, multiplication by area
V^C, V^N	Primitive metric operators, multiplication by volume of cell or node, respectively
$\mathbf{DIV} : \mathcal{H}S \to HC$	Natural discrete analogs of differential operator dive rgence
$\mathbf{GRAD} : HN \to \mathcal{H}L$	Natural discrete analogs of differential operator gradient
$\mathbf{CURL} : \mathcal{H}L \to \mathcal{H}S$	Natural discrete analogs of differential operator curl
$\mathbf{I}_V^V$	Discrete volume integral over volume $\tilde{V}$
$\mathbf{I}_S^S$	Discrete surface integral over surface $\tilde{S}$
$\mathbf{I}_L^L$	Discrete line integral over broken line $\tilde{L}$

1. INTRODUCTION

Solving new and challenging problems with strong nonlinearities, discontinuities, and complex physical processes will require advances in the quality and robustness of numerical algorithms. Experience has confirmed that the best results are usually obtained when the discrete model

preserves the fundamental properties of the original continuum model for the underlying physical problem. Robust, realistic algorithms for large-scale simulations are more capable when they are based on solid mathematical theory and when the discrete model maintains many of the important properties of the continuum model. These properties include conservation laws, symmetries in the solution, and the nondivergence of particular vector fields (they are divergence free).

Developing discrete algorithms that capture all the important characteristics of the physical problem is more difficult as mathematical models become more complex to account for additional physical processes and more complex domains or boundary conditions. The difficulties will be easier to overcome if we are able to derive new discrete algorithms based on a general approach that can be applied to a wide range of physical systems. With this goal in mind, we have developed a discrete analog of vector and tensor calculus that can be used for an accurate approximation of continuum models for a wide range of physical processes.

Most partial differential equations (PDEs) can be formulated in terms of invariant, first-order differential operators, such as the divergence of vectors and tensors, the gradient of scalars and vectors, and curl of vectors. These first-order differential operators are the main objects of vector and tensor analysis and satisfy integral identities that are closely related to the conservation laws of continuum models. We use these coordinate-invariant first-order operators to create high-quality finite-difference methods (FDMs) based on discrete analogs of vector and tensor analysis.

The discrete analogs of integral identities can be used to construct discrete operators satisfying these identities using the support-operator method (SOM) [1-3]. 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 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 identities for differential operators. 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 **GRAD**; **GRAD** is defined to be the negative adjoint of **DIV**.

The SOM FDMs are based on fundamental mathematical principles that correspond to basic physical principles, and these FDMs provide accurate, robust, and stable approximations to differential operators on nonuniform structured and unstructured grids. Because the new FDMs mimic the invariant properties of continuum differential operators, they require fewer points to obtain the same accuracy when compared with many traditional methods. They also lead to a deeper understanding FDMs and of which physical laws are of captured by FDMs.

The properties of the discrete operators, which follow from the construction of FDMs by the SOM, can be used to prove convergence theorems for linear and nonlinear problems [4-8], and to understand the stability of FDMs [9-13], and grids with local refinement [14].

Using the local basis system of components for discrete vector fields is considered in [15-18]. When solving the heat equation, the vector component of heat flux normal to sides of the cells is continuous across discontinuities and is the natural vector component to use when discretizing the vector field. This approach improves accuracy and is especially useful for problems with discontinuous coefficients. For the same reason, in magnetic field diffusion, it is natural to use use the normal components of magnetic field and the tangential components of the electric field.

The SOM has been applied to the equations of magnetic field diffusion [16] and, in particular, for anisotropic conductivity [19], Maxwell equations [20], the biharmonic equation [21], and the static problems of elasticity [22]. The approximation of the general equations of motion, which involve operations on tensor objects, such as the divergence of a tensor and the gradient of vectors, is considered in [2,23]; and applications to the equations of gas dynamics in Eulerian form are considered in [24]. The SOM is used to construct FDMs in a curvilinear orthogonal coordinate system in [25,26]. High-order SOM FDMs are constructed in [27], and the SOM has been used to construct finite-difference schemes on triangular grids [9,28], Voronoi grids [12,13,29,30], and grids with local refinement [14].

Practical applications of the SOM include simulations of controlled laser fusion [31]; the collapse of a quasispherical target in a hard cone [32]; the Rayleigh-Taylor instability for incompressible flows [33]; the compression of a toroidal plasma by a quasispherical liner [34,35]; an overcompressed detonation wave in a conic channel [36]; a magnetic field in a spiral band reel [37]; the magnetic field of a toroidal spiral with a screen [38]; the flows of a viscous incompressible liquid with a free surface [39]; and a microwave plasma generator [40].

The main *goal* of this series of papers is to create a *discrete analog of vector analysis for grid functions associated with logically rectangular, nonorthogonal, nonsmooth grids*. The elements of the theory to achieve this goal have a long history on rectangular and orthogonal grids [41-52].

Mimetic difference operators, which preserve (mimic) the properties of the differential operators, can be investigated using functional analysis. This approach has been successfully applied to the study of problems in mathematical physics. For example, the method of orthogonal projections forms a considerable part of the theory of generalized solutions [53], and Weil's Theorem on orthogonal decomposition plays a fundamental role in solving the Navier-Stokes equations [54]. The difference version of Weil's Theorem, formulated in [52] for square grids in 2-D, can be used to construct high-quality FDMs for these equations [55].

A discrete vector field theory on Delaunay-Voronoi meshes is created in [56] with applications in [57,58]. This theory uses the special geometrical property of the Delaunay-Voronoi meshes that the sides of Delaunay triangulations are orthogonal to the corresponding sides of the Voronoi polygons. The local orthogonality property makes these grids similar to the usual orthogonal grids. Another important property of these grids is that vertices of triangles can be also considered as "centers" of the Voronoi cells. Unfortunately, the theory created in [56] does not cover some very important discretizations of scalar and vectors (see, for example, [59]).

A theoretical foundation does exist for some mimetic FDMs based on the tools and concepts of algebraic topology [41-46,60]. The results from these studies, and history of this approach, are summarized in a recently published book [61]. These methods use exterior differential forms to represent of the equations in invariant form. In this approach, a logically rectangular grid in the plane, used in standard FDMs, is considered as a simplicial complex (in the sense of algebraic topology [62], see, for example, [41,46,63,64]). The operators d and δ, acting on "functions on the complex" and defined by the combinatorial structure, generate difference analogs of the classical operators of mathematical physics (such as gradient, divergence, curl, and the Laplacian).

Applying the algebraic topology to construct the discrete analog of the metric conjuagacy operator "$*$" on nonorthogonal, nonsmooth, logically rectangular grids requires establishing a complex set of definitions and mathematical tools. Moreover, this approach is natural for a specific discretization of the vector field and cannot be easily used for many widely used discretizations, including the usual nodal discretization of the Cartesian components of a vector.

The language and tools of advanced calculus are more widely known and used for formulating the theorems and concepts of vector and tensor analysis than is the language of algebraic topology [65]. This is especially true among the applied numerical researchers in the field of scientific computing, solving systems of PDEs. Because this community is our primary audience, we formulate our discrete vector and tensor analysis without using the language of algebraic topology.

We consider different discrete representations of scalar, vector, and tensor functions on logically rectangular grids and define projection operators between different spaces that preserve some important properties of the functions. We introduce the discrete analog of the line integral, the potential vector, the flux of the vector through a surface, and the circulation of a vector along a contour. We construct discrete analogs for the gradient of scalar functions and investigate discrete analogs for the directional derivative. We define a discrete analog of the divergence operator based on Gauss' Theorem and use Stokes' Theorem to define a discrete curl. We then prove discrete versions of the standard theorems of vector analysis (e.g., [65]).

After introducing notations related to 2-D logically rectangular grids, we describe cell-valued discretization HC, and nodal discretization HN, for scalar functions, and give two "natural" descriptions of discrete vector fields: by the components normal to faces of the cell $\mathcal{HS}$, and by the components aligned with the edges of the cell $\mathcal{HL}$. Here, and later names of spaces of scalar functions begin with H, and names of spaces of vector functions begin with $\mathcal{H}$. These components are natural because they correspond to the natural domain and range of values for discrete operators. (These choices are also clearly based on algebraic topology and geometry of the spaces [61,63,64].)

Next, we use coordinate invariant definitions to define "natural" discrete analogs of the divergence, gradient, and curl. The divergence is defined by

$$\mathbf{div}\,\vec{W} = \lim_{V \to 0} \frac{\oint_{\partial V} \left(\vec{W}, \vec{n}\right)\,dS}{V}, \tag{1.1}$$

where V is a cell volume bounded by surface S and $\vec{n}$ is the outward normal to S. The directional derivative in the direction of the unit vector $\vec{k}$ and related component of vector $\mathbf{grad}\,u$ is defined by

$$\left(\mathbf{grad}\,u, \vec{k}\right) = \frac{\partial u}{\partial k}. \tag{1.2}$$

The curl satisfies

$$\left(\vec{n}, \mathbf{curl}\,\vec{A}\right) = \lim_{S \to 0} \frac{\oint_l \left(\vec{A}, \vec{l}\right)\,dl}{S}, \tag{1.3}$$

where $\vec{n}$ is normal to the surface S, spanning the contour l, and $\vec{l}$ is the unit tangential vector to this contour.

The definitions of discrete operators based on these formulas hold in any coordinate system because they involve only geometrical quantities such as length, area, and volumes, and use only coordinate invariant components of vectors. We will interpret these formulas in terms of curvilinear coordinates, such as lengths of the elements of coordinate curves, areas of the elements of coordinate surfaces, and elementary volumes.

These natural discrete operators derived from coordinate invariant definitions (1.1)–(1.3) have the following domains and ranges of values

$$\mathbf{DIV} : \mathcal{HS} \to HC, \qquad \mathbf{GRAD} : HN \to \mathcal{HL}, \quad \text{and} \quad \mathbf{CURL} : \mathcal{HL} \to \mathcal{HS}. \tag{1.4}$$

Note that, because of the inconsistency in the domains and ranges of these natural operators, the compound operators, such as **DIV GRAD**, **GRAD DIV** or **CURL CURL**, cannot be constructed. In the next paper, in this series, the discrete analogs of divergence, gradient, and curl with following domains and ranges will be constructed

$$\overline{\mathbf{DIV}} : \mathcal{HL} \to HN, \qquad \overline{\mathbf{GRAD}} : HC \to \mathcal{HS}, \quad \text{and} \quad \overline{\mathbf{CURL}} : \mathcal{HS} \to \mathcal{HL}. \tag{1.5}$$

The system of operators (1.4) and (1.5) will allow us to construct all the compound discrete operators.

We introduce the discrete volume integral of scalar functions from HC, the discrete surface integral for vector functions from $\mathcal{HS}$, and the discrete analog of the line integral for vector functions from $\mathcal{HL}$.

Next, we prove a discrete Gauss' Theorem; the discrete analog of 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 discrete analog of theorem that if $\vec{A} = \mathbf{grad}\,\varphi$, then line integral does not depend on path; and if line integral of some vector function is equal to zero for any closed path, then this vector is gradient of some scalar function.

In last section, we introduce the primitive forward and backward difference operators and the primitive metric operator related to multiplications of discrete functions by length of edges, areas of faces, and volumes of 3-D cells. The discrete operators **DIV**, **GRAD**, and **CURL** are expressed in terms of these primitive operators. This formulation helps elucidate the structure of the operators and will be useful in future studies, in particular, for investigating adjoint operators.
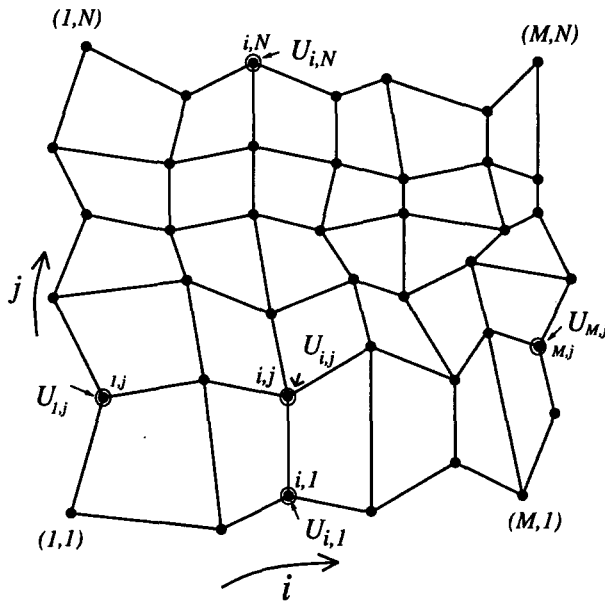
2. DEFINITIONS, GRIDS, AND DISCRETIZATIONS

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 1). The quadrilateral defined by the nodes (i, j), $(i+1, j)$, $(i+1, j+1)$, and $(i, j+1)$ is called the (i, j) cell (see Figure 2).
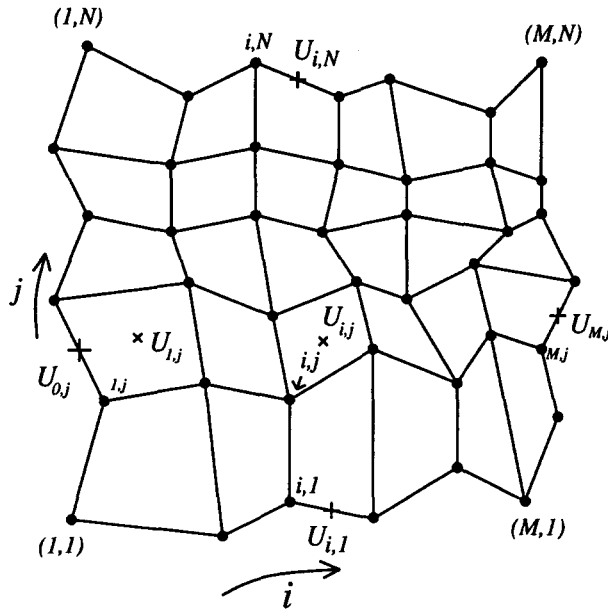
(a)

(b)

Figure 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).

The area of the (i, j) cell is denoted by $VC_{i,j}$, the length of the side that connects the vertices (i, j) and $(i, j+1)$ is denoted $S\xi_{i,j}$, and the length of the side that connects the vertices (i, j)
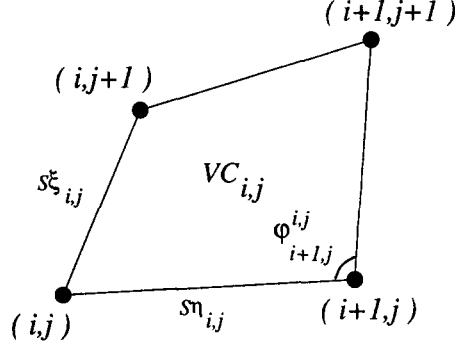
Figure 2. The (i, j) cell in a logically rectangular grid has area $VC_{i,j}$ and sides $S\xi_{i,j}$, $S\eta_{i,j}$, $S\xi_{i+1,j}$, and $S\eta_{i,j+1}$. The interior angle between $S\eta_{i,j}$ and $S\xi_{i+1,j}$ is $\varphi^{i,j}_{i+1,j}$.

and $(i + 1, j)$ is denoted $S\eta_{i,j}$. The angle between any two adjacent sides of cell (i, j) that meet at node (k, l) is denoted $\varphi^{i,j}_{k,l}$.

The parameter h characterizes the density of the grid

$$h = \max\left\{ \frac{1}{M-1}, \frac{1}{N-1} \right\}. \tag{2.1}$$

We assume the mild smoothness condition that the cells are convex, and there exists constants $C^1_{\max}$ and $C^1_{\min}$ independent of h such that

$$C^1_{\min} h^2 \leq VC_{(i,j)} \leq C^1_{\max} h^2, \tag{2.2}$$

that there exists constants $C^2_{\max}$ and $C^2_{\min}$, which do not depend on h such that

$$C^2_{\min} h \leq S\xi_{(i,j)}, \qquad S\eta_{(i,j)} \leq C^2_{\max} h, \tag{2.3}$$

and that there exits a constant $\epsilon > 0$ such that

$$\sin\left(\varphi^{(i,j)}_{(k,l)}\right) > \epsilon, \tag{2.4}$$

where ϵ is constant independent of h.

When we determine discrete differential operators, such as **CURL**, it is useful to consider a grid in 2-D as a projection of a 3-D grid. This approach makes it is easier to later generalize FDMs to 3-D 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 3).

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, the ζ coordinate corresponds to the grid line where the index k is changing (i.e., height of the prism, see Figure 4).

We denote the length of the edge $(i, j, k) - (i+1, j, k)$ by $l\xi_{i,j,k}$, the length of the edge $(i, j, k) - (i, j + 1, k)$ by $l\eta_{i,j,k}$, and the length of the edge $(i, j, k) - (i, j, k + 1)$ by $l\zeta_{i,j,k}$ (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 $S\xi_{i,j,k}$, 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 $S\eta_{i,j,k}$. We use the notation $S\zeta_{i,j,k}$ for the area of 2-D cell (i, j), that is, $S\zeta_{i,j,k} = VC_{i,j}$. Because the artificially constructed 3-D cell is a right prism with unit height, we have

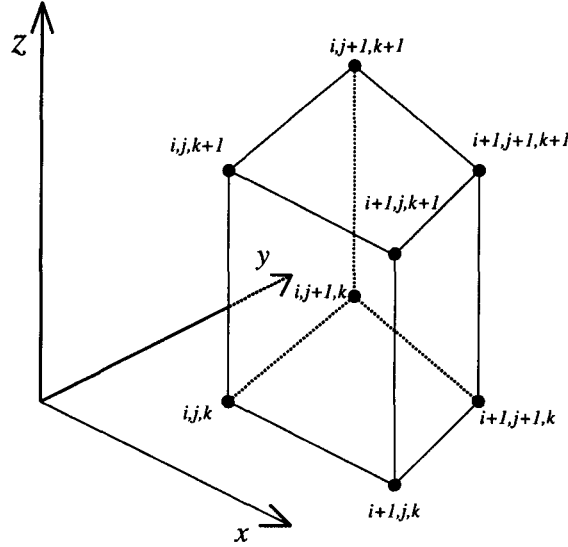$$S\xi_{i,j,k} = l\eta_{i,j,k} \cdot l\zeta_{i,j,k} = l\eta_{i,j,k} \tag{2.5}$$

Figure 3. The 2-D (i,j) cell $(z = 0)$ is interpreted as the base of a 3-D logically cuboid (i,j,k) cell (a prism) with unit height.
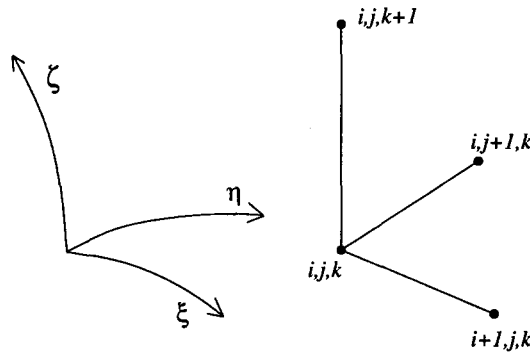

Figure 4. The (ξ, η, ζ) curvilinear coordinate system is approximated by the i, j, and k piecewise linear grid lines.

and

$$S\eta_{i,j,k} = l\xi_{i,j,k} \cdot l\zeta_{i,j,k} = l\xi_{i,j,k}. \tag{2.6}$$

With this 3-D interpretation, the 2-D notations $S\xi_{i,j}$ and $S\eta_{i,j}$ 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 $U_{i,j}$ is defined in the space HC and is given by its values in the cells (see Figure 1a), except at the boundary cells. The treatment of the boundary conditions requires introducing scalar function values at the centers of the boundary segments: $U_{(0,j)}$, $U_{(M,j)}$, where $j = 1, \ldots, N - 1$ and $U_{(i,0)}$, $U_{(i,N)}$, where $i = 1, \ldots, M - 1$. In 3-D, 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 1b). The indices vary in the same range as for coordinates $x_{i,j}$, $y_{i,j}$.

2.3. Discrete Vector Functions

We will 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 5a) 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 6a) where the vectors are defined tangential to the cell edges, is natural for approximations based on Stoke's circulation theorem.
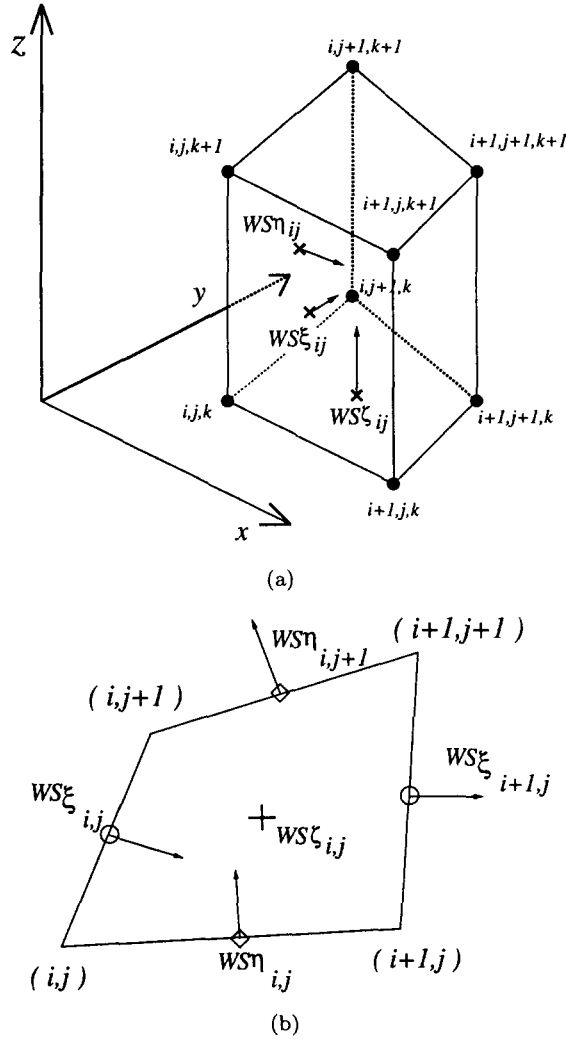

Figure 5. (a) $\mathcal{HS}$ discretization of a vector in 3-D; (b) 2-D interpretation of the $\mathcal{HS}$ discretization of a vector.

The projection of the 3-D $\mathcal{HS}$ vector discretization space into 2-D, results in the vectors being defined perpendicular to the quadrilateral cell sides and in a vertical vector in the cell center (see Figure 5b). We use the notation

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

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

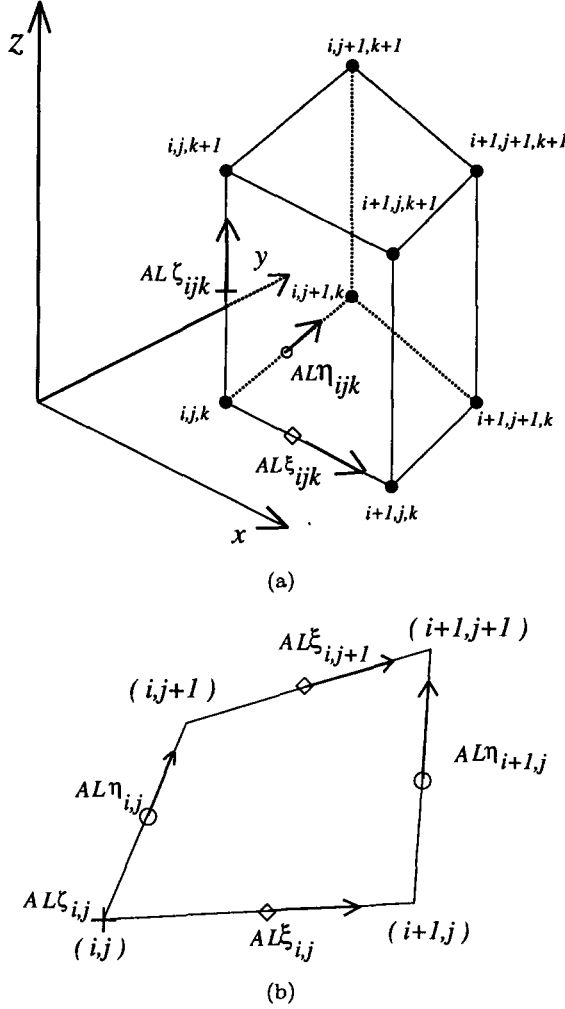$$WS\eta_{(i,j)} : i = 1, \ldots, M - 1; \qquad j = 1, \ldots, N,$$

Figure 6. (a) $\mathcal{HL}$ discretization of vector in 3-D; (b) 2-D interpretation of the $\mathcal{HL}$ discretization of a vector.

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

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

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

The projection of the 3-D $\mathcal{HL}$ vector discretization space into 2-D results in the vectors being defined tangential to the quadrilateral cell sides and in a vertical vector at the nodes (see Figure 6b). We use the notation

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

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

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

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

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

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

3. DISCRETE ANALOGS OF OPERATORS div, grad, AND curl

3.1. Operator DIV

As discussed in the Introduction, the coordinate invariant definition of the **div** operator is based on Gauss' divergence theorem

$$\mathbf{div}\,\vec{W} = \lim_{V \to 0} \frac{\oint_{\partial V} \left(\vec{W}, \vec{n}\right) dS}{V}, \tag{3.1}$$

where $\vec{n}$ is a unit outward normal to ∂V. The corresponding natural definition of the discrete divergence operator is

$$\mathbf{DIV} : \mathcal{H}S \to HC, \tag{3.2}$$

and

$$\left(\mathbf{DIV}\,\vec{W}\right)_{(i,j)} = \frac{1}{VC_{(i,j)}} \left\{ \left(WS\xi_{(i+1,j)}\,S\xi_{(i+1,j)} - WS\xi_{(i,j)}\,S\xi_{(i,j)}\right) \right. \\ \left. + \left(WS\eta_{(i,j+1)}\,S\eta_{(i,j+1)} - WS\eta_{(i,j)}\,S\eta_{(i,j)}\right) \right\}. \tag{3.3}$$

If the grid is smooth, in the sense that there exists a smooth transformation

$$x_{i,j} = x\left(\xi_i, \eta_j\right), \qquad y_{i,j} = y\left(\xi_i, \eta_j\right), \tag{3.4}$$

that maps the uniform grid

$$\xi_i = \frac{i-1}{M-1}, \qquad \eta_i = \frac{j-1}{N-1},$$

to our original grid, then equation (3.3) can be interpreted in terms of general curvilinear coordinates $(\xi, \eta, \zeta = z)$. The expression for **div** in general curvilinear coordinates (using the same description of the vector field, as we are using in the discrete case) is

$$\mathbf{div}\vec{w} = \frac{1}{\sqrt{|g|}} \left\{ \frac{\partial}{\partial \xi} \left(|G_{\xi\xi}|^{1/2}\,ws\xi\right) + \frac{\partial}{\partial \eta} \left(|G_{\eta\eta}|^{1/2}\,ws\eta\right) \right\}. \tag{3.5}$$

Here g is the metric tensor,

$$g = \begin{pmatrix} g_{\xi\xi} & g_{\xi\eta} & 0 \\ g_{\xi\eta} & g_{\eta\eta} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.6}$$

$G_{\xi\xi}$ and $G_{\eta\eta}$ are cofactors of $g_{\xi\xi}$ and $g_{\eta\eta}$, and $\sqrt{|\cdot|}$ is the determinant of the matrix.

The formula for **DIV** can be rewritten in a form similar to equation (3.5):

$$\left(\mathbf{DIV}\,\vec{W}\right)_{i,j}$$
$$= \frac{1}{(VC_{i,j})/\Delta\xi\,\Delta\eta\,\Delta\zeta} \left\{ \left[\frac{WS\xi_{i+1,j}\,(S\xi_{i+1,j}/\Delta\eta\,\Delta\zeta) - WS\xi_{i,j}\,(S\xi_{i,j}/\Delta\eta\,\Delta\zeta)}{\Delta\xi} \right] \right. \\ \left. + \left[\frac{WS\eta_{i,j+1}\,(S\eta_{i,j+1}/\Delta\xi\,\Delta\zeta) - WS\eta_{i,j}\,(S\eta_{i,j}/\Delta\xi\,\Delta\zeta)}{\Delta\eta} \right] \right\}, \tag{3.7}$$

where $\Delta\xi$, $\Delta\eta$, and $\Delta\zeta$ are the arbitrary uniform grid spacings, and are included to clarify the formula.

Comparing equations (3.5) and (3.7) leads to a correspondence between the analytical and discrete quantities:

$$\sqrt{|g|} \sim \frac{VC_{i,j}}{\Delta\xi\,\Delta\eta\,\Delta\zeta}, \qquad |G_{\xi\xi}|^{1/2} \sim \frac{S\xi_{i,j}}{\Delta\eta\,\Delta\zeta}, \qquad |G_{\eta\eta}|^{1/2} \sim \frac{S\eta_{i,j}}{\Delta\xi\,\Delta\zeta},$$

$$\frac{\partial}{\partial\xi}\left(|G_{\xi\xi}|^{1/2}\,ws\xi\right) \sim \left[\frac{WS\xi_{i+1,j}\,(S\xi_{i+1,j}/\Delta\eta\,\Delta\zeta) - WS\xi_{i,j}\,(S\xi_{i,j}/\Delta\eta\,\Delta\zeta)}{\Delta\xi} \right],$$

and

$$\frac{\partial}{\partial\eta}\left(|G_{\eta\eta}|^{1/2}\,ws\eta\right) \sim \left[\frac{WS\eta_{i,j+1}\,(S\eta_{i,j+1}/\Delta\xi\,\Delta\zeta) - WS\eta_{i,j}\,(S\eta_{i,j}/\Delta\xi\,\Delta\zeta)}{\Delta\eta}\right].$$

Also, the elementary volume and surface elements of the coordinate surfaces are

$$dV = \sqrt{|g|}\,d\xi\,d\eta\,d\zeta,$$
$$dS\xi = |G_{\xi\xi}|^{1/2}\,d\eta\,d\zeta,$$

and

$$dS\eta = |G_{\eta\eta}|^{1/2}\,d\xi\,d\zeta.$$

3.2. Operator GRAD

For any direction l, given by the unit vector $\vec{l}$, the directional derivative can be defined as

$$\frac{\partial u}{\partial l} = \left(\mathbf{grad}\,u, \vec{l}\right). \tag{3.8}$$

For function $U_{i,j} \in HN$, this relationship leads to coordinate invariant definition of the natural discrete gradient operator:

$$\mathbf{GRAD} : HN \to \mathcal{HL}. \tag{3.9}$$

The vector $\vec{G} = \mathbf{GRAD}\,U$ is defined as

$$GL\xi_{i,j} = \frac{U_{i+1,j} - U_{i,j}}{l\xi_{i,j}}, \qquad GL\eta_{i,j} = \frac{U_{i,j+1} - U_{i,j}}{l\eta_{i,j}}, \qquad GL\zeta_{i,j} = 0. \tag{3.10}$$

These formulas correspond to components of vector $\mathbf{grad}\,u$, that are orthogonal projections to tangential directions to coordinate curves of the curvilinear coordinate system:

$$\mathbf{grad}\,u = \begin{pmatrix} g_{\xi\xi}^{-1/2}\,\dfrac{\partial u}{\partial\xi} \\[2mm] g_{\eta\eta}^{-1/2}\,\dfrac{\partial u}{\partial\eta} \\[2mm] 0 \end{pmatrix}. \tag{3.11}$$

The correspondence between formulas (3.10) and (3.11) is clear when we recall the identities

$$dl\xi = g_{\xi\xi}^{1/2}, \qquad dl\eta = g_{\eta\eta}^{1/2}, \tag{3.12}$$

where $dl\xi$ and $dl\eta$ are the elements of arcs of coordinate curves.

3.3. Operator CURL

The coordinate invariant definition of the **curl** operator is based on the limit of Stoke's circulation theorem,

$$\left(\vec{n}, \mathbf{curl}\,\vec{B}\right) = \lim_{S\to 0}\frac{\oint_l \left(\vec{B}, \vec{l}\right)\,dl}{S}, \tag{3.13}$$

where S is the surface spanning (based on) the closed curve l, $\vec{n}$ is unit outward normal to S, and $\vec{l}$ is the unit tangential vector to the curve l.

To construct a discrete analog of equation (3.13), we first consider S corresponding to 2-D grid cell $S\zeta_{i,j,k} = VC_{i,j}$; then the contour l consists of the four edges $l\xi_{i,j,k}$, $l\eta_{i+1,j,k}$, $l\xi_{i,j+1,k}$, and $l\eta_{i,j}$, and $(\vec{B}, \vec{l})$ coincides with $BL\xi$ or $BL\eta$ on the corresponding edge. For this choice of S,

we obtain an approximation for the component of the vector **curl** $\vec{B}$, which is the orthogonal projection onto the direction perpendicular to surface $S\zeta_{i,j,k}$. The $RS\zeta$ component of vector $\vec{R} = \textbf{CURL}\,\vec{B}$ has following form:

$$RS\zeta_{i,j} = \frac{(BL\eta_{i+1,j}\,l\eta_{i+1,j} - BL\eta_{i,j}\,l\eta_{i,j}) - (BL\xi_{i,j+1}\,l\xi_{i,j+1} - BL\xi_{i,j}\,l\xi_{i,j})}{S\zeta_{i,j}}. \qquad (3.14)$$

If we will choose $(i,j,k) - (i,j+1,k) - (i,j+1,k+1) - (i,j,k+1)$ as S, and take into account that the integrals over the top and bottom edges cancel because $\vec{B}$ depends only on x and y, we get

$$RS\xi_{i,j} = \frac{BL\zeta_{i,j+1}\,l\zeta_{i,j+1,k} - BL\zeta_{i,j}\,l\zeta_{i,j,k}}{S\xi_{i,j,k}} = \frac{BL\zeta_{i,j+1} - BL\zeta_{i,j}}{l\eta_{i,j}}. \qquad (3.15)$$

Similarly for $S = [(i,j,k) - (i+1,j,k) - (i+1,j,k+1) - (i,j,k+1)]$,

$$RS\eta_{i,j} = -\frac{BL\zeta_{i+1,j,k}\,l\zeta_{i+1,j} - BL\zeta_{i,j}\,l\zeta_{i,j,k}}{S\eta_{i,j,k}} = -\frac{BL\zeta_{i+1,j} - BL\zeta_{i,j}}{l\xi_{i,j}}. \qquad (3.16)$$

Combining these three formulas defines all three components of the natural discrete analog of the **curl** operator:

$$\vec{R} = (RS\xi, RS\eta, RS\zeta) = \textbf{CURL}\,\vec{B},$$

where

$$\textbf{CURL} : \mathcal{HL} \to \mathcal{HS}.$$

In the continuous case, the formulas for these components of the **curl**, in a general curvilinear coordinate system are

$$RS\xi = +\frac{1}{\sqrt{|G_{\xi\xi}|}}\,\frac{\partial}{\partial\eta}\left(BL\zeta\,\sqrt{g_{\zeta\zeta}}\right), \qquad (3.17)$$

$$RS\eta = -\frac{1}{\sqrt{|G_{\eta\eta}|}}\,\frac{\partial}{\partial\xi}\left(BL\zeta\,\sqrt{g_{\zeta\zeta}}\right), \qquad (3.18)$$

and

$$RS\zeta = +\frac{1}{\sqrt{|G_{\zeta\zeta}|}}\left[\frac{\partial}{\partial\xi}\left(BL\eta\,\sqrt{g_{\eta\eta}}\right) - \frac{\partial}{\partial\eta}\left(BL\xi\,\sqrt{g_{\xi\xi}}\right)\right]. \qquad (3.19)$$

The discrete and continuous formulas correspond to each other when we take into account that in 2-D, we have

$$|G_{\zeta\zeta}| = g_{\xi\xi}\,g_{\eta\eta} - g_{\xi\eta}^2, \qquad (3.20)$$

$$|G_{\eta\eta}| = g_{\xi\xi}, \qquad |G_{\xi\xi}| = g_{\eta\eta}, \qquad (3.21)$$

and

$$g_{\zeta\zeta} = 1. \qquad (3.22)$$

4. PROPERTIES OF DIV, GRAD, AND CURL

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

4.1. Discrete Volume Integral of Scalar Function $U \in HC$

In HC, the grid cell is the primitive elementary volume used to construct FDMs; more complex regions will be expressed as a union of these primitive volumes. The discrete analog of the volume integral

$$\int_V u \, dV$$

is expressed as a sum over the primitive cells,

$$\mathbf{I}_V^V(U) = \sum_{\text{cells}} U_{i,j} \, VC_{i,j}, \tag{4.1}$$

where $\tilde{V}$ is the union of the primitive (i,j) cells (discrete volume).

4.2. Discrete Surface Integral of Vector Function $\vec{A} \in \mathcal{HS}$

In $\mathcal{HS}$, we define the primitive surfaces to be the faces of 3-D cells (that is $S\xi_{i,j}$, $S\eta_{i,j}$, $S\zeta_{i,j}$) and express more complex connected surfaces as the union of these surfaces. The discrete analogue of the surface integral of a vector, or the flux of a vector, through a surface

$$\int_S \left(\vec{A}, \vec{n} \right) dS,$$

where $\vec{n}$ is unit outward normal to the surface S, is expressed as

$$\mathbf{I}_{\tilde{S}}^S \left(\vec{A} \right) = \sum_{\xi\text{-surfaces}} WS\xi_{i,j} \, S\xi_{i,j} + \sum_{\eta\text{-surfaces}} WS\eta_{i,j} \, S\eta_{i,j} + \sum_{\zeta\text{-surfaces}} WS\zeta_{i,j} \, S\zeta_{i,j}, \tag{4.2}$$

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

4.3. Discrete Gauss' Theorem

Gauss' Theorem states that the flux of a vector through any closed surface is equal to the volume integral of the divergence,

$$\oint_{\partial V} \left(\vec{A}, \vec{n} \right) dS = \int_V \mathbf{div} \vec{A} \, dV. \tag{4.3}$$

The discrete Gauss' Theorem for elementary cell volumes follows directly from the definitions of **DIV**, of the discrete volume integral, and of the discrete flux of vector:

$$\mathbf{I}_{V_{i,j}}^V \left(\mathbf{DIV} \, \vec{A} \right) = \left(\mathbf{DIV} \, \vec{A} \right)_{i,j} VC_{i,j} = \mathbf{I}_{\partial V_{i,j}}^S \left(\vec{A} \right). \tag{4.4}$$

The discrete Gauss' Theorem for an arbitrary discrete volume $\tilde{V}$,

$$\mathbf{I}_{\tilde{V}}^V \left(\mathbf{DIV} \, \vec{A} \right) = \mathbf{I}_{\partial \tilde{V}}^S \left(\vec{A} \right), \tag{4.5}$$

follows then from the additive property of discrete volume and surface integrals.

4.4. $\mathbf{DIV}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{CURL}\,\vec{B}$

PROOF that $\mathbf{DIV\,CURL} \equiv 0$.

The 2-D **DIV** operator is defined only for vectors that lie in plane (x, y), $\vec{W} = (WS\xi, WS\eta, 0)$. A direct calculation easily verifies that $\mathbf{DIV\,CURL}\,\vec{B} = 0$, when two first components of vector $\mathbf{CURL}\,\vec{B}$ are given by equations (3.15) and (3.16), and the last component is zero:

$$
\left(\mathbf{DIV\,CURL}\,\vec{B}\right)_{i,j}
$$

$$
= \frac{1}{VC_{i,j}}\left\{[RS\xi_{i+1,j}\,S\xi_{i+1,j} - RS\xi_{i,j}\,S\xi_{i,j}] + [RS\eta_{i,j+1}\,S\eta_{i,j+1} - RS\eta_{i,j}\,S\eta_{i,j}]\right\}
$$

$$
= \frac{1}{VC_{i,j}}\left\{\left[\frac{BL\zeta_{i+1,j+1} - BL\zeta_{i+1,j}}{S\xi_{i+1,j}}\,S\xi_{i+1,j} - \frac{BL\zeta_{i,j+1} - BL\zeta_{i,j}}{S\xi_{i,j}}\,S\xi_{i,j}\right] \right.
$$

$$
\left. + \left[-\frac{BL\zeta_{i+1,j+1} - BL\zeta_{i,j+1}}{S\eta_{i,j+1}}\,S\eta_{i,j+1} + \frac{BL\zeta_{i+1,j} - BL\zeta_{i,j}}{S\eta_{i,j}}\,S\eta_{i,j}\right]\right\} \tag{4.6}
$$

$$
= \frac{1}{VC_{i,j}}\left\{[BL\zeta_{i+1,j+1} - BL\zeta_{i+1,j} - BL\zeta_{i,j+1} + BL\zeta_{i,j}]\right.
$$

$$
\left. + [-BL\zeta_{i+1,j+1} + BL\zeta_{i,j+1} + BL\zeta_{i+1,j} - BL\zeta_{i,j}]\right\} = 0.
$$

This property also results from fundamental principles that are clear in the derivations based on algebraic topology [63,64].

PROOF that if $\mathbf{DIV}\,\vec{A} = 0$, then $\vec{A} = \mathbf{CURL}\,\vec{B}$.

We first review the proof for the continuous case. For some differentiable vector $\vec{A}$ with Cartesian components A_x and A_y, if

$$
\mathbf{div}\,\vec{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} = 0, \tag{4.7}
$$

then we must show that there is a vector $\vec{B} = (0, 0, B_z)$, such that $\vec{A} = \mathbf{curl}\,\vec{B}$; that is,

$$
A_x = \frac{\partial B_z}{\partial y} \tag{4.8}
$$

and

$$
A_y = -\frac{\partial B_z}{\partial x}. \tag{4.9}
$$

The general solution of equation (4.8) is

$$
B_z(x, y) = \int_{y_0}^{y} A_x\,(x, \beta)\,d\beta + f(x), \tag{4.10}
$$

where $f(x)$ is an arbitrary function of x. Substituting this expression into equation (4.9) and using equation (4.7), we have

$$
A_y(x, y) = -\frac{\partial B_z}{\partial x} = -\int_{y_0}^{y} \frac{\partial A_x(x, \beta)}{\partial x}\,(x, \beta)\,d\beta - \frac{\partial f}{\partial x}\,(x)
$$

$$
= A_y(x, y) - A_y(x, y_0) - \frac{\partial f}{\partial x}\,(x), \tag{4.11}
$$

or

$$
\frac{\partial f}{\partial x} = -A_y(x, y_0). \tag{4.12}
$$

Substituting the general solution of equation (4.12),

$$
f(x) = -\int_{x_0}^{x} A_y\,(\alpha, y_0)\,d\alpha + \text{const}, \tag{4.13}
$$

into (4.10), and taking constant to be zero gives the explicit formula

$$B_z(x,y) = \int_{y_0}^{y} A_x(x,\beta)\,d\beta - \int_{x_0}^{x} A_y(\alpha,y_0)\,d\alpha, \tag{4.14}$$

and the continuous theorem is proved.

The proof for the discrete case follows an identical line of reasoning. We will not repeat the proof but will present just the final expression for discrete vector $\vec{B}$. If the discrete vector $\vec{A} = (AS\xi, AS\eta, 0)$ satisfies $\mathbf{DIV}\,\vec{A} = 0$, that is,

$$(AS\xi_{i+1,j}\,S\xi_{i+1,j} - AS\xi_{i,j}\,S\xi_{i,j}) = -(AS\eta_{i,j+1}\,S\eta_{i,j} - AS\eta_{i,j+1}\,S\eta_{i,j}), \tag{4.15}$$

the corresponding discrete vector $\vec{B} = (0,0,BL\zeta)$ such that $\vec{A} = \mathbf{CURL}\,\vec{B}$ is defined by

$$BL\zeta_{i,j} = \sum_{j'=1}^{j-1} AS\xi_{i,j'}\,S\xi_{i,j'} - \sum_{i'=1}^{i-1} AS\eta_{i',1}\,S\eta_{i',1}. \tag{4.16}$$

To verify that

$$AS\xi_{i,j} = \left((\mathbf{CURL}\,\vec{B}S\xi)\right)_{i,j} = \frac{BL\zeta_{i,j+1} - BL\zeta_{i,j}}{S\xi_{i,j}}$$

$$= \frac{\left\{\left[\sum_{j'=1}^{j} AS\xi_{i,j'}\,S\xi_{i,j'} - \sum_{i'=1}^{i-1} AS\eta_{i',1}\,S\eta_{i',1}\right] - \left[\sum_{j'=1}^{j-1} AS\xi_{i,j'}\,S\xi_{i,j'} - \sum_{i'=1}^{i-1} AS\eta_{i',1}\,S\eta_{i',1}\right]\right\}}{S\xi_{i,j}},$$

note that the second and fourth terms within the braces cancel, and that, the first and third term in braces, after division by $S\xi_{i,j}$, give us desired result.

To verify that

$$AS\eta_{i,j} = ((\mathbf{CURL}\,\vec{B})S\eta)_{i,j} = -\frac{BL\zeta_{i+1,j} - BL\zeta_{i,j}}{S\eta_{i,j}}$$

$$= \frac{\left\{\left[\sum_{j'=1}^{j-1} AS\xi_{i+1,j'}S\xi_{i+1,j'} - \sum_{i'=1}^{i} AS\eta_{i',1}S\eta_{i',1}\right] - \left[\sum_{j'=1}^{j-1} AS\xi_{i,j'}S\xi_{i,j'} - \sum_{i'=1}^{i-1} AS\eta_{i',1}S\eta_{i',1}\right]\right\}}{S\eta_{i,j}}$$

$$= \frac{-\left\{\left[\sum_{j'=1}^{j-1}(AS\xi_{i+1,j}\,S\xi_{i+1,j} - AS\xi_{i,j}\,S\xi_{i,j})\right] - AS\eta_{i,1}\,S\eta_{i,1}\right\}}{S\eta_{i,j}}, \tag{4.17}$$

use equation (4.15) to transform the expression in square brackets

$$\sum_{j'=1}^{j-1}(AS\xi_{i+1,j}\,S\xi_{i+1,j} - AS\xi_{i,j}\,S\xi_{i,j}) = -\sum_{j'=1}^{j-1}(AS\eta_{i,j+1}\,S\eta_{i,j+1} - AS\eta_{i,j}\,S\eta_{i,j})$$

$$= -AS\eta_{i,j}\,S\eta_{i,j} + AS\eta_{i,1}\,S\eta_{i,1}. \tag{4.18}$$

The desired result follows directly from equations (4.17) and (4.18).

4.5. $\mathbf{CURL}\,\vec{A} = 0$ if and only if $\vec{A} = \mathbf{GRAD}\,U$

Proof that $\mathbf{CURL\,GRAD}\,U \equiv 0$.

In 2-D, the third component of the discrete gradient, defined by equation (3.10), is zero: $GL\zeta \equiv 0$. Consequently, from equations (3.15) and (3.16), the components $RS\xi$ and $RS\eta$ of the vector $\vec{R} = \mathbf{CURL\,GRAD}\,U$ are zero, and we have only to consider the $RS\zeta$ component defined by equation (3.14).

Direct substitution into equation (3.14) proves the result:

$$RS\zeta_{i,j} = \frac{\left[\left(\frac{U_{i+1,j+1}-U_{i+1,j}}{l\eta_{i+1,j}}l\eta_{i+1,j} - \frac{U_{i,j+1}-U_{i,j}}{l\eta_{i,j}}l\eta_{i,j}\right)\left(\frac{U_{i+1,j+1}-U_{i,j+1}}{l\xi_{i,j+1}}l\xi_{i,j+1} - \frac{U_{i+1,j}-U_{i,j}}{l\xi_{i,j}}l\xi_{i,j}\right)\right]}{S\zeta_{i,j}}$$

$$= \frac{[((U_{i+1,j+1} - U_{i+1,j}) - (U_{i,j+1} - U_{i,j}) - (U_{i+1,j+1} - U_{i,j+1}) - (U_{i+1,j} - U_{i,j}))]}{S\zeta_{i,j}} \equiv 0.$$

PROOF that if **CURL** $\vec{A} = 0$, then $\vec{A} = $ **GRAD** U.

For the space of nodal scalar discrete functions, HN, we can naturally define the discrete analog of the directional derivative using the unique set of directions given by the directions of the edges of cells. At each node, two discrete directional derivatives,

$$\frac{\delta U}{\delta l\xi_{i,j}} = \frac{U_{i+1,j} - U_{i,j}}{l\xi_{i,j}} \tag{4.19}$$

and

$$\frac{\delta U}{\delta l\eta_{i,j}} = \frac{U_{i,j+1} - U_{i,j}}{l\eta_{i,j}}, \tag{4.20}$$

coincide with the components of **GRAD** U, defined in equation (3.10).

In the space $\mathcal{HL}$, we introduce the discrete analog of line integral,

$$\int_L \left(\vec{A}, \vec{l}\right) \, dl.$$

The discrete analog of the line integral is defined naturally in $\mathcal{HL}$, where the vector field is described by its orthogonal projections onto the directions of the edges. These projections coincide with expression of the integrand in the line integral. In the discrete case, all the possible paths, L_{discrete}, are given by a connected combination of the edges; that is, the end of one edge is the beginning of next edge (see Figure 7).
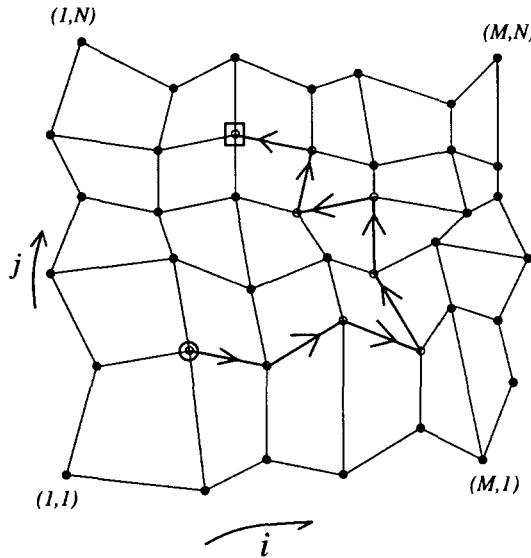

Figure 7. The discrete analog of the line integral starting at the ○ node and ending at the □ node, follows a connected combination of cell edges.

We will denote the discrete analog of the line integral as

$$\mathbf{I}_{\tilde{L}}^L\left(\vec{A}\right) = \sum_{\xi\text{-edges}} AL\xi_{i,j}\, l\xi_{i,j} + \sum_{\eta\text{-edges}} AL\eta_{i,j}\, l\eta_{i,j}, \tag{4.21}$$

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

THEOREM. *The discrete line integral of the vector function* $\vec{A} = $ **GRAD** U *over an arbitrary connected path is equal to the difference between function values at the first and last nodes of the path.*

The discrete line integral of **GRAD** *U over one edge of the path is equal to the difference of the function values at the ends of this edge. For example, for edge $l\xi_{i,j}$,*

$$\mathbf{I}^{L}_{l\xi_{i,j}} (\mathbf{GRAD}) = \frac{U_{i+1,j} - U_{i,j}}{l\xi_{i,j}} \, l\xi_{i,j} = U_{i+1,j} - U_{i,j}. \tag{4.22}$$

The complete line integral can be expressed as the sum of the edge integrals. Because the end of one edge is the beginning of next edge in the path, all the function values in the sum of these pieces cancel, except for the first and last node. Therefore, the value of line integral of **GRAD** *U does not depend on the path, and in particular, the line integral of* **GRAD** *U over the closed path is zero.*   ∎

The reverse of this theorem is also true.

THEOREM. *If the discrete line integral of the vector function $\vec{A} \in \mathcal{HL}$ is zero for any closed path, then this vector function is the discrete gradient of some scalar function in HN; that is, $\vec{A} = \mathbf{GRAD}\, U$.*

Consider the two paths L and L' that start at the node (i_0, j_0) and end at the node (i, j). By the condition of the theorem,

$$\mathbf{I}^{L}_{L[(i_0,j_0)\to(i,j)]}\left(\vec{A}\right) + \mathbf{I}^{L}_{L'[(i,j)\to(i_0,j_0)]}\left(\vec{A}\right) = 0, \tag{4.23}$$

where the notation explicitly indicates the first and last node in each path. When we change the direction of the line integral, the sign changes. Hence,

$$\mathbf{I}^{L}_{L[(i_0,j_0)\to(i,j)]}\left(\vec{A}\right) = \mathbf{I}^{L}_{L'[(i_0,j_0)\to(i,j)]}\left(\vec{A}\right). \tag{4.24}$$

That is, the line integral is independent of the path from a fixed node node (i_0, j_0), and it can be expressed as a single-valued function,

$$U_{(i,j)} = \mathbf{I}^{L}_{L[(i_0,j_0)\to(i,j)]}\left(\vec{A}\right), \tag{4.25}$$

where L can be any path connecting nodes (i_0, j_0) and (i, j).

Then for the neighboring node $(i+1, j)$,

$$U_{(i+1,j)} - U_{(i,j)} = \mathbf{I}^{L}_{L[(i_0,j_0)\to(i+1,j)]}\left(\vec{A}\right) - \mathbf{I}^{L}_{L[(i_0,j_0)\to(i,j)]}\left(\vec{A}\right) = \mathbf{I}^{L}_{L[(i,j)\to(i+1,j)]}\left(\vec{A}\right), \quad (4.26)$$

which also does not depend on path. Along the edge $l\xi_{i,j}$,

$$U_{(i+1,j)} - U_{(i,j)} = \mathbf{I}^{L}_{l\xi_{i,j}}\left(\vec{A}\right) = AL\xi_{i,j}\, l\xi_{i,j}, \tag{4.27}$$

or

$$AL\xi_{i,j} = \frac{U_{(i+1,j)} - U_{(i,j)}}{l\xi_{i,j}}. \tag{4.28}$$

Similarly, for the edge $l\eta_{i,j}$, we have

$$AL\eta_{i,j} = \frac{U_{(i,j+1)} - U_{(i,j)}}{l\eta_{i,j}}. \tag{4.29}$$

Hence,

$$\vec{A} = \mathbf{GRAD}\, U. \tag{4.30} \quad ∎$$

Also, given the vector function $\vec{A}$, we can explicitly construct the scalar function U. Because the line integral does not depend on the path, we can define

$$U_{(i,j)} = \sum_{i'=i_0}^{i} AL\xi_{i',j}\, l\xi_{i',j} + \sum_{j'=j_0}^{j} AL\eta_{i,j'},\, l\eta_{i,j'}, \tag{4.31}$$

where i_0 and j_0 are arbitrary indices.

The **CURL** $\vec{B}$, given by equations (3.15), (3.16), and (3.14), can be expressed in terms of line integrals over the 3-D grid as

$$RS\xi_{i,j} = \frac{\mathbf{I}^L_{\partial S\xi_{i,j,k}}\left(\vec{B}\right)}{S\xi_{i,j,k}}, \qquad RS\eta_{i,j} = \frac{\mathbf{I}^L_{\partial S\eta_{i,j,k}}\left(\vec{B}\right)}{S\eta_{i,j,k}}, \qquad RS\zeta_{i,j} = \frac{\mathbf{I}^L_{\partial S\zeta_{i,j,k}}(\vec{B})}{S\zeta_{i,j,k}}. \tag{4.32}$$

The condition **CURL** $\vec{A} = 0$, requires

$$\mathbf{I}^L_{\partial S\xi_{i,j,k}}\left(\vec{A}\right) = 0, \qquad \mathbf{I}^L_{\partial S\eta_{i,j,k}}\left(\vec{A}\right) = 0, \qquad \mathbf{I}^L_{\partial S\zeta_{i,j,k}}(\vec{A}) = 0, \tag{4.33}$$

for any (i,j). That is, the line integral of vector $\vec{A}$ for each primitive closed path (each of them contains edges which are the base for a face) are zero. Because any closed path can be formed by the union of primitive closed paths, the line integral of $\vec{A}$ over any closed path is zero, and, the previous theorem implies $\vec{A} = \mathbf{GRAD}\,U$. ∎

5. DIFFERENCING IN TERMS OF PRIMITIVE OPERATORS

5.1. Primitive Differencing and Metric Operators

For a better understanding of the structure of the discrete operators **GRAD**, **DIV**, and **CURL**, it is useful to introduce them in terms of primitive difference and metric operators.

We define the *primitive forward difference operators* by

$$(D\xi\,U)_{i,j} = U_{i+1,j} - U_{i,j}, \qquad (D\eta\,U)_{i,j} = U_{i,j+1} - U_{i,j}, \tag{5.1}$$

and the *backward difference operators* by

$$\left(\overline{D\xi}\,U\right)_{i,j} = U_{i,j} - U_{i-1,j}, \qquad \left(\overline{D\eta}\,U\right)_{i,j} = U_{i,j} - U_{i,j-1}. \tag{5.2}$$

Note that we are being a little vague in these definitions. The function U can have different meanings: it can be a scalar function in HC or HN or the component of a vector function in $\mathcal{HS}$ or $\mathcal{HL}$.

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

$$(L\xi\,U)_{i,j} = l\xi_{i,j}\,U_{i,j},\, (L\eta\,U)_{i,j} = l\eta_{i,j}\,U_{i,j},\, (L\zeta\,U)_{i,j} = l\zeta_{i,j}\,U_{i,j}, \tag{5.3}$$

$$(S\xi\,U)_{i,j} = S\xi_{i,j}\,U_{i,j},\, (S\eta\,U)_{i,j} = S\eta_{i,j}\,U_{i,j},\, (S\zeta\,U)_{i,j} = S\zeta_{i,j}\,U_{i,j}, \tag{5.4}$$

$$\left(V^C(U)\right)_{i,j} = VC_{i,j}\,U_{i,j}, \tag{5.5}$$

and

$$\left(V^N(U)\right)_{i,j} = VN_{i,j}\,U_{i,j}. \tag{5.6}$$

5.2. Expressions for GRAD, DIV, and CURL in Terms of of Primitive Operators

We will interpret the vector functions as column vectors. For example, the vector function in $\mathcal{HS}$ is represented as

$$\vec{W} = \begin{pmatrix} WS\xi \\ WS\eta \\ WS\zeta \end{pmatrix}.$$

Also, we will form block operators from the previously defined primitive operators. The rules of operation for block operators will be the same as the ones for matrices.

The operator **GRAD**, given by formula (3.10), can be represented as

$$\mathbf{GRAD} = \begin{pmatrix} L\xi^{-1} & 0 \\ 0 & L\eta^{-1} \end{pmatrix} \cdot \begin{pmatrix} D\xi \\ D\eta \end{pmatrix},$$

the operator **DIV** can be represented as

$$\mathbf{DIV} = (V^C)^{-1} \cdot (D\xi, D\eta) \cdot \begin{pmatrix} S\xi & 0 \\ 0 & S\eta \end{pmatrix},$$

and the operator **CURL** as

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

6. CONCLUSION

We introduced notations for 2-D logically rectangular grids, described both cell-valued and nodal discretizations for scalar functions, and constructed the natural discretizations of vector fields, using the vector components normal and tangential to the cell boundaries. We then defined natural discrete analogs of the divergence, gradient, and curl operators based on coordinate-invariant definitions.

We introduced the discrete volume integral of scalar functions, the discrete surface integral, and a discrete analog of the line integral and proved discrete versions of the main theorems relating these objects. These theorems include the the discrete analogs of following:

- **div** $\vec{A} = 0$ if and only if $\vec{A} = \mathbf{curl}\,\vec{B}$;
- **curl** $\vec{A} = 0$ if and only if $\vec{A} = \mathbf{grad}\varphi$;
- if $\vec{A} = \mathbf{grad}\,\varphi$, then the line integral does not depend on path;
- 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.

The natural discrete operators alone are not sufficient to construct discrete analogs of the second-order operators **div grad**, **grad div**, and **curl curl**, because of inconsistencies in domains and range of values. In the next paper [66], we will use the support-operators method to construct additional discrete analogs of the divergence, gradient, and curl with complementary domains and ranges. These new discrete operators are adjoints to the natural operators, and when combined with natural operators defined in this paper, allow all the compound operators to be constructed. By construction all of these operators satisfy discrete analogs of the integral identities satisfied by the differential operators. We will prove that adjoints operators satisfy similar theorems as natural operators.

APPENDIX

FORMULAS FOR DISCRETE OPERATORS ON RECTANGULAR GRIDS

In this appendix, we present formulas for the discrete operators **DIV**, **GRAD**, and **CURL** on a nonuniform 2-D, tensor-product, rectangular grid with spatial steps hX_i and hY_j (see Figure A.1).

Operator DIV

At the internal cells (i, j), where $i = 1, \ldots, M-1$ and $j = 1, \ldots, N-1$, the formula for operator **DIV** is given by

$$\left(\mathbf{DIV}\,\vec{W}\right)_{i,j} = \frac{WS\xi_{i+1,j} - WS\xi_{i,j}}{hX_i} + \frac{WS\eta_{i,j+1} - WS\eta_{i,j}}{hY_j}, \tag{A.1}$$

which has the stencil shown in Figure A.2.

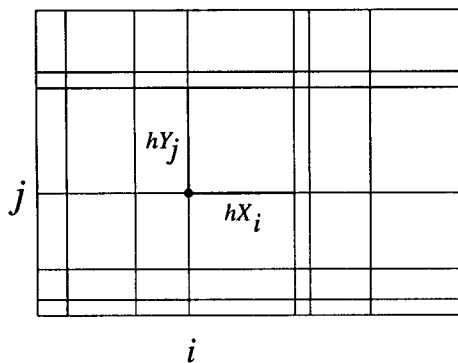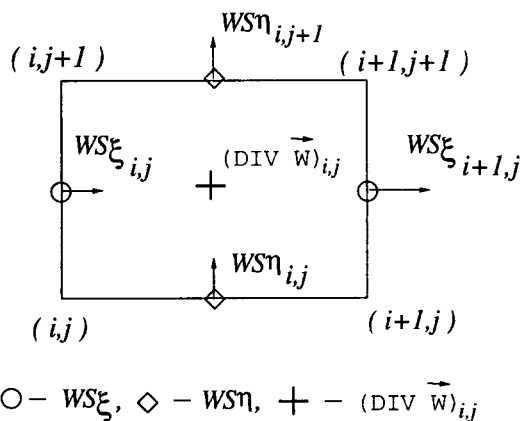Figure A.1. Tensor product, rectangular grid.

Figure A.2. Stencil for operator **DIV**.

Operator GRAD

The two components of the vector $\vec{G} = \mathbf{GRAD}\,U = (GL\xi, GL\eta)$, are defined on corresponding edges by

$$GL\xi_{i,j} = \frac{U_{i+1,j} - U_{i,j}}{hX_i}, \qquad i = 1, \ldots, M-1, \quad j = 1, \ldots, N, \qquad (A.2)$$

and

$$GL\eta_{i,j} = \frac{U_{i,j+1} - U_{i,j}}{hY_j}, \qquad i = 1, \ldots, M, \qquad j = 1, \ldots, N-1, \qquad (A.3)$$

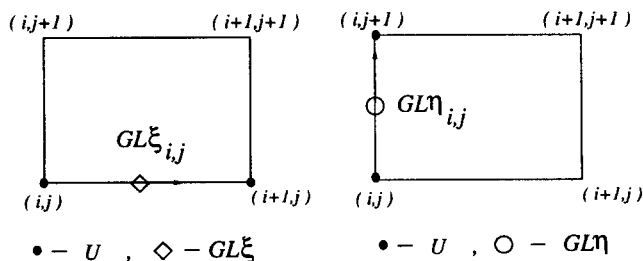and have the stencils shown in Figure A.3.

Figure A.3. Stencils for operator **GRAD**.

Operator CURL

The three components of the vector $\vec{R} = \mathbf{CURL}\, B = \vec{R} = (RS\xi, RS\eta, RS\zeta)$, are defined on corresponding faces by

$$RS\xi_{i,j} = \frac{BL\zeta_{i,j+1} - BL\zeta_{i,j}}{hY_j}, \qquad i = 1, \dots, M, \qquad j = 1, \dots, N-1, \qquad (A.4)$$

$$RS\eta_{i,j} = -\frac{BL\zeta_{i+1,j} - BL\zeta_{i,j}}{hX_i}, \qquad i = 1, \dots, M-1, \quad j = 1, \dots, N, \qquad (A.5)$$

and

$$RS\zeta_{i,j} = \frac{BL\eta_{i+1,j} - BL\eta_{i,j}}{hX_i} - \frac{BL\xi_{i,j+1} - BL\xi_{i,j}}{hY_j}. \qquad i = 1, \dots, M-1, \quad j = 1, \dots, N-1. \quad (A.6)$$

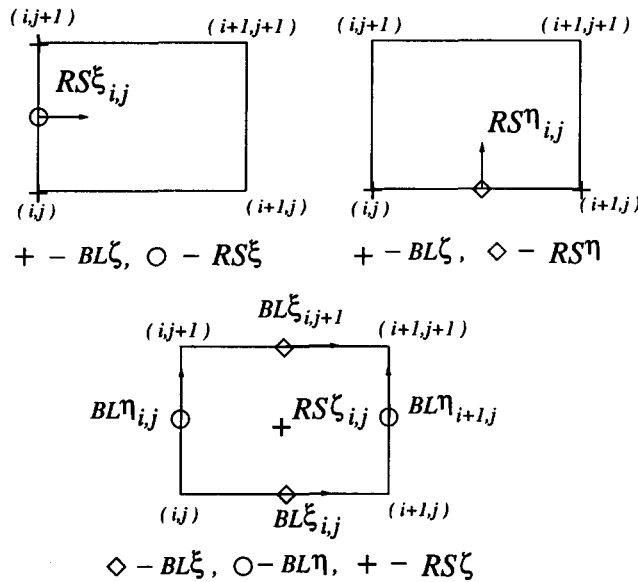The stencils for these components are shown on Figure A.4.

Figure A.4. Stencils for operator CURL.

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