

THE ORTHOGONAL DECOMPOSITION THEOREMS FOR MIMETIC FINITE DIFFERENCE METHODS*

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This paper is dedicated to the fond memory of Ami Harten.

Abstract. Accurate discrete analogs of differential operators that satisfy the identities and theorems of vector and tensor calculus provide reliable finite difference methods for approximating the solutions to a wide class of partial differential equations. These methods mimic many fundamental properties of the underlying physical problem including conservation laws, symmetries in the solution, and the nondivergence of particular vector fields (i.e., they are divergence free) and should satisfy a discrete version of the orthogonal decomposition theorem. This theorem plays a fundamental role in the theory of generalized solutions and in the numerical solution of physical models, including the Navier–Stokes equations and in electrodynamics. We are deriving mimetic finite difference approximations of the divergence, gradient, and curl that satisfy discrete analogs of the integral identities satisfied by the differential operators. We first define the natural discrete divergence, gradient, and curl operators based on coordinate invariant definitions, such as Gauss’s theorem, for the divergence. Next we use the formal adjoints of these natural operators to derive compatible divergence, gradient, and curl operators with complementary domains and ranges of values. In this paper we prove that these operators satisfy discrete analogs of the orthogonal decomposition theorem and demonstrate how a discrete vector can be decomposed into two orthogonal vectors in a unique way, satisfying a discrete analog of the formula $\vec{A} = \mathbf{grad} \varphi + \mathbf{curl} \vec{B}$. We also present a numerical example to illustrate the numerical procedure and calculate the convergence rate of the method for a spiral vector field.

Key words. discrete vector analysis, discrete orthogonal decomposition theorem, mimetic finite difference methods

AMS subject classifications. 65N06, 65P05, 53A45

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1. Introduction. We are developing a discrete analog of vector and tensor calculus that can be used to accurately approximate continuum models for a wide range of physical processes on logically rectangular, nonorthogonal, nonsmooth grids. These finite difference methods preserve fundamental properties of the original continuum differential operators and allow the discrete approximations of partial differential equations (PDEs) to mimic critical properties of the underlying physical problem including conservation laws, symmetries in the solution, and the nondivergence of particular vector fields (i.e., they are divergence free). These discrete analogs of differential operators satisfy the identities and theorems of vector and tensor calculus and are providing new reliable finite difference methods for a wide class of PDEs.

The orthogonal decomposition theorem plays a fundamental role in the theory of generalized solutions and in the numerical approximation of physical models, including the Navier–Stokes equations and in electrodynamics. In this paper, we will prove discrete analogs of the orthogonal decomposition theorem for the discretization of a vector field. That is, we prove that for given discrete divergence and curl, a discrete vector can be decomposed into two orthogonal vectors in a unique way satisfying

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a discrete analog of the formula $\vec{A} = \mathbf{grad} \varphi + \mathbf{curl} \vec{B}$ if its normal or tangential component is given on the boundary.

In [16], we defined the natural discrete divergence, gradient, and curl operators based on coordinate invariant definitions, such as Gauss’s theorem, for the divergence. We introduced notations for two-dimensional (2-D) logically rectangular grids, defined analogues of line, surface, and volume integrals, described both cell 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.

The domains and ranges of the natural discrete operators arise “naturally” from discrete analogs of Stokes’s theorem. To form second-order nontrivial combinations of these operators, which are discrete analogs of $\mathbf{div grad}$, $\mathbf{grad div}$, and $\mathbf{curl curl}$, the range of the first operator must be equal to the domain of the second operator. The natural operators alone are not sufficient to construct discrete analogs of the second-order operators $\mathbf{div grad}$, $\mathbf{grad div}$, and $\mathbf{curl curl}$ because of inconsistencies in domains and range of values.

In [17], we used the formal adjoints of these natural operators to derive compatible divergence, gradient, and curl operators with complementary domains and ranges of values. These new discrete operators are adjoints to the natural operators and, when combined with natural operators, 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.

In [16] and [17], we proved discrete analogs of main theorems of vector analysis for both the natural and adjoint discrete operators. These theorems include Gauss’s theorem; the theorem that $\mathbf{div} \vec{A} = 0$ if and only if $\vec{A} = \mathbf{curl} \vec{B}$; the theorem that $\mathbf{curl} \vec{A} = 0$ 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.

The discrete analogs of the differential operators are derived and analyzed using the *support-operators method* (SOM) [33, 35, 36]. 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’s theorem. This initial discrete operator, called the *prime* operator, then *supports* the construction of other discrete operators, using discrete formulations of the integral identities

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

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

For example, if the initial discretization is defined for the divergence (*prime operator*), it should satisfy a discrete form of Gauss’s theorem. This prime discrete divergence, DIV, is then used to *support* the *derived* discrete operator GRAD satisfying a discrete version of the integral identity (1.1). The derived operator GRAD would then also be the negative adjoint of DIV.

The SOM uses the discrete versions of integral identities as a basis to construct discrete operators with compatible domains and ranges and is used to extend the set of discrete operators by forcing discrete analogs of the integral identities (1.1) or (1.2). In the simplest case, when boundary integrals vanish, the above entities imply

$\mathbf{div} = -\mathbf{grad}^*$ and $\mathbf{curl} = \mathbf{curl}^*$ in the sense of the inner products

$$(1.3) \quad (u, v)_H = \int_V u v dV, \quad (\vec{A}, \vec{B})_{\mathcal{H}} = \int_V (\vec{A}, \vec{B}) dV.$$

The natural discrete divergence is defined as a discrete operator from the space \mathcal{HS} of discrete vector functions, defined by their orthogonal projections onto directions perpendicular to the face of the cell, to the space HC of discrete scalar functions, given by their values in the cell (see [16] and section 3 of this paper for details)

$$\text{DIV} : \mathcal{HS} \rightarrow HC.$$

The discrete gradient,

$$\overline{\text{GRAD}} : HC \rightarrow \mathcal{HS},$$

is constructed as a negative adjoint to DIV,

$$(1.4) \quad \overline{\text{GRAD}} = -\text{DIV}^*,$$

where we have indicated the derived adjoint operator by the overbar.

The natural discrete gradient GRAD is defined as a discrete operator from space HN of discrete scalar functions, given by their values in the nodes, to the space \mathcal{HL} of discrete vector functions, defined by their orthogonal projections onto directions of the edges of the cell

$$\text{GRAD} : HN \rightarrow \mathcal{HL}.$$

The discrete divergence,

$$\overline{\text{DIV}} : \mathcal{HL} \rightarrow HN,$$

is constructed as a negative adjoint to GRAD,

$$(1.5) \quad \overline{\text{DIV}} = -\text{GRAD}^*.$$

In a similar way, the natural $\text{CURL} : \mathcal{HL} \rightarrow \mathcal{HS}$ is used to construct another discrete curl,

$$(1.6) \quad \overline{\text{CURL}} : \mathcal{HS} \rightarrow \mathcal{HL}, \quad \overline{\text{CURL}} = \text{CURL}^*.$$

These operators satisfy the main discrete theorems of vector analysis [16, 17].

The natural operators alone can be combined only to construct the *trivial* operators:

$$(1.7) \quad \text{DIV CURL} : \mathcal{HL} \rightarrow HC, \quad \text{DIV CURL} \equiv 0,$$

$$(1.8) \quad \text{CURL GRAD} : HN \rightarrow \mathcal{HS}, \quad \text{CURL GRAD} \equiv 0.$$

For example, we cannot apply DIV to GRAD because the range of values of GRAD does not coincide with the domain of operator DIV, and so on.

Similarly, the adjoint operators alone can be combined only to construct the *trivial* operators:

$$(1.9) \quad \overline{\text{DIV}} \overline{\text{CURL}} : \mathcal{HS} \rightarrow HN, \quad \overline{\text{DIV}} \overline{\text{CURL}} \equiv 0,$$

$$(1.10) \quad \overline{\text{CURL}} \overline{\text{GRAD}} : HC \rightarrow \mathcal{HL}, \quad \overline{\text{CURL}} \overline{\text{GRAD}} \equiv 0.$$

However, the natural and adjoint operators together can be combined to form all the *nontrivial* high-order operators:

$$(1.11) \quad \text{DIV } \overline{\text{GRAD}} : HC \rightarrow HC, \quad \overline{\text{DIV}} \text{ GRAD} : HN \rightarrow HN,$$

$$(1.12) \quad \text{CURL } \overline{\text{CURL}} : \mathcal{HS} \rightarrow \mathcal{HS}, \quad \overline{\text{CURL}} \text{ CURL} : \mathcal{HL} \rightarrow \mathcal{HL},$$

$$(1.13) \quad \text{GRAD } \overline{\text{DIV}} : \mathcal{HL} \rightarrow \mathcal{HL}, \quad \overline{\text{GRAD}} \text{ DIV} : \mathcal{HS} \rightarrow \mathcal{HS}.$$

In this paper, we use results from [16, 17] to prove discrete analogs of one of the most important theorems of vector analysis, i.e., the orthogonal decomposition theorem for vector fields. This theorem states that a vector function \vec{a} in a bounded domain, V , is uniquely determined by its divergence, curl, and values of normal component on the boundary:

$$(1.14) \quad \mathbf{div} \vec{a} = \rho, \quad (x, y, z) \in V,$$

$$(1.15) \quad \mathbf{curl} \vec{a} = \vec{\omega}, \quad (x, y, z) \in V,$$

and

$$(1.16) \quad (\vec{a}, \vec{n}) = \beta, \quad (x, y, z) \in \partial V.$$

Moreover, any vector \vec{a} can be represented in the form

$$(1.17) \quad \vec{a} = \mathbf{grad} \varphi + \mathbf{curl} \vec{B}.$$

This decomposition forms a considerable part of the theory of generalized solutions [41], and Weyl’s theorem on orthogonal decomposition plays a fundamental role in solving the Navier–Stokes equations [12, 19, 21, 40, 41] and in electrodynamics [15]. The discrete version of Weyl’s theorem, formulated in [39] for square grids in two dimensions, can be used to construct high-quality finite-difference methods (FDMs) for Navier–Stokes equations [3, 4]. The orthogonal decomposition theorem has been proved for discrete vector fields on both orthogonal grids [8, 22, 23, 24, 20, 32] and Voronoi grids [27, 28, 14]. Similar results for the finite-element method can be found in [12, 26]. The orthogonal decomposition theorem has been applied in numerical simulation to remove artificial vorticity from a velocity vector field [10]. Some general results for discrete models can also be found in [6, 7].

The discrete analog of the orthogonal decomposition theorem for vectors from the space \mathcal{HS} grids states that any discrete vector function $\vec{A} \in \mathcal{HS}$, where

$$(1.18) \quad \text{DIV } \vec{A} = \rho^h, \quad \overline{\text{CURL}} \vec{A} = \omega^h,$$

where the normal component of the vector \vec{A} is given on the boundary (for $\vec{A} \in \mathcal{HS}$ these are the components used to describe discrete vector field) and can be represented in the form

$$(1.19) \quad \vec{A} = \overline{\text{GRAD}} \varphi + \text{CURL} \vec{B},$$

where $\varphi \in HC$ and $\vec{B} \in \mathcal{HL}$. As in the continuous case, the discrete vector functions $\overline{\text{GRAD}} \varphi$ and $\text{CURL} \vec{B}$ are orthogonal to each other.

The theorem also holds for any discrete vector function $\vec{A} \in \mathcal{HL}$, where

$$(1.20) \quad \overline{\text{DIV}} \vec{A} = \rho^h, \quad \text{CURL} \vec{A} = \omega^h.$$

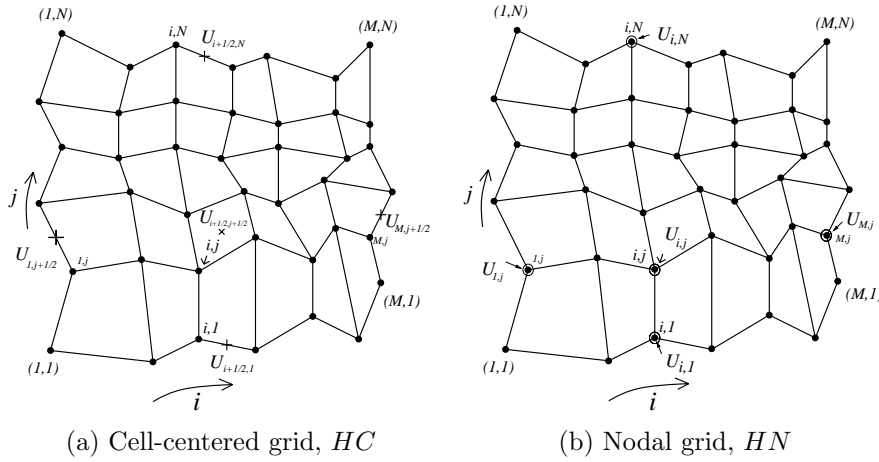


FIG. 2.1. On a logically rectangular grid, the scalar function values can be either cell-centered (HC), as in (a), or defined at the nodes (HN), as in (b).

Here the tangential component of the vector \vec{A} is given on the boundary (for $\vec{A} \in \mathcal{H}\mathcal{L}$ these are the components used to describe discrete vector field) and can be presented in the form

$$(1.21) \quad \vec{A} = \text{GRAD } \varphi + \overline{\text{CURL}} \vec{B},$$

where $\varphi \in HN$ and $\vec{B} \in \mathcal{H}\mathcal{S}$, and the discrete vector functions $\text{GRAD } \varphi$ and $\overline{\text{CURL}} \vec{B}$ are orthogonal to each other.

The discrete orthogonal decomposition theorem can be viewed from two different perspectives. In the first case, we can consider the solution of the discrete problem (1.18) as an approximation to the solution of the corresponding continuous problem (1.14), (1.15), (1.16). In the second case, we have a pure discrete problem: for a given discrete vector, $\vec{A} \in \mathcal{H}\mathcal{S}$, find its representation in the form (1.19), or for the vector $\vec{A} \in \mathcal{H}\mathcal{L}$, find its representation in the form (1.21).

After describing the grid, discretizations of scalar and vector functions, and inner products in spaces of discrete functions, we will review the derivation of the natural and adjoint finite difference analogs for the divergence, gradient, and curl. Next we prove the discrete orthogonal decomposition theorems for discrete vector functions from $\mathcal{H}\mathcal{S}$ and $\mathcal{H}\mathcal{L}$. Finally, we present a numerical example for the orthogonal decomposition of a spiral vector field and demonstrate a second-order convergence rate in max norm for the recovered (reconstructed) discrete vector function $\vec{A} \in \mathcal{H}\mathcal{S}$.

2. Spaces of 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 by $S\xi_{i, j+1/2}$, and the length of the side that connects the vertices (i, j) and $(i + 1, j)$ is denoted by $S\eta_{i+1/2, j}$. The angle between any two adjacent sides of cell (i, j) that meet at node (k, l) is denoted by $\varphi_{k, l}^{i+1/2, j+1/2}$.

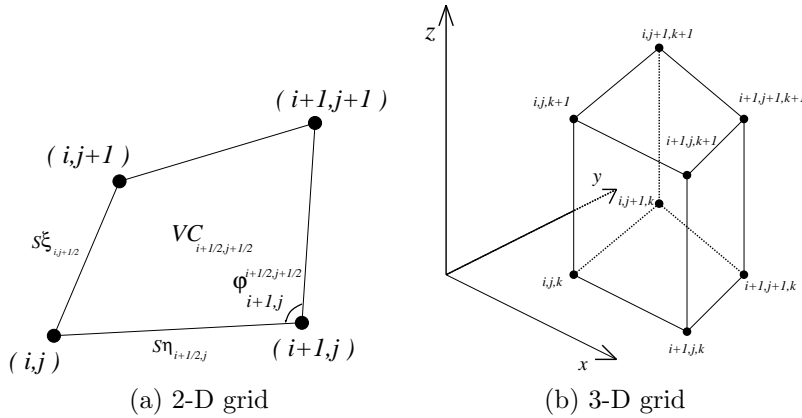


FIG. 2.2. (a) The $(i + 1/2, j + 1/2)$ cell in a logically rectangular grid has area $VC_{i+1/2,j+1/2}$ and sides $S\xi_{i+1/2}$, $S\eta_{i+1/2,j}$, $S\xi_{i+1/2,j+1/2}$, and $S\eta_{i+1/2,j+1}$. The interior angle between $S\eta_{i+1/2,j}$ and $S\xi_{i+1/2,j+1/2}$ is $\varphi_{i+1/2,j+1/2}$. (b) The 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.

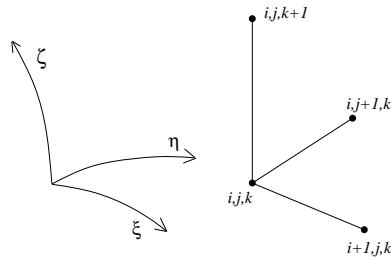


FIG. 2.3. The (ξ, η, ζ) curvilinear coordinate system is approximated by the i, j , and k piecewise linear grid lines.

When defining discrete differential operators, such as CURL, it is convenient to consider a 2-D grid as the projection of a three-dimensional (3-D) grid. This approach eliminates any ambiguity in the notation and simplifies generalizing the FDMs to 3-D. In this paper, we consider functions of the coordinates x and y and extend the grid into a third dimension, z , 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, η , or ζ coordinate corresponds to the grid line where the index i, j , or k is changing, respectively (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 $(i, j, k) - (i, j + 1, k) - (i, j, k + 1) - (i, j + 1, k + 1)$, denoted by $S\xi_{i,j+1/2,k+1/2}$, 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

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

and

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

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 and vector 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 at the centers of the boundary segments: $U_{(1,j+1/2)}, U_{(M,j+1/2)}$, where $j = 1, \dots, N - 1$, and $U_{(i+1/2,1)}, U_{(i+1/2,N)}$, where $i = 1, \dots, M - 1$. 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 $x_{i,j}, y_{i,j}$.

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 face vectors being defined perpendicular to the quadrilateral cell sides and in the cell-centered vertical vectors being defined perpendicular to the 2-D plane (see Figure 2.4 (b)). We use the notation

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

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

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

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

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

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

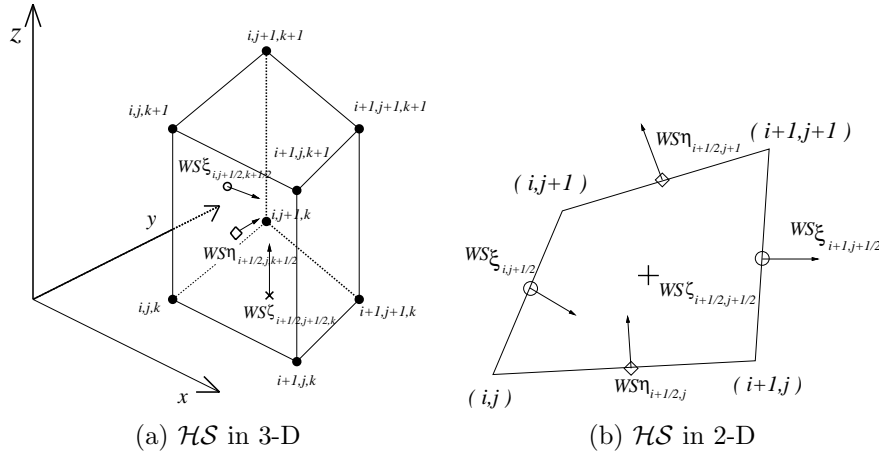


FIG. 2.4. (a) $\mathcal{H}\mathcal{S}$ discretization of a vector in three dimensions. (b) 2-D interpretation of the $\mathcal{H}\mathcal{S}$ discretization of a vector results in the face vectors being defined perpendicular to the cell sides and the vertical vectors being defined at cell centers perpendicular to the plane.

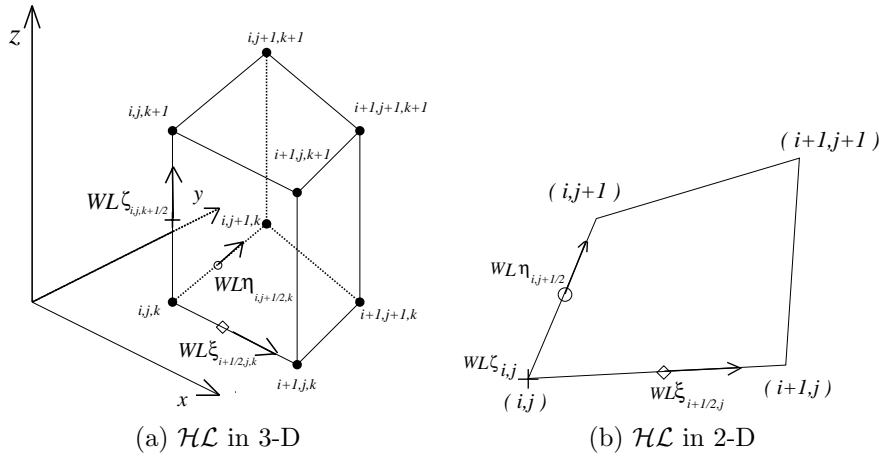


FIG. 2.5. (a) $\mathcal{H}\mathcal{L}$ discretization of a vector in three dimensions. (b) 2-D interpretation of the $\mathcal{H}\mathcal{L}$ discretization of a vector results in the edge vectors tangential to the cell sides and the vertical vectors being defined at cell nodes.

The projection of the 3-D $\mathcal{H}\mathcal{L}$ 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

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

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

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

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

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

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 notation.

2.3. Discrete inner products. In the space of discrete scalar functions, HC , (functions defined in the cell centers), the *natural* inner product corresponding to the continuous inner product

$$(2.1) \quad (u, v)_H = \int_V u v dV + \oint_{\partial V} u v dV$$

is

$$(2.2) \quad \begin{aligned} (U, V)_{HC} &= \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} U_{(i+1/2, j+1/2)} V_{(i+1/2, j+1/2)} VC_{(i+1/2, j+1/2)} \\ &+ \sum_{i=1}^{M-1} U_{(i+1/2, 1)} V_{(i+1/2, 1)} S\eta_{(i+1/2, 1)} + \sum_{j=1}^{N-1} U_{(M, j+1/2)} V_{(M, j+1/2)} S\xi_{(M, j+1/2)} \\ &+ \sum_{i=1}^{M-1} U_{(i+1/2, N)} V_{(i+1/2, N)} S\eta_{(i+1/2, N)} + \sum_{j=1}^{N-1} U_{(1, j+1/2)} V_{(1, j+1/2)} S\xi_{(1, j+1/2)}. \end{aligned}$$

In our future consideration, we will use the subspace of HN , HN^0 , where discrete functions are equal to zero on the boundary:

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

(the notation of “zero” above the name of a space indicates the subspace where the functions are equal to zero on the boundary), with the inner product defined as

$$(2.3) \quad (U, V)_{HN^0} \stackrel{def}{=} \sum_{i=2}^{M-1} \sum_{j=2}^{N-1} U_{(i,j)} V_{(i,j)} VN_{(i,j)},$$

where $VN_{(i,j)}$ is the nodal volume.

In the space of vector functions \mathcal{HS} , the *natural* inner product corresponding to the continuous inner product (3.14) is

$$(2.4) \quad (\vec{A}, \vec{B})_{\mathcal{HS}} = \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} (\vec{A}, \vec{B})_{(i+1/2, j+1/2)} VC_{(i+1/2, j+1/2)},$$

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 2.6). 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 $WS\xi$

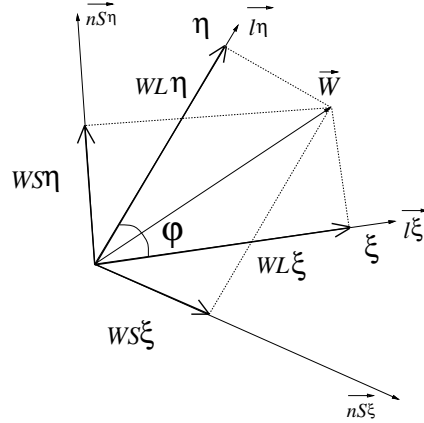


FIG. 2.6. The grid lines (ξ, η) form a local nonorthogonal coordinate system with unit vectors $\vec{l}_\xi, \vec{l}_\eta$ and corresponding unit normals to these directions, $n\vec{S}_\xi$ and $n\vec{S}_\eta$. In this basis, the components (WL_ξ, WL_η) of vector \vec{W} are the orthogonal projections onto the grid lines, and the components (WS_ξ, WS_η) are the orthogonal projections to the normal directions.

and WS_η of \vec{W} onto the normal vectors. The expression for the dot product of $\vec{A} = (AS_\xi, AS_\eta)$ and $\vec{B} = (BS_\xi, BS_\eta)$ is

$$(2.5) \quad (\vec{A}, \vec{B}) = \frac{AS_\xi BS_\xi + AS_\eta BS_\eta + (AS_\xi BS_\eta + AS_\eta BS_\xi) \cos \varphi}{\sin^2 \varphi},$$

where φ is the angle between these axes (see Figure 2.6).

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

$$(2.6) \quad (\vec{A}, \vec{B})_{(i+1/2, j+1/2)} = \sum_{k, l=0}^1 \frac{V_{(i+k, j+l)}^{(i+1/2, j+1/2)}}{\sin^2 \varphi_{(i+k, j+l)}} \cdot \left[AS_\xi_{(i+k, j+1/2)} BS_\xi_{(i+k, j+1/2)} + AS_\eta_{(i+1/2, j+l)} BS_\eta_{(i+1/2, j+l)} \right. \\ \left. + (-1)^{k+l} (AS_\xi_{(i+k, j+1/2)} BS_\eta_{(i+1/2, j+l)} + AS_\eta_{(i+1/2, j+l)} BS_\xi_{(i+k, j+1/2)}) \cos \varphi_{(i+k, j+l)} \right],$$

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

$$(2.7) \quad V_{(i+k, j+l)}^{(i+1/2, j+1/2)} \geq 0, \quad \sum_{k, l=0}^1 V_{(i+k, j+l)}^{(i+1/2, j+1/2)} = 1.$$

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.

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

$$(2.8) \quad (\vec{A}, \vec{B})_{\mathcal{HL}} = \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} (\vec{A}, \vec{B})_{(i+1/2, j+1/2)} VC_{(i+1/2, j+1/2)},$$

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 2.6). 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 the coordinate axes. If $\vec{A} = (AL\xi, AL\eta)$ and $\vec{B} = (BL\xi, BL\eta)$, then the dot product is

$$(2.9) \quad (\vec{A}, \vec{B}) = \frac{AL\xi BL\xi + AL\eta BL\eta - (AL\xi BL\eta + AL\eta BL\xi) \cos \varphi}{\sin^2 \varphi}.$$

From a formal point of view, the only difference between this formula and the one for the surface components (see (2.5)) is the minus sign before the third term. This difference can be easily understood by taking into account that the basis vectors of the nonorthogonal local systems are perpendicular to each other.

Equation (2.9) is used to approximate the dot product in a cell:

$$(2.10) \quad (\vec{A}, \vec{B})_{(i+1/2, j+1/2)} = \sum_{k, l=0}^1 \frac{V_{(i+k, j+l)}^{(i+1/2, j+1/2)}}{\sin^2 \varphi_{(i+k, j+l)}^{(i+1/2, j+1/2)}} \cdot \left[AL\xi_{(i+1/2, j+l)} BL\xi_{(i+1/2, j+l)} + AL\eta_{(i+k, j+1/2)} BL\eta_{(i+k, j+1/2)} - (-1)^{k+l} (AL\xi_{(i+1/2, j+l)} BL\eta_{(i+k, j+1/2)} + AL\eta_{(i+k, j+1/2)} BL\xi_{(i+1/2, j+l)}) \cos \varphi_{(i+k, j+l)}^{(i+1/2, j+1/2)} \right],$$

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

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

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

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

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

The natural and formal inner products satisfy the relationships

$$(2.11) \quad (U, V)_{HC} = [\mathcal{C}U, V]_{HC} \quad \text{and} \quad (\vec{A}, \vec{B})_{\mathcal{HS}} = [\mathcal{S}\vec{A}, \vec{B}]_{\mathcal{HS}},$$

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

$$(2.12) \quad [\mathcal{C}U, V]_{HC} = [U, \mathcal{C}V]_{HC} \quad \text{and} \quad [\mathcal{C}U, U]_{HC} > 0,$$

and therefore

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

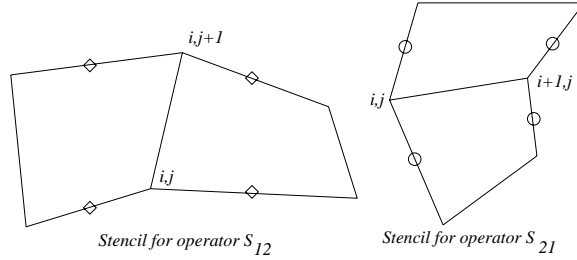


FIG. 2.7. The stencils of the components S_{12} and S_{21} of the symmetric positive operator \mathcal{S} that connects the natural and formal inner products $(\vec{A}, \vec{B})_{\mathcal{H}\mathcal{S}} = [\mathcal{S} \vec{A}, \vec{B}]_{\mathcal{H}\mathcal{S}}$.

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

$$(2.13) \quad \mathcal{S} \vec{A} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} AS\xi \\ AS\eta \end{pmatrix} = \begin{pmatrix} S_{11} AS\xi + S_{12} AS\eta \\ S_{21} AS\xi + S_{22} AS\eta \end{pmatrix},$$

and is symmetric and positive in the formal inner product

$$(2.14) \quad [\mathcal{S} \vec{A}, \vec{B}]_{\mathcal{H}\mathcal{S}} = [\vec{A}, \mathcal{S} \vec{B}]_{\mathcal{H}\mathcal{S}}, \quad [\mathcal{S} \vec{A}, \vec{A}]_{\mathcal{H}\mathcal{S}} > 0.$$

By comparing the formal and natural inner products

$$(2.15) \quad \begin{aligned} (\vec{A}, \vec{B})_{\mathcal{H}\mathcal{S}} &= [\mathcal{S} \vec{A}, \vec{B}]_{\mathcal{H}\mathcal{S}} = \sum_{i=1}^M \sum_{j=1}^{N-1} [(S_{11} AS\xi)_{(i,j+1/2)} + (S_{12} AS\eta)_{(i,j+1/2)}] BS\xi_{(i,j+1/2)} \\ &+ \sum_{i=1}^{M-1} \sum_{j=1}^N [(S_{21} AS\xi)_{(i+1/2,j)} + (S_{22} AS\eta)_{(i+1/2,j)}] BS\eta_{(i+1/2,j)}, \end{aligned}$$

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

$$(2.16) \quad \begin{aligned} (S_{11} AS\xi)_{(i,j+1/2)} &= \left(\sum_{k=\pm 1/2; l=0,1} \frac{V_{(i,j+l)}^{(i+k,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i+k,j+1/2)}} \right) AS\xi_{(i,j+1/2)}, \\ (S_{12} AS\eta)_{(i,j+1/2)} &= \sum_{k=\pm 1/2; l=0,1} (-1)^{k+\frac{1}{2}+l} \frac{V_{(i,j+l)}^{(i+k,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i+k,j+1/2)}} \cos \varphi_{(i,j+l)}^{(i+k,j+1/2)} AS\eta_{(i+k,j+l)}, \\ (S_{21} AS\xi)_{(i+1/2,j)} &= \sum_{k=\pm 1/2; l=0,1} (-1)^{k+\frac{1}{2}+l} \frac{V_{(i+l,j)}^{(i+1/2,j+k)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j+k)}} \cos \varphi_{(i+l,j)}^{(i+1/2,j+k)} AS\xi_{(i+l,j+k)}, \\ (S_{22} AS\eta)_{(i+1/2,j)} &= \left(\sum_{k=\pm 1/2; l=0,1} \frac{V_{(i+l,j)}^{(i+1/2,j+k)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j+k)}} \right) AS\eta_{(i+1/2,j)}. \end{aligned}$$

The operators S_{11} and S_{22} are diagonal, and the stencils for the operators S_{12} and S_{21} are shown on Figure 2.7. These formulas are valid only for sides of the grid cells interior to the domain. They can be applied at the sides on the domain boundary if the grid and discrete functions are first extended to a row of points outside the domain by using the appropriate boundary conditions.

The relationship between the natural and formal inner products in H^0_N is

$$(2.17) \quad (U, V)_{HN}^0 = [\mathcal{N}U, V]_{HN}^0,$$

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

$$(2.18) \quad [\mathcal{N}U, V]_{HN} = [U, \mathcal{N}V]_{HN}, \quad [\mathcal{N}U, U]_{HN} > 0,$$

and

$$(2.19) \quad (\mathcal{N}U)_{(i,j)} = VN_{(i,j)}U_{(i,j)}, \quad i = 2, \dots, M-1, \quad j = 2, \dots, N-1.$$

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

$$(2.20) \quad \mathcal{L}\vec{A} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} AL\xi \\ AL\eta \end{pmatrix} = \begin{pmatrix} L_{11}AL\xi + L_{12}AL\eta \\ L_{21}AL\xi + L_{22}AL\eta \end{pmatrix}.$$

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

$$(2.21) \quad [\mathcal{L}\vec{A}, \vec{B}]_{\mathcal{H}\mathcal{L}} = [\vec{A}, \mathcal{L}\vec{B}]_{\mathcal{H}\mathcal{L}}, \quad [\mathcal{L}\vec{A}, \vec{A}]_{\mathcal{H}\mathcal{L}} > 0.$$

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

$$\begin{aligned} (L_{11}AL\xi)_{(i+1/2,j)} &= \left(\sum_{k=\pm\frac{1}{2}; l=0,1} \frac{V_{(i+l,j)}^{(i+1/2,j+k)}}{\sin^2 \varphi_{(i,j+l)}^{(i+1/2,j+k)}} \right) AL\xi_{(i+1/2,j)}, \\ (L_{12}AL\eta)_{(i+1/2,j)} &= - \sum_{k=\pm\frac{1}{2}; l=0,1} (-1)^{k+\frac{1}{2}+l} \frac{V_{(i+l,j)}^{(i+1/2,j+k)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j+k)}} \cos \varphi_{(i+l,j)}^{(i+1/2,j+k)} AL\eta_{(i+l,j+k)}, \\ (2.22) \quad (L_{21}AL\xi)_{(i,j+1/2)} &= - \sum_{k=\pm\frac{1}{2}; l=0,1} (-1)^{k+\frac{1}{2}+l} \frac{V_{(i,j+l)}^{(i+k,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i+k,j+1/2)}} \cos \varphi_{(i,j+l)}^{(i+k,j+1/2)} AL\xi_{(i+k,j+l)}, \\ (L_{22}AL\eta)_{(i,j+1/2)} &= \left(\sum_{k=\pm\frac{1}{2}; l=0,1} \frac{V_{(i,j+l)}^{(i+k,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i+k,j+1/2)}} \right) AL\eta_{(i,j+1/2)}. \end{aligned}$$

The operators L_{11} and L_{22} are diagonal, and the stencils for the operators L_{21} and L_{12} (in 2-D) are the same as for the operators S_{12} and S_{21} (see Figure 2.7).

These discrete inner products satisfy the axioms of inner products; that is,

- $(A, B)_{H_h} = (B, A)_{H_h}$,
- $(\lambda A, B)_{H_h} = \lambda(A, B)_{H_h}$ (for all real numbers λ),
- $(A_1 + A_2, B)_{H_h} = (A_1 B)_{H_h} + (A_2 B)_{H_h}$,
- $(A, A)_{H_h} \geq 0$ and $(A, A)_{H_h} = 0$ if and only if $A = 0$.

In these axioms, A and B are either discrete scalar or discrete vector functions and $(\cdot, \cdot)_{H_h}$ is the appropriate discrete inner product.

Therefore the discrete inner products are true inner products and not just approximations of the continuous inner products. Also, discrete spaces are Euclidean spaces.

3. Discrete analogs of div, grad, and curl.

3.1. Natural operators.

3.1.1. Natural operator DIV. The coordinate invariant definition of the **div** operator is based on Gauss's divergence theorem:

$$(3.1) \quad \mathbf{div} \vec{W} = \lim_{V \rightarrow 0} \frac{\oint_{\partial V} (\vec{W}, \vec{n}) dS}{V},$$

where \vec{n} is a unit outward normal to boundary ∂V . To extend the operator **div** to the boundary, we define the extended divergence operator **d** as

$$(3.2) \quad \mathbf{d}\vec{w} = \begin{cases} +\mathbf{div} \vec{w}, & (x, y) \in V, \\ -(\vec{w}, \vec{n}), & (x, y) \in \partial V. \end{cases}$$

The corresponding natural definition of the discrete divergence operator is

$$(3.3) \quad \text{DIV} : \mathcal{HS} \rightarrow \mathcal{HC},$$

where

$$(3.4) \quad \begin{aligned} & (\text{DIV} \vec{W})_{(i+1/2, j+1/2)} \\ &= \frac{1}{VC_{(i,j)}} \{ (WS\xi_{(i+1, j+1/2)}) S\xi_{(i+1, j+1/2)} - WS\xi_{(i, j+1/2)} S\xi_{(i, j+1/2)} \\ &+ (WS\eta_{(i+1/2, j+1)}) S\eta_{(i+1/2, j+1)} - WS\eta_{(i+1/2, j)} S\eta_{(i+1/2, j)} \}. \end{aligned}$$

The discrete operator DIV is also extended to the boundary, and we denote the extended operator as **D**. This operator coincides with DIV, $(\mathbf{D} \vec{W})_{(i+1/2, j+1/2)} = (\text{DIV} \vec{W})_{(i+1/2, j+1/2)}$ on the internal cells and is defined on the boundary by

$$(3.5) \quad \begin{aligned} (\mathbf{D} \vec{W})_{(i+1/2, 1)} &= -WS\eta_{(i+1/2, 1)}, \quad i = 1, \dots, M-1, \\ (\mathbf{D} \vec{W})_{(i+1/2, N)} &= +WS\eta_{(i+1/2, N)}, \quad i = 1, \dots, M-1, \\ (\mathbf{D} \vec{W})_{(1, j+1/2)} &= -WS\xi_{(1, j+1/2)}, \quad j = 1, \dots, N-1, \\ (\mathbf{D} \vec{W})_{(M, j+1/2)} &= +WS\xi_{(M, j+1/2)}, \quad j = 1, \dots, N-1. \end{aligned}$$

3.1.2. Natural operator GRAD. For any direction l given by the unit vector \vec{l} , the directional derivative can be defined as

$$(3.6) \quad \frac{\partial u}{\partial \vec{l}} = (\mathbf{grad} u, \vec{l}).$$

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

$$(3.7) \quad \text{GRAD} : HN \rightarrow \mathcal{HL}.$$

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

$$(3.8) \quad GL\xi_{i+1/2, j} = \frac{U_{i+1, j} - U_{i, j}}{l\xi_{i+1/2, j}}, \quad GL\eta_{i, j+1/2} = \frac{U_{i, j+1} - U_{i, j}}{l\eta_{i, j+1/2}}, \quad GL\zeta_{i, j} = 0.$$

Note that if $\text{GRAD} U = 0$, then scalar discrete function U is a constant, and vice versa.

3.1.3. Natural operator CURL. The coordinate invariant definition of the **curl** operator is based on Stokes’s circulation theorem,

$$(3.9) \quad (\vec{n}, \mathbf{curl} \vec{B}) = \lim_{S \rightarrow 0} \frac{\oint_l (\vec{B}, \vec{l}) dl}{S},$$

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

Using the discrete analog of (3.9), we can obtain expressions for components of vector $\vec{R} = (RS\xi, RS\eta, RS\zeta) = \text{CURL} \vec{B}$, where

$$\text{CURL} : \mathcal{HL} \rightarrow \mathcal{HS},$$

and

$$(3.10) \quad \begin{aligned} RS\xi_{i,j+1/2} &= \frac{BL\zeta_{i,j+1} l\zeta_{i,j+1,k+1/2} - BL\zeta_{i,j} l\zeta_{i,j,k+1/2}}{S\xi_{i,j+1/2,k+1/2}} \\ &= \frac{BL\zeta_{i,j+1} - BL\zeta_{i,j}}{l\eta_{i,j+1/2}}, \end{aligned}$$

$$(3.11) \quad \begin{aligned} RS\eta_{i+1/2,j} &= -\frac{BL\zeta_{i+1,j,k+1/2} l\zeta_{i+1,j,k+1/2} - BL\zeta_{i,j,k+1/2} l\zeta_{i,j,k+1/2}}{S\eta_{i+1/2,j,k+1/2}} \\ &= -\frac{BL\zeta_{i+1,j} - BL\zeta_{i,j}}{l\xi_{i+1/2,j}}, \end{aligned}$$

and

$$(3.12) \quad \begin{aligned} RS\zeta_{i+1/2,j+1/2} &= \{ (BL\eta_{i+1,j+1/2} l\eta_{i+1,j+1/2} - BL\eta_{i,j+1/2} l\eta_{i,j+1/2}) - \\ &\quad (BL\xi_{i+1/2,j+1} l\xi_{i+1/2,j+1} - BL\xi_{i+1/2,j} l\xi_{i+1/2,j}) \} / S\zeta_{i+1/2,j+1/2} \end{aligned}$$

(see [16] for details).

Note that if $\vec{B} = (0, 0, BL\zeta)$, then the condition $\text{CURL} \vec{B} = 0$ is equivalent to $BL\zeta_{i,j} = \text{const}$. This follows since for any such vector \vec{B} we have that $RS\zeta_{i,j} = 0$, and from (3.10), (3.11) we can conclude that $RS\xi_{i,j}$ and $RS\eta_{i,j}$ equal zero only if $BL\zeta_{i,j} = \text{const}$.

3.1.4. Properties of natural discrete operators. The natural discrete operators satisfy discrete analogs of the theorems of vector analysis [16], including Gauss’s theorem; the theorem that $\mathbf{div} \vec{A} = 0$ if and only if $\vec{A} = \mathbf{curl} \vec{B}$; the theorem that $\mathbf{curl} \vec{A} = 0$ 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.

In this paper we use two theorems:

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

$\text{CURL} \vec{A} = 0$ if and only if $\vec{A} = \text{GRAD} U$, where $\vec{A} \in \mathcal{HL}$ and $U \in \mathcal{HN}$.

3.2. Adjoint operators. In [17], we use the SOM to derive the operators $\overline{\text{DIV}}$, $\overline{\text{GRAD}}$, and $\overline{\text{CURL}}$ 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.

3.2.1. Operator $\overline{\text{GRAD}}$. To construct the operator $\overline{\text{GRAD}}$ we use a discrete analog of the identity (1.1). If we introduce the space of scalar functions H with the inner product

$$(3.13) \quad (u, v)_H = \int_V u v dV + \oint_{\partial V} u v dS, \quad u, v \in H,$$

and the space of vector functions \mathbf{H} with inner product defined as

$$(3.14) \quad (\vec{A}, \vec{B})_{\mathbf{H}} = \int_V (\vec{A}, \vec{B}) dV, \quad \vec{A}, \vec{B} \in \mathbf{H},$$

then the identity (1.1) implies

$$(3.15) \quad \mathbf{d} = -\mathbf{grad}^*$$

or

$$(3.16) \quad \begin{aligned} (\mathbf{d} \vec{w}, u)_H &= \int_V u \mathbf{div} \vec{w} dV - \oint_{\partial V} u (\vec{w}, \vec{n}) dS \\ &= - \int_V (\vec{w}, \mathbf{grad} u) dV \\ &= (\vec{w}, -\mathbf{grad} u)_{\mathbf{H}}. \end{aligned}$$

We will base the definition of $\overline{\text{GRAD}}$ on a discrete analog of (3.14). In section 3.1.1, we defined the operator \mathbf{D} as the discrete analog of the continuous operator \mathbf{d} . Therefore the derived gradient operator is defined by $\overline{\text{GRAD}} \stackrel{def}{=} -\mathbf{D}^*$, 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).

Because $\mathbf{D} : \mathcal{HS} \rightarrow HC$, the adjoint operator is defined in terms of the inner products

$$(3.17) \quad (\mathbf{D} \vec{W}, U)_{HC} = (\vec{W}, \mathbf{D}^* U)_{\mathcal{HS}},$$

which can be translated into the formal inner products as

$$(3.18) \quad [\mathbf{D} \vec{W}, \mathcal{C} U]_{HC} = [\vec{W}, \mathcal{S} \mathbf{D}^* U]_{\mathcal{HS}}.$$

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

$$(3.19) \quad [\vec{W}, \mathbf{D}^\dagger \mathcal{C} U]_{\mathcal{HS}} = [\vec{W}, \mathcal{S} \mathbf{D}^* U]_{\mathcal{HS}}.$$

This relationship must be true for all \vec{W} and U . Therefore $\mathbf{D}^\dagger \mathcal{C} = \mathcal{S} \mathbf{D}^*$ or $\mathbf{D}^* = \mathcal{S}^{-1} \mathbf{D}^\dagger \mathcal{C}$, and the discrete analog of the operator **grad** can be represented as

$$(3.20) \quad \overline{\text{GRAD}} = -\mathbf{D}^* = -\mathcal{S}^{-1} \mathbf{D}^\dagger \mathcal{C}.$$

Because the operator \mathcal{S} is banded, its inverse \mathcal{S}^{-1} is full on nonorthogonal grids, and it is not possible to derive explicit formulas for the components of the operator $\overline{\text{GRAD}}$. Consequently, $\overline{\text{GRAD}}$ has a *nonlocal* stencil.

The discrete flux,

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

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

$$(3.21) \quad \mathcal{S} \vec{W} = \mathbf{D}^\dagger \mathcal{C} U,$$

where the right-hand side, $F = (FS\xi, FS\eta) = \mathbf{D}^\dagger \mathcal{C} U$, is

$$(3.22) \quad \begin{aligned} FS\xi_{i,j+1/2} &= -S\xi_{i,j+1/2} (U_{i+1/2,j+1/2} - U_{i-1/2,j+1/2}), \\ FS\eta_{i+1/2,j} &= -S\eta_{i+1/2,j} (U_{i+1/2,j+1/2} - U_{i+1/2,j-1/2}). \end{aligned}$$

The discrete operator \mathcal{S} is symmetric positive definite and can be represented as matrix with five nonzero elements in each row (see (2.16) and Figure 2.7).

To prove that $\overline{\text{GRAD}} U$ is zero if and only if U is constant, note that (3.22) implies that if U is a constant, then $\mathcal{D}^\dagger \mathcal{M} U = 0$ and therefore $\overline{\text{GRAD}} U = \mathcal{S}^{-1} \mathcal{D}^\dagger \mathcal{M} U = 0$. Conversely, if we assume $\overline{\text{GRAD}} U = 0$, then (3.20) and the fact that \mathcal{S} is positive definite imply

$$(3.23) \quad \mathcal{D}^\dagger \mathcal{M} U = 0.$$

This and (3.22) then give

$$\begin{aligned} U_{(i+1/2,j+1/2)} - U_{(i-1/2,j+1/2)} &= 0; & i = 1, \dots, M, \quad j = 1, \dots, N-1, \\ U_{(i+1/2,j+1/2)} - U_{(i+1/2,j-1/2)} &= 0; & i = 1, \dots, M-1, \quad j = 1, \dots, N, \end{aligned}$$

which implies that U is a constant. Therefore the null space of the discrete operator $\overline{\text{GRAD}}$ is composed only of the constant functions.

3.2.2. Operator $\overline{\text{DIV}}$. The operator $\overline{\text{DIV}}$ is defined as the negative adjoint to the natural operator GRAD . In the subspace of scalar functions, $\overset{0}{H}$, where $u(x, y) = 0$, $(x, y) \in \partial V$, the boundary term in integral identity (1.1) is zero, and therefore

$$(3.24) \quad \int_V (\vec{W}, \mathbf{grad} u) dV = - \int_V u \mathbf{div} \vec{W} dV.$$

That is, in this subspace \mathbf{div} is the negative adjoint of \mathbf{grad} in the sense of

$$(3.25) \quad (u, v)_{\overset{0}{H}} = \int_V u v dV \quad \text{and} \quad (\vec{A}, \vec{B})_{\mathcal{H}} = \int_V (\vec{A}, \vec{B}) dV.$$

The discrete adjoint operator $\overline{\text{DIV}} : \mathcal{H}\mathcal{L} \rightarrow \overset{0}{H}N$ is defined as the negative adjoint of the discrete natural operator $\text{GRAD} : \overset{0}{H}N \rightarrow \mathcal{H}\mathcal{L}$,

$$(3.26) \quad \overline{\text{DIV}} \stackrel{def}{=} -\text{GRAD}^*.$$

Using the connections between the formal and natural inner products,

$$(3.27) \quad \overline{\text{DIV}} = -\mathcal{N}^{-1} \cdot \text{GRAD}^\dagger \cdot \mathcal{L}.$$

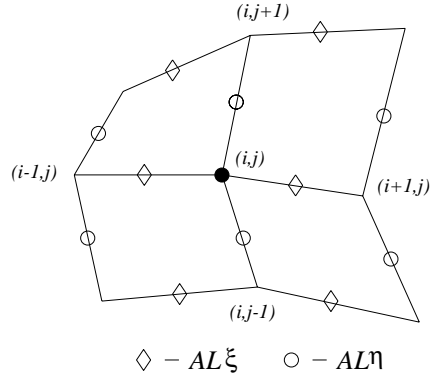


FIG. 3.1. Stencil for the operator $\overline{\text{DIV}} = -\text{GRAD}^* : \mathcal{HL} \rightarrow \mathcal{HN}$.

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

$$-\text{GRAD}^\dagger \vec{A} = \left(\frac{AL\xi_{i+1/2,j}}{l\xi_{i+1/2,j}} - \frac{AL\xi_{i-1/2,j}}{l\xi_{i-1/2,j}} \right) + \left(\frac{AL\eta_{i,j+1/2}}{l\eta_{i,j+1/2}} - \frac{AL\eta_{i,j-1/2}}{l\eta_{i,j-1/2}} \right).$$

The stencil for $\overline{\text{DIV}}$ at the interior nodes (shown in Figure 3.1) is obtained by combining this formula with the stencil for operators L_{11} , L_{12} , L_{21} , and L_{22} defined in (2.22).

3.2.3. Operator $\overline{\text{CURL}}$. In the subspace of vectors \vec{A} , where the surface integral in (1.2) on the right-hand side vanishes, we have

$$(3.28) \quad \int_V (\mathbf{curl} \vec{A}, \vec{B}) dV = \int_V (\vec{A}, \mathbf{curl} \vec{B}) dV.$$

That is, in this subspace of vector functions, \mathbf{curl} is self-adjoint,

$$(3.29) \quad \mathbf{curl} = \mathbf{curl}^*,$$

in the inner product

$$(3.30) \quad (\vec{A}, \vec{B})_{\mathcal{H}} = \int_V (\vec{A}, \vec{B}) dV.$$

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

$$(3.31) \quad \overline{\text{CURL}} \stackrel{\text{def}}{=} \text{CURL}^*.$$

That is,

$$(3.32) \quad (\text{CURL} \vec{A}, \vec{B})_{\mathcal{HS}} = (\vec{A}, \overline{\text{CURL}} \vec{B})_{\mathcal{HL}}.$$

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

$$(3.33) \quad \overline{\text{CURL}} = \mathcal{L}^{-1} \cdot \text{CURL}^\dagger \cdot \mathcal{S}$$

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

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

$$(3.34) \quad \mathcal{L} \vec{\mathbf{C}} = \text{CURL}^\dagger \cdot \mathcal{S} \vec{\mathbf{B}},$$

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

When $\vec{\mathbf{B}} = (0, 0, BS\zeta)$, it easy to prove that the condition $\overline{\text{CURL}} \vec{\mathbf{B}} = 0$ implies that $BS\zeta_{i,j} = \text{const}$. The proof is similar to one for $\overline{\text{GRAD}}$.

3.2.4. Properties of adjoint discrete operators. The vector analysis theorems for adjoint operators are proved in [17]. In this paper we use two theorems:

$\overline{\text{DIV}} \vec{\mathbf{A}} = 0$ if and only if $\vec{\mathbf{A}} = \overline{\text{CURL}} \vec{\mathbf{B}}$, where $\vec{\mathbf{A}} \in \mathcal{HL}$ and $\vec{\mathbf{B}} \in \mathcal{HS}$;
 $\overline{\text{CURL}} \vec{\mathbf{A}} = 0$ if and only if $\vec{\mathbf{A}} = \overline{\text{GRAD}} U$, where $\vec{\mathbf{A}} \in \mathcal{HS}$ and $U \in \mathcal{HC}$.

4. Orthogonal decomposition of discrete vector functions.

4.1. Continuous case. The orthogonal decomposition theorem for continuous operators states that we can find the unique vector $\vec{\mathbf{a}}$, which satisfies the system of equations

$$(4.1) \quad \mathbf{div} \vec{\mathbf{a}} = \rho, \quad (x, y, z) \in V,$$

$$(4.2) \quad \mathbf{curl} \vec{\mathbf{a}} = \vec{\omega}, \quad (x, y, z) \in V,$$

and one of the boundary conditions,

$$(4.3) \quad (\vec{\mathbf{a}}, \vec{\mathbf{n}}) = \beta, \quad (x, y, z) \in \partial V,$$

where ∂V is the boundary of V , $\vec{\mathbf{n}}$ is the outward unit normal to ∂V , or

$$(4.4) \quad [\vec{\mathbf{a}} \times \vec{\mathbf{n}}] = \vec{\gamma}, \quad (x, y, z) \in \partial V,$$

where the tangential components of vector $\vec{\mathbf{a}}$ are given on the boundary.

In addition the vector $\vec{\omega}$ must satisfy

$$(4.5) \quad \mathbf{div} \vec{\omega} = 0$$

because $\mathbf{div} \vec{\omega} = \mathbf{div} \mathbf{curl} \vec{\mathbf{a}} \equiv 0$, and there are additional compatibility conditions that depend on the boundary conditions (see, for example, [12, 19, 21]). When the normal components of the vector are on the boundary, the additional compatibility condition needed is

$$(4.6) \quad \int_V \rho dV = \oint_{\partial V} \beta dS.$$

When the tangential components of the vector are on the boundary, the compatibility condition is

$$(4.7) \quad \int_S (\vec{\omega}, \vec{\mathbf{n}}) dS = \oint_{\partial S} (\vec{\gamma}, \vec{\mathbf{l}}) dl,$$

where S is the part of ∂V , spanned by the contour ∂S , and $\vec{\mathbf{l}}$ is the unit tangential vector to ∂S .

Moreover, the vector $\vec{\mathbf{a}}$ can be represented in the form

$$(4.8) \quad \vec{\mathbf{a}} = \vec{\mathbf{a}}_1 + \vec{\mathbf{a}}_2,$$

where

$$(4.9) \quad \mathbf{div} \vec{a}_1 = \rho, \quad \mathbf{curl} \vec{a}_1 = 0,$$

$$(4.10) \quad \mathbf{div} \vec{a}_2 = 0, \quad \mathbf{curl} \vec{a}_2 = \vec{\omega}.$$

From these equations, we can conclude that there is a scalar function φ and a vector function \vec{b} such that

$$(4.11) \quad \vec{a}_1 = \mathbf{grad} \varphi, \quad \vec{a}_2 = \mathbf{curl} \vec{b},$$

and the vector \vec{a} can be decomposed into two orthogonal parts:

$$(4.12) \quad \vec{a} = \mathbf{grad} \varphi + \mathbf{curl} \vec{b}.$$

For the case where the normal component of \vec{a} is given on the boundary, we have

$$(4.13) \quad \mathbf{div} \mathbf{grad} \varphi = \rho, \quad (x, y, z) \in V,$$

$$(4.14) \quad (\mathbf{grad} \varphi, \vec{n}) = \beta, \quad (x, y, z) \in \partial V,$$

and

$$(4.15) \quad \mathbf{curl} \mathbf{curl} \vec{b} = \vec{\omega}, \quad (x, y, z) \in V,$$

$$(4.16) \quad (\mathbf{curl} \vec{b}, \vec{n}) = 0, \quad (x, y, z) \in \partial V.$$

The representation (4.12) is called the orthogonal decomposition of \vec{a} because the vector functions \vec{a}_1 and \vec{a}_2 are orthogonal to each other, $(\vec{a}_1, \vec{a}_2)_{\mathbf{H}} = 0$, in the sense of the inner product. In fact,

$$(4.17) \quad (\vec{a}_1, \vec{a}_2)_{\mathbf{H}} \stackrel{def}{=} \int_V (\vec{a}_1, \vec{a}_2) dV$$

$$(4.18) \quad \begin{aligned} &= \int_V (\mathbf{grad} \varphi, \mathbf{curl} \vec{b}) dV \\ &= - \int_V \varphi \mathbf{div} \mathbf{curl} \vec{b} dV + \oint_{\partial V} \varphi (\vec{n}, \mathbf{curl} \vec{b}) dS \\ &= 0. \end{aligned}$$

This follows from the boundary condition (4.16) and the fact that $\mathbf{div} \mathbf{curl} \vec{b} = 0$ for any vector \vec{b} .

The Neumann boundary condition (4.14) allows the scalar function φ to be determined only up to an arbitrary constant. Note that if \vec{b} is set equal to zero on the boundary, then it automatically satisfies the Dirichlet-type boundary condition (4.16) for \vec{b} .

When the tangential components of \vec{a} are given on the boundary, φ and \vec{b} satisfy the equations

$$(4.19) \quad \mathbf{div} \mathbf{grad} \varphi = \rho, \quad (x, y, z) \in V,$$

$$(4.20) \quad [\mathbf{grad} \varphi \times \vec{n}] = \vec{0}, \quad (x, y, z) \in \partial V,$$

and

$$(4.21) \quad \mathbf{curl} \mathbf{curl} \vec{b} = \vec{\omega}, \quad (x, y, z) \in V,$$

$$(4.22) \quad [\mathbf{curl} \vec{b} \times \vec{n}] = \vec{\gamma}, \quad (x, y, z) \in \partial V.$$

Here again, the vector functions \vec{a}_1 and \vec{a}_2 are orthogonal to each other:

$$\begin{aligned}
 (4.23) \quad (\vec{a}_1, \vec{a}_2)_{\mathbf{H}} &= \int_V (\mathbf{grad} \varphi, \mathbf{curl} \vec{b}) \, dV \\
 &= \int_V (\mathbf{curl} \mathbf{grad} \varphi, \vec{b}) \, dV - \oint_{\partial V} (\vec{b}, [\mathbf{grad} \varphi \times \vec{n}]) \\
 &= 0.
 \end{aligned}$$

This follows from the boundary condition (4.20) and the fact $\mathbf{curl} \mathbf{grad} \varphi = 0$ for any scalar function φ .

We can take the function φ equal to zero on the boundary to satisfy the Dirichlet boundary condition (4.20). For the Neumann boundary condition (4.22) for \vec{b} , we can determine \vec{b} up to the gradient of an arbitrary scalar function.

In this paper, we consider only the 2-D case when the vector \vec{a} depends on (x, y) and lies in (x, y) plane. For simplicity, we will call these 2-D vectors.

For the 2-D vector \vec{a} , the vector $\vec{\omega} = \mathbf{curl} \vec{a}$ has only the ω_z component, which we, for simplicity, will denote by ω . Also the first compatibility condition in (4.5), $\mathbf{div} \vec{\omega} = 0$, is always satisfied because vector ω_z is independent of z . In the 2-D case, vector $[\vec{a} \times \vec{n}] = \vec{\gamma}$ in the boundary condition (4.4) has a single component and can be considered a scalar, which we denote by γ . The compatibility condition (4.7) reduces to the case where S is a 2-D domain, and ∂S is the boundary contour. Note that (4.15) and (4.21) are scalar equations in the 2-D case.

We will now consider the orthogonal decomposition of discrete vector functions for both the case where the normal component of the vector for discrete vector functions from the space \mathcal{HS} is given or where the tangential component of the vector for discrete vector functions from the space \mathcal{HL} is given.

4.2. Orthogonal decomposition of vector functions in \mathcal{HS} . We first consider the orthogonal decomposition of 2-D vector functions $\vec{A} \in \mathcal{HS}$, where $\vec{A} = (AS\xi, AS\eta, 0)$.

The discrete orthogonal decomposition states that we can find a vector function $\vec{A} \in \mathcal{HS}$, satisfying the conditions

$$(4.24) \quad (\text{DIV} \vec{A})_{i+1/2, j+1/2} = \rho_{i+1/2, j+1/2}, \quad \begin{cases} i = 1, \dots, M-1, \\ j = 1, \dots, N-1, \end{cases}$$

$$(4.25) \quad (\overline{\text{CURL}} \vec{A})_{i, j} = \omega_{i, j}, \quad \begin{cases} i = 2, \dots, M-1, \\ j = 2, \dots, N-1, \end{cases}$$

$$(4.26) \quad \begin{aligned} AS\xi_{1, j+1/2} &= \beta L_{j+1/2}, & AS\xi_{M, j+1/2} &= \beta R_{j+1/2}, & j &= 1, \dots, N-1, \\ AS\eta_{i+1/2, 1} &= \beta B_{i+1/2}, & AS\eta_{i+1/2, N} &= \beta T_{i+1/2}, & i &= 1, \dots, M-1. \end{aligned}$$

That is, the equation $\text{DIV} \vec{A} = \rho$ is satisfied in all the cells, the equation $\overline{\text{CURL}} \vec{A} = \omega$ is satisfied at all the internal nodes, and the components of vector \vec{A} on the boundary faces are given.

The discrete compatibility condition (and analog of (4.6)) for ρ and β is

$$\begin{aligned}
 (4.27) \quad \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} \rho_{i+1/2, j+1/2} VC_{i+1/2, j+1/2} &= \sum_{j=1}^{N-1} (\beta R_{j+1/2} S\xi_{M, j+1/2} - \beta L_{j+1/2} S\xi_{1, j+1/2}) \\
 &+ \sum_{i=1}^{M-1} (\beta T_{i+1/2} S\eta_{i+1/2, N} - \beta B_{i+1/2} S\eta_{i+1/2, 1}).
 \end{aligned}$$

The discrete analog of the condition $\mathbf{div} \vec{\omega} = 0$ is always satisfied because the vector ω has only a z component, which depends only on (x, y) .

THEOREM 4.1. *The solution to (4.24)–(4.27) is unique.*

Proof. We prove that the solution is unique by contradiction. Assume \vec{A}_1 and \vec{A}_2 are two different solutions, then $\vec{\varepsilon} = \vec{A}_1 - \vec{A}_2$ satisfies

$$(4.28) \quad \text{DIV } \vec{\varepsilon} = 0,$$

$$(4.29) \quad \overline{\text{CURL}} \vec{\varepsilon} = 0,$$

$$(4.30) \quad \begin{aligned} \varepsilon S \xi_{1,j+1/2} = 0, & \quad \varepsilon S \xi_{M,j+1/2} = 0, & j = 1, \dots, N-1, \\ \varepsilon S \eta_{i+1/2,1} = 0, & \quad \varepsilon S \eta_{i+1/2,N} = 0, & i = 1, \dots, M-1. \end{aligned}$$

From (4.29), we can conclude

$$(4.31) \quad \vec{\varepsilon} = \overline{\text{GRAD}} \varphi$$

on the internal faces. Normal components of vector $\vec{\varepsilon}$ are equal to zero on the boundary (4.30). We know that for the subspace of vector functions with zero normal components on the boundary, the discrete divergence is the negative adjoint of the gradient

$$(4.32) \quad \text{DIV} = -\overline{\text{GRAD}}^*,$$

or

$$(4.33) \quad (\text{DIV } \vec{\varepsilon}, \varphi)_{\mathcal{HC}} + (\overline{\text{GRAD}} \varphi, \vec{\varepsilon})_{\mathcal{HS}} = 0.$$

Using (4.28), (4.31), and (4.33), we can conclude

$$(\overline{\text{GRAD}} \varphi, \overline{\text{GRAD}} \varphi)_{\mathcal{HS}} = 0,$$

which implies

$$\overline{\text{GRAD}} \varphi = 0.$$

Therefore $\vec{\varepsilon} = 0$ both on the internal faces (4.31), and on the boundary faces (4.30). Hence $\vec{A}_1 = \vec{A}_2$, and the solution is unique. \square

THEOREM 4.2. *There exists a solution of problem (4.24)–(4.27).*

Proof. We will find the solution of (4.24)–(4.27) in the form

$$(4.34) \quad \vec{A} = \vec{G} + \vec{C},$$

where the vectors \vec{G} and \vec{C} satisfy the equations

$$(4.35) \quad \overline{\text{CURL}} \vec{G} = 0,$$

$$(4.36) \quad \text{DIV } \vec{G} = \rho,$$

$$(4.37) \quad \begin{aligned} GS \xi_{1,j+1/2} = \beta L_{j+1/2}, & \quad GS \xi_{M,j+1/2} = \beta R_{j+1/2}, & j = 1, \dots, N-1, \\ GS \eta_{i+1/2,1} = \beta B_{i+1/2}, & \quad GS \eta_{i+1/2,N} = \beta T_{i+1/2}, & i = 1, \dots, M-1; \end{aligned}$$

$$(4.38) \quad \text{DIV } \vec{C} = 0,$$

$$(4.39) \quad \overline{\text{CURL}} \vec{C} = \omega,$$

$$(4.40) \quad \begin{aligned} CS \xi_{1,j+1/2} = 0, & \quad CS \xi_{M,j+1/2} = 0, & j = 1, \dots, N-1, \\ CS \eta_{i+1/2,1} = 0, & \quad CS \eta_{i+1/2,N} = 0, & i = 1, \dots, M-1. \end{aligned}$$

By linearity, if the problems for \vec{G} and \vec{C} have a solutions, then $\vec{A} = \vec{G} + \vec{C}$ is the solution of our original problem.

First we note that at the internal faces (4.35) can be replaced by

$$(4.41) \quad \vec{G} = \overline{\text{GRAD}} \varphi.$$

Equations (4.36) and (4.41) with boundary conditions (4.37) give the discrete Poisson equation with Neumann boundary conditions and can be solved by eliminating \vec{G} and moving all known values of \vec{G} on the boundary to the right-hand side of (4.36). From a formal point of view, the transformed equations are equivalent to a problem with zero Neumann boundary conditions and a modified right-hand side, where the operator DIV is defined on the subspace of vector functions with zero normal components on the boundary

$$(4.42) \quad \text{DIV } \overline{\text{GRAD}} \varphi = \tilde{\rho}.$$

Because $\text{DIV} = -\overline{\text{GRAD}}^*$ on the subspace of vector functions with zero normal components on the boundary, $\text{DIV } \overline{\text{GRAD}}$ is a self-adjoint operator. The number of linear equations for $\varphi_{i,j}$ in system (4.42) is equal to the number of unknowns (and equal to number of cells), $(M-1) \times (N-1)$.

Equation (4.42) also can be written as

$$(4.43) \quad \text{DIV } \vec{G} = \tilde{\rho},$$

$$(4.44) \quad \vec{G} = \overline{\text{GRAD}} \varphi,$$

$$(4.45) \quad \begin{aligned} \vec{G} S \xi_{1,j+1/2} = 0, & \quad \vec{G} S \xi_{M,j+1/2} = 0, & j = 1, \dots, N-1, \\ \vec{G} S \eta_{i+1/2,1} = 0, & \quad \vec{G} S \eta_{i+1/2,N} = 0, & i = 1, \dots, M-1, \end{aligned}$$

where $\vec{G} \equiv \vec{G}$ on all the internal faces. The compatibility condition (4.27) is

$$(4.46) \quad \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} \tilde{\rho}_{i+1/2,j+1/2} V C_{i+1/2,j+1/2} = 0.$$

When the number of unknowns is equal to the number of equations, then a system of linear equations has a solution if and only if the right-hand side is orthogonal to all the solutions of the homogeneous adjoint equation [38].

The homogeneous adjoint problem

$$(4.47) \quad \text{DIV } \vec{F} = 0,$$

$$(4.48) \quad \vec{F} = \overline{\text{GRAD}} \psi,$$

$$(4.49) \quad \begin{aligned} F S \xi_{1,j+1/2} = 0, & \quad F S \xi_{M,j+1/2} = 0, & j = 1, \dots, N-1, \\ F S \eta_{i+1/2,1} = 0, & \quad F S \eta_{i+1/2,N} = 0, & i = 1, \dots, M-1, \end{aligned}$$

has $\psi = \text{const.}$ as a solution. To prove this is the *only* solution, notice that if ψ is the solution of homogeneous system, then $\text{DIV } \overline{\text{GRAD}} \psi = 0$. Because $\text{DIV} = -\overline{\text{GRAD}}^*$, we have

$$(4.50) \quad 0 = (\text{DIV } \overline{\text{GRAD}} \psi, \psi)_{HC} = (\overline{\text{GRAD}} \psi, \overline{\text{GRAD}} \psi)_{HS},$$

and therefore $\overline{\text{GRAD}} \psi = 0$, which requires $\psi = \text{const.}$

The right-hand side $\tilde{\rho}$ of (4.43) is orthogonal to the constant function, which is equal to one in all cells; $I = I_{i,j} = \text{const.}$;

$$(4.51) \quad (\tilde{\rho}, I)_{HC} = \text{constant} \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} \tilde{\rho}_{i+1/2, j+1/2} VC_{i+1/2, j+1/2} = 0,$$

using compatibility conditions (4.46). Therefore there is a solution to our original problem for \vec{G} . Furthermore, as in the continuous case, φ is defined up to a constant, and because $\overline{\text{GRAD}} I = 0$, the vector $\vec{G} = \overline{\text{GRAD}} \varphi$ is unique.

Next we show that there is a unique vector \vec{C} satisfying (4.38)–(4.40).

From condition (4.38) we know that $\vec{C} = \text{CURL } \vec{B}$ on all faces. Because \vec{C} is a 2-D vector, the vector \vec{B} has a single component, $BL\zeta$; then

$$(4.52) \quad CS\xi_{i, j+1/2} = \frac{BL\zeta_{i, j+1} - BL\zeta_{i, j}}{l\eta_{i, j+1/2}},$$

$$(4.53) \quad CS\eta_{i+1/2, j} = -\frac{BL\zeta_{i+1, j} - BL\zeta_{i, j}}{l\xi_{i+1/2, j}},$$

and we can satisfy the boundary conditions (4.40) by choosing $BL\zeta_{i, j}$ equal to zero on the boundary.

The equations for \vec{C} are equivalent to the problem for the vector \vec{B} ;

$$(4.54) \quad \overline{\text{CURL}} \text{CURL } \vec{B} = \omega,$$

$$(4.55) \quad \begin{aligned} BL\zeta_{1, j} &= 0, & BL\zeta_{M, j} &= 0, & j &= 1, \dots, N, \\ BL\zeta_{i, 1} &= 0, & BL\zeta_{i, N} &= 0, & i &= 1, \dots, M. \end{aligned}$$

If we know $BL\zeta_{i, j}$, then \vec{C} is determined by (4.52), (4.53).

To show that the solution of (4.54), (4.55) is unique, note that for vector functions with zero boundary conditions $\text{CURL} = \overline{\text{CURL}}^*$, and therefore

$$(4.56) \quad (\overline{\text{CURL}} \text{CURL } \vec{B}, \vec{B})_{\mathcal{H}\mathcal{L}} = (\text{CURL } \vec{B}, \text{CURL } \vec{B})_{\mathcal{H}\mathcal{S}} \geq 0,$$

or

$$\overline{\text{CURL}} \text{CURL} \geq 0.$$

If

$$(4.57) \quad (\overline{\text{CURL}} \text{CURL } \vec{B}, \vec{B})_{\mathcal{H}\mathcal{L}} = (\text{CURL } \vec{B}, \text{CURL } \vec{B})_{\mathcal{H}\mathcal{S}} = 0,$$

then $\text{CURL } \vec{B} = 0$, and because \vec{B} has only one component, $BL\zeta$, $BL\zeta_{i, j} = \text{const.}$ Also, because of $BL\zeta_{i, j} = 0$ on the boundary, then $BL\zeta_{i, j} = 0$ everywhere. This implies that the operator $\overline{\text{CURL}} \text{CURL}$ is positive; $\overline{\text{CURL}} \text{CURL} > 0$.

Positive operators are invertible in a finite-dimensional space. Therefore $\overline{\text{CURL}} \text{CURL}$ has an inverse, and the system (4.54), (4.55) has a unique solution. \square

THEOREM 4.3. $\overline{\text{GRAD}} \varphi$ is orthogonal to $\text{CURL } \vec{B}$.

Proof. Because of the zero boundary conditions for \vec{B} ,

$$(4.58) \quad \left(\overline{\text{GRAD}} \varphi, \text{CURL } \vec{B} \right)_{\mathcal{H}\mathcal{S}} = \left(\overline{\text{CURL}} \overline{\text{GRAD}} \varphi, \vec{B} \right)_{\mathcal{H}\mathcal{L}},$$

and since $\overline{\text{CURL}} \overline{\text{GRAD}} \varphi = 0$ for any φ , we have

$$(4.59) \quad \left(\overline{\text{GRAD}} \varphi, \text{CURL } \vec{B} \right)_{\mathcal{H}\mathcal{S}} = 0,$$

proving that $\overline{\text{GRAD}} \varphi$ is orthogonal to $\text{CURL } \vec{B}$. \square

4.3. Orthogonal decomposition of vector functions in \mathcal{HL} . We now consider the orthogonal decomposition of vector functions $\vec{A} \in \mathcal{HL}$, where $\vec{A} = (AL\xi, AL\eta, 0)$, and its tangential components $AL\xi, AL\eta$ are given on corresponding parts of the boundary.

The goal is to find vector function $\vec{A} \in \mathcal{HL}$, satisfying the conditions

$$(4.60) \quad (\overline{\text{DIV}} \vec{A})_{i,j} = \rho_{i,j}, \quad \begin{cases} i = 1, \dots, M-1, \\ j = 1, \dots, N-1, \end{cases}$$

$$(4.61) \quad (\text{CURL} \vec{A})_{i+1/2, j+1/2} = \omega_{i+1/2, j+1/2}, \quad \begin{cases} i = 1, \dots, M-1, \\ j = 1, \dots, N-1, \end{cases}$$

$$(4.62) \quad \begin{aligned} AL\eta_{1, j+1/2} &= \beta L_{j+1/2}, & AL\eta_{M, j+1/2} &= \beta R_{j+1/2}, & j &= 1, \dots, N-1, \\ AL\xi_{i+1/2, 1} &= \beta B_{i+1/2}, & AL\xi_{i+1/2, N} &= \beta T_{i+1/2}, & i &= 1, \dots, M-1. \end{aligned}$$

That is, the equation $\overline{\text{DIV}} \vec{A} = \rho$ is satisfied at all the internal nodes, the equation $\text{CURL} \vec{A} = \omega$ is satisfied in all the cells, and the tangential components of the vector \vec{A} are given on the boundary edges. The discrete compatibility condition for ω and β 's,

$$(4.63) \quad \begin{aligned} \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} \omega_{i+1/2, j+1/2} VC_{i+1/2, j+1/2} &= \sum_{j=1}^{N-1} (\beta R_{j+1/2} S\xi_{M, j+1/2} - \beta L_{j+1/2} S\xi_{1, j+1/2}) \\ &- \sum_{i=1}^{M-1} (\beta T_{i+1/2} S\eta_{i+1/2, N} - \beta B_{i+1/2} S\eta_{i+1/2, 1}), \end{aligned}$$

also has to be satisfied.

THEOREM 4.4. *The solution to (4.60)–(4.62) is unique.*

Proof. We prove the uniqueness of the solution contradiction. If \vec{A}_1 and \vec{A}_2 are two different solutions, then $\vec{\varepsilon} = \vec{A}_1 - \vec{A}_2$ satisfies

$$(4.64) \quad \overline{\text{DIV}} \vec{\varepsilon} = 0,$$

$$(4.65) \quad \text{CURL} \vec{\varepsilon} = 0,$$

$$(4.66) \quad \begin{aligned} \varepsilon L\eta_{1, j+1/2} &= 0, & \varepsilon L\eta_{M, j+1/2} &= 0, & j &= 1, \dots, N-1, \\ \varepsilon L\xi_{i+1/2, 1} &= 0, & \varepsilon L\xi_{i+1/2, N} &= 0, & i &= 1, \dots, M-1. \end{aligned}$$

From (4.64), we can conclude

$$(4.67) \quad \vec{\varepsilon} = \overline{\text{CURL}} \vec{B}$$

on the internal edges.

The tangential components of the vector $\vec{\varepsilon}$ are zero on the boundary by (4.66). In the subspace of vector functions with zero tangential components on the boundary, the discrete operators CURL and $\overline{\text{CURL}}$ are adjoint to each other, $\text{CURL} = \overline{\text{CURL}}^*$, or

$$(4.68) \quad (\text{CURL} \vec{\varepsilon}, \vec{B})_{\mathcal{HS}} + (\overline{\text{CURL}} \vec{B}, \vec{\varepsilon})_{\mathcal{HL}} = 0.$$

Using (4.65) and (4.67), we conclude that $(\overline{\text{CURL}} \vec{B}, \overline{\text{CURL}} \vec{B})_{\mathcal{HL}} = 0$, and therefore $\overline{\text{CURL}} \vec{B} = 0$. Because $\vec{\varepsilon} = \overline{\text{CURL}} \vec{B} = 0$ on the internal edges, and it is equal to zero on the boundary (4.66), then $\vec{\varepsilon} = 0$, and the solution is unique. \square

THEOREM 4.5. *There exists the solution of problem (4.60)–(4.62).*

Proof. We will find the solution of (4.60)–(4.62) in the form

$$(4.69) \quad \vec{A} = \vec{G} + \vec{C},$$

where the vector \vec{G} satisfies the equations

$$(4.70) \quad \text{CURL } \vec{G} = 0,$$

$$(4.71) \quad \overline{\text{DIV}} \vec{G} = \rho,$$

$$(4.72) \quad \begin{aligned} GL\eta_{1,j} &= 0, & GL\eta_{M,j} &= 0, & j &= 1, \dots, N-1, \\ GL\xi_{i,1} &= 0, & GL\xi_{i,N} &= 0, & i &= 1, \dots, M-1, \end{aligned}$$

and the vector \vec{C} satisfies the equations

$$(4.73) \quad \overline{\text{DIV}} \vec{C} = 0, X$$

$$(4.74) \quad \text{CURL } \vec{C} = \omega,$$

$$(4.75) \quad \begin{aligned} CL\eta_{1,j+1/2} &= \beta L_{j+1/2}, & CL\eta_{M,j+1/2} &= \beta R_{j+1/2}, & j &= 1, \dots, N-1, \\ CL\xi_{i+1/2,1} &= \beta B_{i+1/2}, & CL\xi_{i+1/2,N} &= \beta T_{i+1/2}, & i &= 1, \dots, M-1. \end{aligned}$$

We first consider the problem for \vec{G} and replace (4.70) by the equation

$$\vec{G} = \text{GRAD } \varphi.$$

Because the components $GL\xi_{i,j}, GL\eta_{i,j}$ of the vector $\text{GRAD } \varphi$ are equal to

$$(4.76) \quad GL\xi_{i+1/2,j} = \frac{\varphi_{i+1,j} - \varphi_{i,j}}{l_{\xi_{i+1/2,j}}}, \quad GL\eta_{i,j+1/2} = \frac{\varphi_{i,j+1} - \varphi_{i,j}}{l_{\eta_{i,j+1/2}}},$$

the boundary conditions (4.72) will be satisfied if we choose $\varphi_{i,j} = 0$ on the boundary.

Therefore, instead of the original problem, we can consider

$$(4.77) \quad \overline{\text{DIV}} \vec{G} = \rho,$$

$$(4.78) \quad \vec{G} = \text{GRAD } \varphi,$$

$$(4.79) \quad \begin{aligned} \varphi_{1,j} &= 0, & \varphi_{M,j} &= 0, & j &= 1, \dots, N, \\ \varphi_{i,1} &= 0, & \varphi_{i,N} &= 0, & i &= 1, \dots, M. \end{aligned}$$

This is a discrete Poisson's equation with Dirichlet boundary conditions. It can easily be shown that the solution is unique using the fact that $\overline{\text{DIV}}$ and GRAD are negative adjoint to each other in the subspace of discrete scalar functions that are zero on the boundary. The proof is almost identical to one for the Dirichlet problem in the case of \mathcal{HS} vectors.

Now let us consider problem (4.70)–(4.72) for the vector \vec{C} . The condition (4.73) implies that $\vec{C} = \overline{\text{CURL}} \vec{B}$ on the internal edges. Because the vector \vec{C} is a 2-D vector, the vector \vec{B} has only one component, $BS\zeta$.

This Neumann boundary problem is self-adjoint, and the compatibility condition (4.63) guarantees that the right-hand side of the nonhomogeneous equation is orthogonal to all solutions (constants) of the adjoint homogeneous equation. The proof that this problem has a unique (up to constant) solution and that the vector \vec{C} is unique follows from a simple modification of the proof for the \mathcal{HS} case with Neumann boundary conditions. \square

THEOREM 4.6. $\text{GRAD } \varphi$ is orthogonal to $\overline{\text{CURL}} \vec{B}$.

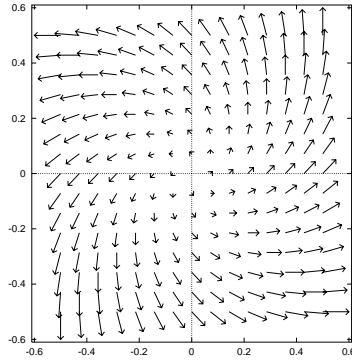


FIG. 5.1. Continuous spiral vector field \vec{a} .

Proof. Because of the zero boundary conditions for the scalar function φ ,

$$(4.80) \quad \left(\text{GRAD } \varphi, \overline{\text{CURL } \vec{B}} \right)_{\mathcal{HL}} = \left(\varphi, \overline{\text{DIV } \text{CURL } \vec{B}} \right)_{HN},$$

and because $\overline{\text{DIV } \text{CURL } \vec{B}} = 0$ for any \vec{B} ,

$$(4.81) \quad \left(\text{GRAD } \varphi, \overline{\text{CURL } \vec{B}} \right)_{\mathcal{HL}} = 0.$$

Hence $\text{GRAD } \varphi$ and $\overline{\text{CURL } \vec{B}}$ are orthogonal. \square

5. Numerical example. We will illustrate these theorems on the orthogonal decomposition of a spiral vector field. The continuous spiral vector field \vec{a} given by its Cartesian components $(a_x(x, y), a_y(x, y))$,

$$(5.1) \quad a_x(x, y) = x - y, \quad a_y(x, y) = x + y,$$

is shown in Figure 5.1 in the square $[-0.5, 0.5] \times [-0.5, 0.5]$.

This vector field satisfies

$$(5.2) \quad \text{div } \vec{a} = 2, \quad \text{curl } \vec{a} = 2,$$

and the values of the normal components of the vector on the boundary can be obtained from the exact solution.

We first consider approximation of problem (5.2) in space \mathcal{HS} :

$$(5.3) \quad \text{DIV } \vec{A} = 2, \quad \overline{\text{CURL } \vec{A}} = 2,$$

where $\vec{A} \in \mathcal{HS}$ and the components of \vec{A} are given on the boundary, and then solve for the orthogonal decomposition of $\vec{A} = \overline{\text{GRAD } \varphi} + \text{CURL } \vec{B}$, satisfying (4.35)–(4.40).

We solve (5.3) on the smooth grid (shown in Fig. 5.2 (a)) obtained by mapping the uniform grid in square $[-0.5, 0.5] \times [-0.5, 0.5]$ in the space (ξ, η) into the same square in computational space $x(\xi, \eta), y(\xi, \eta)$:

$$x(\xi, \eta) = \xi + 0.1 \sin(2\pi\xi) \sin(2\pi\eta), \quad y(\xi, \eta) = \eta + 0.1 \sin(2\pi\xi) \sin(2\pi\eta).$$

The numerical solution of 5.3 for $M = N = 17$ is shown in Figure 5.2 (b).

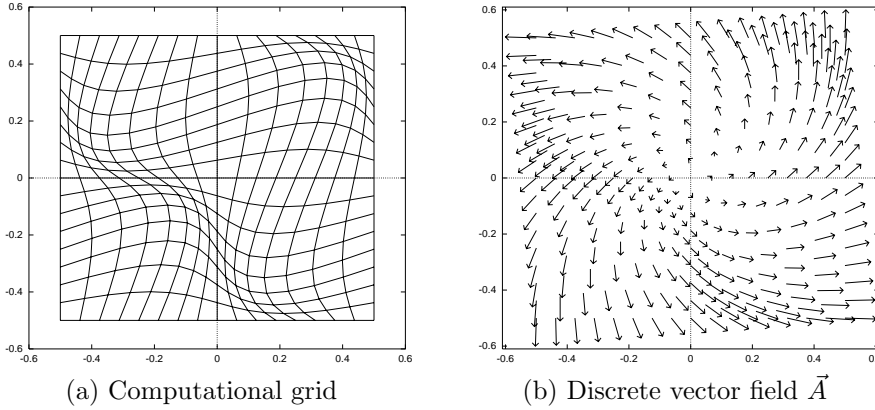


FIG. 5.2. (a) The smooth computational grid, used in solution of (5.3). (b) The recovered (reconstructed) discrete vector field \vec{A} .

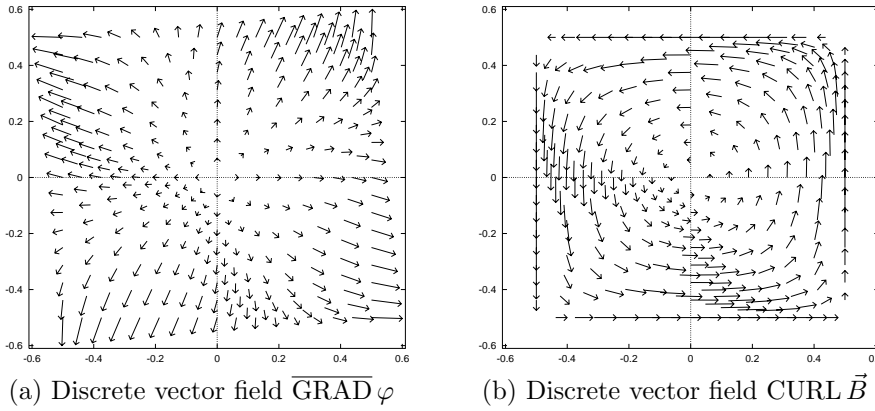


FIG. 5.3. The orthogonal decomposition of vector $\vec{A} = \overline{\text{GRAD}} \varphi + \text{CURL } \vec{B}$ satisfying (5.3). (a) Vector function $\overline{\text{GRAD}} \varphi$, $M = N = 17$. (b) Vector function $\text{CURL } \vec{B}$, $M = N = 17$.

To solve discrete equations we use the multigrid-preconditioned conjugate-gradient method described in [25].

The results of orthogonal decomposition, vector functions $\overline{\text{GRAD}} \varphi$ and $\text{CURL } \vec{B}$, are shown in Figure 5.3 (a) and (b).

Table 5.1 verifies the second-order convergence rate for the approximate vector field \vec{A} to the exact solution in the max norm

$$(5.4) \quad \psi = \max\left\{\max_{i,j} |AS\xi_{i,j+1/2} - AS\xi_{i,j+1/2}^E|, \max_{i,j} |AS\eta_{i+1/2,j} - AS\eta_{i+1/2,j}^E|\right\},$$

where $AS\xi_{i,j+1/2}, AS\eta_{i+1/2,j}$ are the approximate solutions, and $AS\xi_{i,j+1/2}^E, AS\eta_{i+1/2,j}^E$ are the projections of the exact spiral vector field, defined by

$$(5.5) \quad \begin{aligned} AS\xi_{i,j+1/2}^E &= n\xi_{i,j+1/2}^x 0.5 [a_x(x_{i,j+1}, y_{i,j+1}) + a_x(x_{i,j}, y_{i,j})] \\ &+ n\xi_{i,j+1/2}^y 0.5 [a_y(x_{i,j+1}, y_{i,j+1}) + a_y(x_{i,j}, y_{i,j})], \end{aligned}$$

TABLE 5.1
 Convergence rate for the approximate vector field \vec{A} to the exact solution

$M = N$	17	33	65
max norm	1.11E-2	3.05E-3	7.85E-4
q_{max}	1.86	1.95	-

$$(5.6) \quad AS\eta_{i+1/2,j}^E = n\eta_{i+1/2,j}^x 0.5 [a_x(x_{i+1,j}, y_{i+1,j}) + a_x(x_{i,j}, y_{i,j})] \\ + n\eta_{i+1/2,j}^y 0.5 [a_y(x_{i+1,j}, y_{i+1,j}) + a_y(x_{i,j}, y_{i,j})],$$

where $(n\xi_{i,j+1/2}^x, n\xi_{i,j+1/2}^y)$ and $(n\eta_{i+1/2,j}^x, n\eta_{i+1/2,j}^y)$ are Cartesian components of the unit normal vectors to the faces $S\xi_{i,j+1/2}$ and $S\eta_{i+1/2,j}$.

6. Discussion. The orthogonal decomposition theorem of a vector field is one of the most important theorems of vector analysis. In this paper, we proved that the new mimetic discrete approximations of the divergence, gradient, and curl derived using the SOM automatically satisfy discrete analogs of the theorem for vectors from spaces \mathcal{HL} of discrete vector functions defined by their orthogonal projections onto directions of the edges of the cell and \mathcal{HS} of discrete vector functions defined by their orthogonal projections onto directions perpendicular to face of the cell. That is, any vector $\vec{A} \in \mathcal{HS}$ can be represented uniquely as

$$(6.1) \quad \vec{A} = \overline{\text{GRAD}} \varphi + \text{CURL } \vec{B},$$

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

$$(6.2) \quad \vec{A} = \text{GRAD } \varphi + \overline{\text{CURL}} \vec{B},$$

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

The approximations for **div**, **grad**, and **curl** described in detail in [16, 17] include the natural discrete divergence, gradient, and curl operators based on coordinate invariant definitions, such as Gauss's theorem, for the divergence, and the formal adjoints of these operators. The operators have compatible domains and ranges and can be combined to form all the compound operators **div grad**, **grad div**, and **curl curl**. By construction, all of these operators satisfy discrete analogs of the integral identities satisfied by the differential operators. Furthermore, all the discrete operators defined by this self-consistent approach satisfy analogs of the major theorems of vector analysis relating the differential operators. These discrete operators have proven to be effective in solving the heat conduction equation [36], [37], [18], Maxwell equations [9], [1], and the equations of magnetic field diffusion [34]. In our continuing quest to create a discrete analog of vector analysis on logically rectangular, nonorthogonal, nonsmooth grids, we are comparing the accuracy and stability of the SOM methods with the commonly used FDM and finite-element methods and are investigating higher-order methods on nonuniform grids. We will use the theorems in this paper to investigate the stability and accuracy of SOM methods using the energy method in an approach similar to what has been used in [13], [30], [31] for rectangular grids.

These new methods have great potential for solving complex, nonlinear PDEs on nonuniform grids and preserving the conservation laws and geometric properties of the underlying physical problem.

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