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Approximation of Boundary Conditions for Mimetic Finite-Difference Methods

J. M. HYMAN AND M. SHASHKOV
Los Alamos National Laboratory, T-7, MS B284
Los Alamos, NM 87545, U.S.A.
<jh><shashkov>@lanl.gov

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Abstract—The numerical solution of partial differential equations solved with finite-difference approximations that mimic the symmetry properties of the continuum differential operators and satisfy discrete versions of the appropriate integral identities are more likely to produce physically faithful results. Furthermore, those properties are often needed when using the energy method to prove convergence and stability of a particular difference approximation. Unless special care is taken, mimetic difference approximations derived for the interior grid points will fail to preserve the symmetries and identities between the gradient, curl, and divergence operators at the computational boundary. In this paper, we describe how to incorporate boundary conditions into finite-difference methods so the resulting approximations mimic the identities for the differential operators of vector and tensor calculus. The approach is valid for a wide class of partial differential equations of mathematical physics and will be described for Poisson's equation with Dirichlet, Neumann, and Robin boundary conditions. We prove that the resulting difference approximation is symmetric and positive definite for each of these boundary conditions. Published by Elsevier Science Ltd.

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

1. INTRODUCTION

Mimetic finite-difference methods retain or mimic the main properties of the continuum problem. We have developed a discrete analog of vector and tensor calculus [1–3], based on the Support Operator Method (SOM) [4–7], that can be used to accurately approximate continuum models on nonuniform grids for a wide range of physical processes. The SOM defines discrete mimetic approximations of the divergence, gradient, and curl operators that satisfy discrete analogs of the coordinate invariant integral identities, such as Gauss' or Stoke's theorem, responsible for the conservative properties of the continuum model. These initial discrete operators, called the *prime* operators, then ***support*** the construction of other discrete operators, using discrete formulations of the integral identities. That is, we use the formal adjoints of the natural operators to derive compatible divergence, gradient, and curl operators with complementary domains and ranges of values.

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

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support the *derived* discrete operator **GRAD**, thus satisfying a discrete version of the integral identity relating the **DIV** and **GRAD**. Because the derived operator **GRAD** is defined to be the negative adjoint of **DIV**, the discrete Laplacian operator **DIV**$\cdot$ **GRAD** is guaranteed to be a positive symmetric operator. Finite-difference methods derived for nonuniform grids by the SOM automatically preserve discrete versions of the integral identities for the gradient, curl, and divergence operators and satisfy discrete analogs of many of the theorems of vector and tensor calculus, including Stoke's theorem and a discrete orthogonal decomposition theorem.

For these methods to provide reliable approximations to the solutions for a wide class of partial differential equations, they must retain these properties when the boundary conditions of the partial differential equation being approximated is incorporated into the discrete model. For example, when solving Poisson's equation, if the discrete operator, including the boundary conditions, is symmetric and positive, then we can investigate the stability and accuracy by applying an approach similar to that what has been used in [8–10]. In addition, powerful iteration methods for solving linear systems often require symmetric and positive discrete equations [11].

We will demonstrate how to incorporate boundary conditions into the finite-difference methods on nonsmooth, logically rectangular grids and still preserve the integral identities and symmetries of the original differential equation. We demonstrate the main ideas by constructing a finite-difference method that preserves the symmetry and is a positive definite approximation of the stationary heat equation

$$-\,\mathbf{div}\,\mathbf{grad}\,u = f, \qquad (x,y) \in V. \tag{1.1}$$

This equation arises in solving for the pressure in the incompressible flow equations, in solving for the temperature in the steady-state heat equation, and in solving for mass concentration in the steady-state diffusion equation. Here V is a two-dimensional region, **div** is the divergence, **grad** is the gradient, and $f = f(x,y)$ is a given function.

The boundary conditions may be general Robin (or mixed):

$$(\mathbf{grad}\,u, \vec{n}) + \alpha u = \psi, \qquad (x,y) \in \partial V, \tag{1.2}$$

where $\vec{n}$ is the vector of the unit outward normal to the boundary ∂V, and α and ψ are functions given on ∂V. These boundary conditions include the Neumann boundary condition

$$(\mathbf{grad}\,u, \vec{n}) = \psi, \qquad (x,y) \in \partial V, \tag{1.3}$$

when α is zero. We will consider the Dirichlet boundary conditions when the solution $u(x,y)$ is given on the boundary

$$u(x,y) = \psi(x,y), \qquad (x,y) \in \partial V. \tag{1.4}$$

The boundary conditions (1.2) and (1.3) are *natural* boundary conditions because they can be taken into account by changing the definition of the inner product in the functional spaces without imposing the boundary conditions on the solution $u(x,y)$. The Dirichlet boundary condition (1.4) is called an *essential* boundary condition and has to be explicitly imposed on the function space where we are looking for the solution.

We incorporate Robin boundary conditions into the discrete problem by defining an inner product in the space of discrete scalar functions, which includes a discrete analog of boundary integral.

We begin by analyzing the continuum problem for Poisson's equation with Dirichlet, Neumann, and Robin boundary conditions to illuminate the properties, such as symmetry and positiveness, of the operators that we wish to preserve in the discrete case. Next, we introduce the notation for nonuniform staggered grids, the discretizations of scalar and vector functions, and the appropriate discrete inner products for the space of scalar discrete functions for each type of boundary condition. We describe SOM for approximating the **div** and **grad** on nonuniform grids, and we provide a detailed analysis proving that the approximations for the Dirichlet, Neumann, and Robin boundary value problems are symmetric positive operators.

2. PROPERTIES OF THE CONTINUUM PROBLEM

We begin by analyzing the continuum problem for Poisson's equation with Dirichlet, Neumann, and Robin boundary conditions and emphasize the properties of differential operators that we want to retain in the discrete case.

2.1. Dirichlet Boundary Value Problem

The Dirichlet boundary value problem,

$$\begin{aligned} -\operatorname{\mathbf{div}}\operatorname{\mathbf{grad}} u &= f, \qquad && (x,y) \in V, \\ u(x,y) &= \psi(x,y), \qquad && (x,y) \in \partial V, \end{aligned} \tag{2.1}$$

can be transformed into an equivalent problem with zero boundary conditions if we assume that the shape of the domain satisfies the *extensibility or continuability* condition [12]. Then there is a smooth function $\Psi(x,y)$ which coincides with $\psi(x,y)$ on the boundary $\Psi(x,y) = \psi(x,y)$, $(x,y) \in \partial V$.

We introduce the new unknown function

$$\tilde{u}(x,y) = u(x,y) - \Psi(x,y), \tag{2.2}$$

and reformulate (2.1) as

$$\begin{aligned} -\operatorname{\mathbf{div}}\operatorname{\mathbf{grad}} \tilde{u} &= \tilde{f}, \qquad && (x,y) \in V, \\ \tilde{u}(x,y) &= 0, \qquad && (x,y) \in \partial V, \end{aligned} \tag{2.3}$$

where

$$\tilde{f} = f + \operatorname{\mathbf{div}}\operatorname{\mathbf{grad}} \Psi. \tag{2.4}$$

This transformed problem has zero Dirichlet boundary conditions and a modified right-hand side.

We restate this problem in operator notation by introducing the space of scalar functions that are equal to zero on the boundary; that is,

$$\overset{0}{H} = \{v(x,y) \in H,\ v(x,y) = 0 \in \partial V\}, \tag{2.5}$$

with the following inner product:

$$(u,v)_{\overset{0}{H}} = \int_V uv\, dV. \tag{2.6}$$

The problem now is to find $\tilde{u} \in \overset{0}{H}$, which satisfies the equation

$$A\tilde{u} = \tilde{f}, \qquad A = -\operatorname{\mathbf{div}}\operatorname{\mathbf{grad}}, \tag{2.7}$$

where the operator **grad** is defined on the subspace $\overset{0}{H}$ of the space H.

To show that the operator A is symmetric and positive, we note that the identity

$$\int_V \phi\, \operatorname{\mathbf{div}} \vec{w}\, dV + \int_V (\vec{w}, \operatorname{\mathbf{grad}} \phi)\, dV = \oint_S \phi\, (\vec{w}, \vec{n})\, dS \tag{2.8}$$

reduces to

$$\int_V \phi\, \operatorname{\mathbf{div}} \vec{w}\, dV + \int_V (\vec{w}, \operatorname{\mathbf{grad}} \phi)\, dV = 0, \tag{2.9}$$

for the scalar functions in $\overset{0}{H}$. In addition,

$$\begin{aligned}(Au, v)_{\overset{0}{H}} &= -\int_V v \,\mathbf{div}\,\mathbf{grad}\, u \, dV \\ &= \int_V (\mathbf{grad}\, u, \mathbf{grad}\, v) \, dV,\end{aligned} \tag{2.10}$$

and hence,

$$(Au, v)_{\overset{0}{H}} = (u, Av)_{\overset{0}{H}}, \qquad (Au, u)_{\overset{0}{H}} > 0. \tag{2.11}$$

If we introduce the inner product in the space of vector functions $\mathcal{H}$ as

$$\left(\vec{A}, \vec{B}\right)_{\mathcal{H}} = \int_V \left(\vec{A}, \vec{B}\right) dV, \tag{2.12}$$

then the identity (2.9) implies

$$\left(\mathbf{div}\,\vec{A}, u\right)_{\overset{0}{H}} = \left(\vec{A}, \mathbf{grad}\, u\right)_{\mathcal{H}}, \tag{2.13}$$

and the operators **div** and $-$**grad** are adjoint to each other in these function spaces,

$$\mathbf{div} = -\,\mathbf{grad}^*. \tag{2.14}$$

2.2. Neumann Boundary Value Problem

The Neumann boundary value problem is defined as

$$\begin{aligned} -\,\mathbf{div}\,\mathbf{grad}\, u &= f, && (x, y) \in V, \\ (\mathbf{grad}\, u, \vec{n})|_{(x,y)} &= \psi(x, y), && (x, y) \in \partial V,\end{aligned} \tag{2.15}$$

where $\vec{n}$ is the unit outward normal to ∂V. The divergence theorem

$$\int_V \mathbf{div}\, \vec{W} \, dV = \oint \left(\vec{W}, \vec{n}\right) dS, \tag{2.16}$$

requires the compatibility condition

$$-\int_V f \, dV = \oint_{\partial V} \psi \, dS, \tag{2.17}$$

for the Neumann problem to have a unique solution (up to constant).

We analyze the Neumann problem from two different approaches: the modified inner-product approach (where we embed the boundary integral in inner-product space), and flux form approach (used for the Dirichlet boundary conditions).

2.2.1. Modified inner-product approach

In the modified inner-product approach, we rewrite (2.15) in operator form as

$$\mathbf{A}u = \mathbf{F}, \tag{2.18}$$

where

$$\mathbf{A}u = \begin{cases} -\,\mathbf{div}\,\mathbf{grad}\, u, & (x, y) \in V, \\ (\mathbf{grad}\, u, \vec{n}), & (x, y) \in \partial V,\end{cases} \tag{2.19}$$

and

$$\mathbf{F} = \begin{cases} f, & (x,y) \in V, \\ \psi, & (x,y) \in \partial V. \end{cases} \tag{2.20}$$

Next, we introduce an inner product in the space of the scalar functions, which includes the boundary integral

$$(u,v)_H \stackrel{\text{def}}{=} \int_V uv\, dV + \oint_{\partial V} uv\, dS, \tag{2.21}$$

(from here on, we use the notation $\stackrel{\text{def}}{=}$ when we define a new object) and leave the values of $u(x,y)$ unrestricted on the boundary.

In this inner product, the Neumann problem is symmetric and nonnegative because

$$\begin{aligned}(\mathbf{A}u,v)_H &= -\int_V \mathbf{div}\,\mathbf{grad}\, uv\, dV + \oint_{\partial V} (\mathbf{grad}\, u, v)\, dS \\ &= \int_V (\mathbf{grad}\, u, \mathbf{grad}\, v)\, dV.\end{aligned} \tag{2.22}$$

The Neumann boundary conditions are called *natural* boundary conditions in this approach because they can be embedded in a natural way into the definition of the inner product, or in finite-element methods, by changing the variational functional or variational identity.

If we extend the divergence operator to the boundary and define the operator $\mathbf{d} : \mathcal{H} \to H$ as

$$\mathbf{d}\vec{w} = \begin{cases} +\mathbf{div}\,\vec{w}, & (x,y) \in V, \\ -(\vec{w},\vec{n}), & (x,y) \in \partial V, \end{cases} \tag{2.23}$$

we can express (2.19) in compact form,

$$\mathbf{A} = -\mathbf{d} \cdot \mathbf{grad}, \tag{2.24}$$

and (2.15) can be written as the first-order system

$$\mathbf{d}\vec{w} = F, \qquad \vec{w} = -\,\mathbf{grad}\, u. \tag{2.25}$$

From the definition of operator $\mathbf{d}$, the definition (2.21) for the inner product in the space H, and the integral identity (2.8), we have

$$\begin{aligned}(\mathbf{d}\vec{w},u)_H &= \int_V u\, \mathbf{div}\, \vec{w}\, dV - \oint_{\partial V} u\,(\vec{w},\vec{n})\, dS \\ &= -\int_V (\vec{w}, \mathbf{grad}\, u)\, dV \\ &= (\vec{w}, -\,\mathbf{grad}\, u)_{\mathcal{H}}\end{aligned} \tag{2.26}$$

or

$$\mathbf{d} = -\,\mathbf{grad}^*. \tag{2.27}$$

This is a crucial relationship, which we must retain in our discrete approximation. An immediate benefit of (2.27) is that the operator A,

$$A = -\mathbf{d}\ \mathbf{grad} = \mathbf{d}\mathbf{d}^* \tag{2.28}$$

is symmetric and nonnegative.

2.2.2. Flux form approach

In the flux form approach, we first rewrite problem (2.15) in *flux* or *mixed* form as the first-order system

$$\mathbf{div}\,\vec{W} = f, \qquad (x,y) \in V, \tag{2.29a}$$

$$\vec{W} = -\,\mathbf{grad}\,u, \qquad (x,y) \in V, \tag{2.29b}$$

$$-\left(\vec{W},\vec{n}\right)\Big|_{(x,y)} = \psi(x,y), \qquad (x,y) \in V, \tag{2.29c}$$

where $\vec{W}$ is flux.

If we assume that we can find a scalar function ϕ, where

$$(\mathbf{grad}\,\phi,\vec{n})|_{(x,y)} = \psi(x,y), \qquad (x,y) \in \partial V, \tag{2.30}$$

then we can reformulate problem expressed as (2.29a)–(2.29c) as

$$\mathbf{div}\,\vec{\tilde{W}} = \tilde{f}, \qquad (x,y) \in V, \tag{2.31a}$$

$$\vec{\tilde{W}} = -\,\mathbf{grad}\,\tilde{u}, \qquad (x,y) \in V, \tag{2.31b}$$

$$-\left(\vec{\tilde{W}},\vec{n}\right)\Big|_{(x,y)} = 0, \qquad (x,y) \in V, \tag{2.31c}$$

where

$$\begin{gathered} \tilde{u} = u - \phi, \\ \vec{\tilde{W}} = \vec{W} - \vec{\Phi}, \qquad \vec{\Phi} = \mathbf{grad}\,\phi, \\ \tilde{f} = f - \mathbf{div}\,\vec{\Phi}. \end{gathered} \tag{2.32}$$

Now, we now need only consider the problem expressed as (2.31a) and (2.31b) in the space $H \times \overset{0}{\mathcal{H}}$, where

$$\overset{0}{\mathcal{H}} = \left\{\vec{W} \in \mathcal{H},\ \left(\vec{W},\vec{n}\right)\Big|_{(x,y)} = 0,\ (x,y) \in \partial V\right\}.$$

That is, in the flux formulation, the Neumann boundary condition is an essential boundary condition, which must be imposed on the solution.

The operator **div**, defined on the subspace $\overset{0}{\mathcal{H}}$, satisfies

$$\mathbf{div} = -\,\mathbf{grad}^*\,.$$

That is, either when we consider **grad** on subspace $\overset{0}{H}$ or when we consider **div** on subspace $\overset{0}{\mathcal{H}}$, we have $\mathbf{div} = -\,\mathbf{grad}^*$ in an inner product that does not include the boundary integral in (2.8). This boundary integral no longer contributes to the inner product because the problem has been reformulated in subspaces where the boundary integral vanishes.

2.3. Robin Boundary Value Problem

The Robin boundary value problem can be formulated as

$$\begin{aligned} -\,\mathbf{div}\,\mathbf{grad}\,u &= f, \qquad (x,y) \in V, \\ (\mathbf{grad}\,u,\vec{n}) + \alpha u &= \psi, \qquad (x,y) \in \partial V, \quad \alpha > 0, \end{aligned} \tag{2.33}$$

or in operator form as

$$\mathbf{A}u = \mathbf{F}. \tag{2.34}$$

Here, $\mathbf{A}$ is defined by

$$\mathbf{A} : H \to H, \qquad \mathbf{Au} = \begin{cases} -\operatorname{\mathbf{div}} \operatorname{\mathbf{grad}} u, & (x,y) \in V, \\ (\operatorname{\mathbf{grad}} u, \vec{n}\,) + \alpha u, & (x,y) \in \partial, \end{cases} \tag{2.35}$$

and

$$\mathbf{F} = \begin{cases} f, & (x,y) \in V, \\ \psi, & (x,y) \in \partial V. \end{cases} \tag{2.36}$$

We can easily prove that $\mathbf{A}$ is symmetric and positive, that is,

$$(\mathbf{A}u, v)_H = (u, \mathbf{A}v)_H, \qquad (\mathbf{A}u, u)_H > 0, \tag{2.37}$$

with a proof similar to the one for Neumann boundary conditions and using the identity

$$\begin{aligned} (Au, v)_H &= -\int_V \operatorname{\mathbf{div}} \operatorname{\mathbf{grad}} uv\, dV + \oint_{\partial V} (\operatorname{\mathbf{grad}} u, v)\, dS + \oint_{\partial V} \alpha uv\, dS \\ &= \int_V (\operatorname{\mathbf{grad}} u, \operatorname{\mathbf{grad}} v)\, dV + \oint_{\partial V} \alpha uv\, dS. \end{aligned} \tag{2.38}$$

The operator $\mathbf{A}$ can be represented in the form

$$\mathbf{A} = \Omega - \mathbf{d} \cdot \operatorname{\mathbf{grad}}, \tag{2.39}$$

where the operator $\mathbf{d}$ is defined by (2.23) and $\Omega : H \to H$ is defined as

$$\Omega u = \begin{cases} 0, & (x,y) \in V, \\ \alpha u, & (x,y) \in \partial V. \end{cases} \tag{2.40}$$

It can be useful to formulate problem (2.33) in terms of first-order operators as

$$\begin{aligned} \operatorname{\mathbf{div}} \vec{w} &= f, && (x,y) \in V, \\ \vec{w} &= -\operatorname{\mathbf{grad}} u, && (x,y) \in V, \\ -(\vec{w}, \vec{n}\,) + \alpha u &= \psi, && (x,y) \in \partial V, \end{aligned} \tag{2.41}$$

or in terms of first-order operators as

$$\Omega u + \mathbf{d}\vec{w} = F, \qquad \vec{w} = -\operatorname{\mathbf{grad}} u. \tag{2.42}$$

Because $\mathbf{A} = \Omega + \mathbf{d} \cdot \mathbf{d}^*$ and $\Omega = \Omega^* \geq 0$, the properties (2.37) follow from the properties of the operators Ω, $\mathbf{d}$, and $-\operatorname{\mathbf{grad}}$. The boundary conditions are included in definitions of the operators and spaces of functions in a natural way.

3. SPACES OF DISCRETE FUNCTIONS

3.1. Grid Notations

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 $(i+1/2, j+1/2)$ cell (see Figure 2a). 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 $(i+1/2, j+1/2)$ that meet at node (k,l) is denoted by $\varphi_{k,l}^{i+1/2,j+1/2}$.

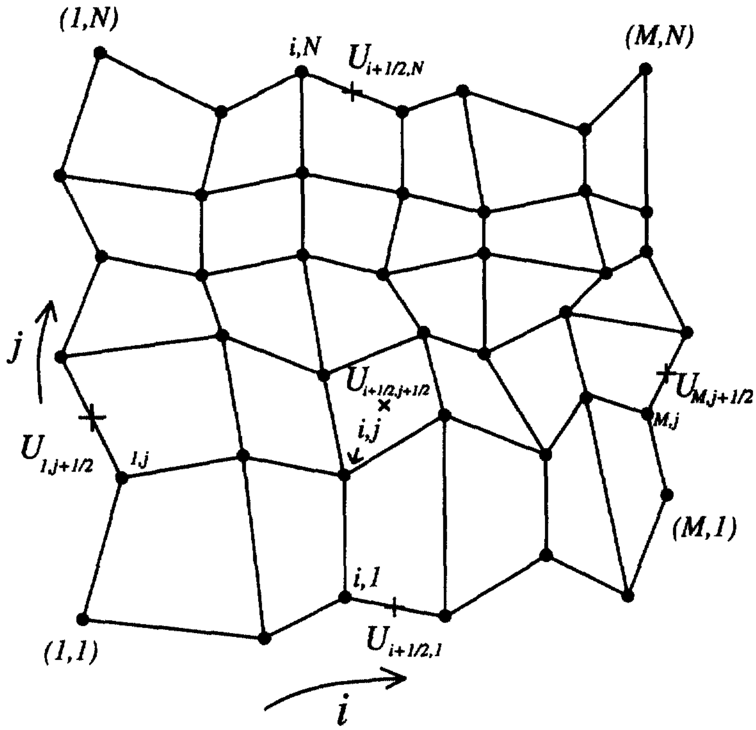


Figure 1. Cell-centered discretization of the scalar functions (HC) on a logically rectangular grid.

When defining discrete differential operators, such as **CURL**, it is convenient to consider a 2-D grid as the projection of a 3-D grid. This approach simplifies the notation and generalizing finite-difference methods to three dimensions. Here 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 2b).

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.

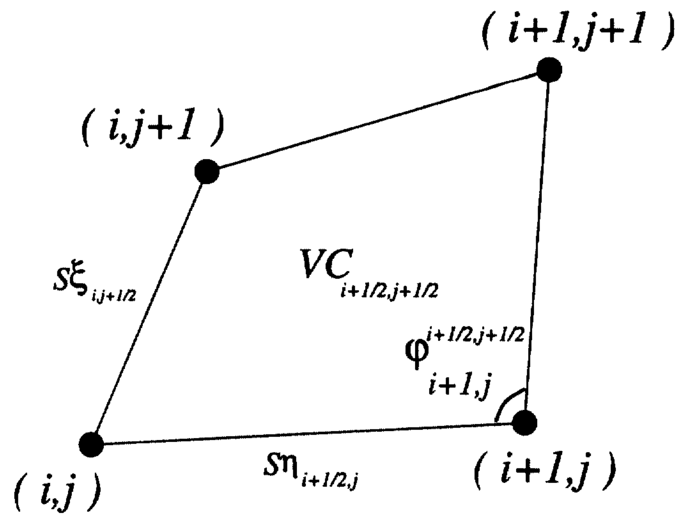
Using this analogy, we denote the length of the edge $(i,j,k)-(i+1,j,k)$ by $l\xi_{i+1/2,j,k}$, the length of the edge $(i,j,k)-(i,j+1,k)$ by $l\eta_{i,j+1/2,k}$, and the length of the edge $(i,j,k)-(i,j,k+1)$ by $l\zeta_{i,j,k+1/2}$ (which we have chosen to be equal to 1). The area of the surface $(i,j,k)-(i,j+1,k)-(i,j,k+1)-(i,j+1,k+1)$, 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

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

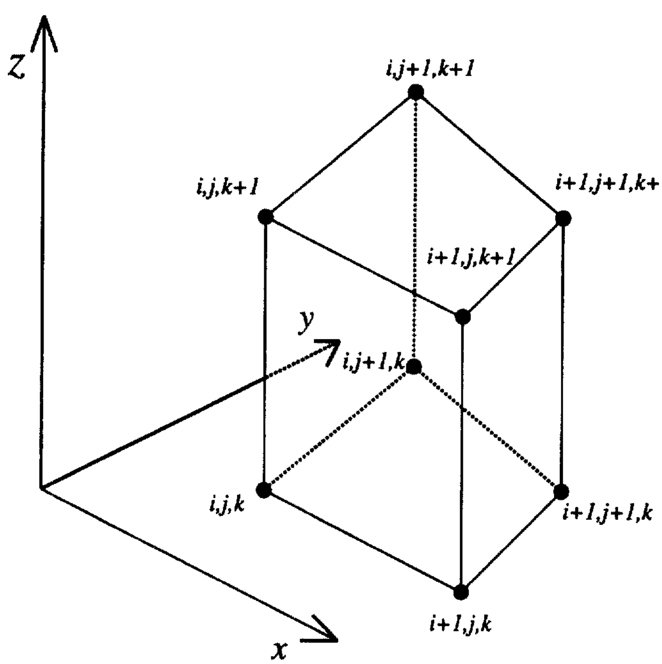
and

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

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.



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



(b) The 2-D $(i + 1/2, j + 1/2)$ cell $(z = 0)$ is interpreted as the base of a 3-D, logical cuboid $(i + 1/2, j + 1/2, k + 1/2)$ cell (a prism) with unit height.

Figure 2.

3.2. Discrete Scalar and Vector Functions

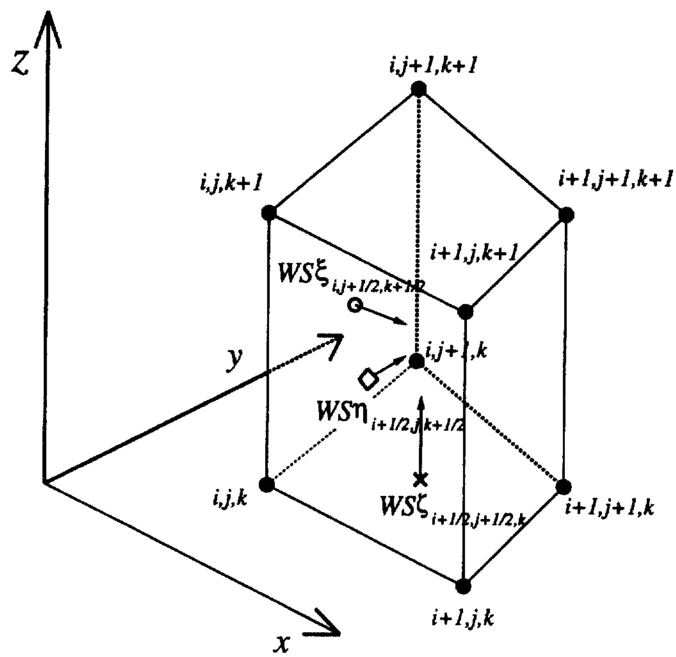
In a cell-centered discretization, the discrete scalar function $U_{i+1/2,j+1/2}$ is defined in the space HC and is given by its values in the cells (see Figure 1), except at the boundary cells. The treatment of the boundary conditions requires introducing scalar function values at the centers of the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

We define the subspace $\overset{0}{HC}$ of HC to be the scalar functions that are zero on the boundary

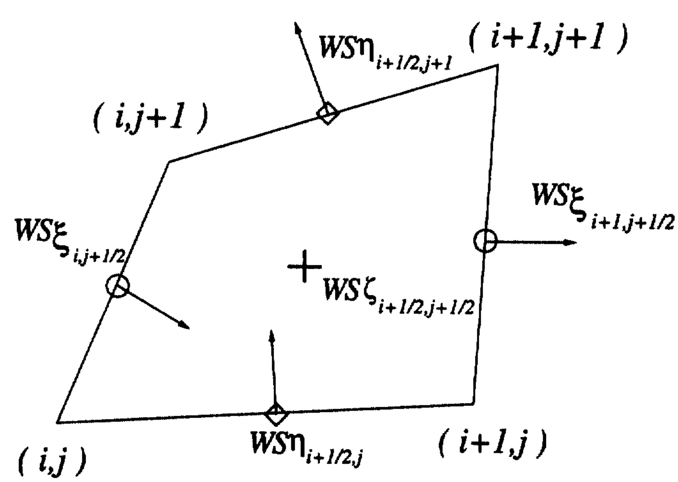
$$U_{(1,j+1/2)} = 0, \quad U_{(M,j+1/2)} = 0, \qquad j = 1, \dots, N-1, \tag{3.1}$$

$$U_{(i+1/2,1)} = 0, \quad U_{(i+1/2,N)} = 0, \qquad i = 1, \dots, M-1. \tag{3.2}$$

The vectors can have three components, but in our 2-D analysis, the components depend on only two spatial coordinates, x and y. The $\mathcal{HS}$ space (see Figure 3a), where the vector components are defined perpendicular to the cell faces, is the natural space when the approximations are based on Gauss' divergence theorem.



(a) $\mathcal{HS}$ discretization of a vector in three dimensions is defined at the center of the faces of the prism.



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

Figure 3.

The projection of the 3-D $\mathcal{HS}$ vector space into two dimensions results in the face vectors defined perpendicular to the quadrilateral cell sides and cell-centered vertical vector perpendicular to 2-D plane (see Figure 3b).

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 $V_{i+1/2,j+1/2}$).

Here, we will consider 2-D vector functions that have only the $WS\xi$, $WS\eta$ components.

3.3. Discrete Inner Products

In the space of discrete scalar functions defined in the cell centers HC, the *natural* inner product corresponding to the continuous inner product (2.21) is

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

The inner product in $\overset{0}{HC}$,

$$(U,V)_{\overset{0}{HC}} = \sum_{i=1}^{M-1}\sum_{j=1}^{N-1} U_{(i+1/2,j+1/2)}V_{(i+1/2,j+1/2)}VC_{(i+1/2,j+1/2)} \tag{3.3}$$

is analogous to the continuous inner product (2.6) for $(u,v)_{\overset{0}{H}}$.

In the space of vector functions $\mathcal{HS}$, the *natural* inner product corresponding to the continuous inner product (2.12) is

$$\left(\vec{A},\vec{B}\right)_{\mathcal{HS}} = \sum_{i=1}^{M-1}\sum_{j=1}^{N-1}\left(\vec{A},\vec{B}\right)_{(i+1/2,j+1/2)} VC_{(i+1/2,j+1/2)}, \tag{3.4}$$

where $(\vec{A},\vec{B})$ is the dot product of two vectors. The dot product must be defined for vectors in $\mathcal{HS}$ (Figure 4). Suppose the axes ξ and η form a nonorthogonal basis and φ is the angle between these axes. If the unit normals to the axes are $n\vec{S}\xi$ and $n\vec{S}\eta$, then the components of the vector $\vec{W}$ in this basis are the orthogonal projections $WS\xi$ and $WS\eta$ of $\vec{W}$ onto the normal vectors. The expression for the dot product of $\vec{A} = (AS\xi, AS\eta)$ and $\vec{B} = (BS\xi, BS\eta)$ is

$$\left(\vec{A},\vec{B}\right) = \frac{AS\xi BS\xi + AS\eta BS\eta + (AS\xi BS\eta + AS\eta BS\xi)\cos\varphi}{\sin^2\varphi}. \tag{3.5}$$

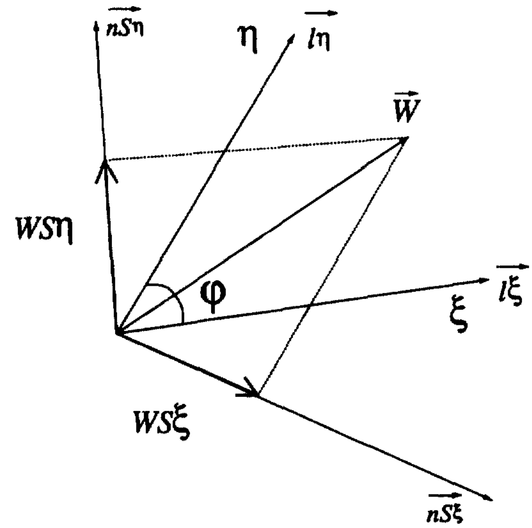


Figure 4. The grid lines (ξ, η) form a local nonorthogonal coordinate system with unit vectors $\vec{l\xi}$, $\vec{l\eta}$ and corresponding unit normals to these directions $n\vec{S}\xi$ and $n\vec{S}\eta$. In this basis, the components $(WS\xi, WS\eta)$ are orthogonal projections to normal directions.

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

$$\begin{aligned}\left(\vec{A}, \vec{B}\right)_{(i+1/2,j+1/2)} = \sum_{k,l=0}^{1} & \frac{V_{(i+k,j+l)}^{(i+1/2,j+1/2)}}{\sin^2 \varphi_{(i+k,j+l)}^{(i+1/2,j+1/2)}} \\ & \cdot \left[AS\xi_{(i+k,j+1/2)} BS\xi_{(i+k,j+1/2)} + AS\eta_{(i+1/2,j+l)} BS\eta_{(i+1/2,j+l)}\right. \\ & + (-1)^{k+l} \left(AS\xi_{(i+k,j+1/2)} BS\eta_{(i+1/2,j+l)}\right. \\ & \left.\left. + \; AS\eta_{(i+1/2,j+l)} BS\xi_{(i+k,j+1/2)}\right) \cos \varphi_{(i+k,j+l)}^{(i+1/2,j+1/2)}\right],\end{aligned} \tag{3.6}$$

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

$$V_{(i+k,j+l)}^{(i+1/2,j+1/2)} \geq 0, \qquad \sum_{k,l=0}^{1} V_{(i+k,j+l)}^{(i+1/2,j+1/2)} = 1. \tag{3.7}$$

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 those for angles between the cell edges.

The inner product in $\overset{0}{\mathcal{H}S}$ is defined by the same equations as those that define the inner product in $\mathcal{H}S$ if we eliminate $WS\xi_{(i,j+1/2)}$, $WS\eta_{(i+1/2,j)}$ (which are equal to zero in $\overset{0}{\mathcal{H}S}$).

When we compute the adjoint relationships between the discrete operators, it is helpful to introduce the *formal* inner products (which we denote by square brackets $[\cdot,\cdot]$) in the spaces of scalar and vector functions:

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

In $\overset{0}{HC}$, the formal inner product is

$$[U, V]_{\overset{0}{HC}} = \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} U_{(i+1/2,j+1/2)} V_{(i+1/2,j+1/2)}, \tag{3.8}$$

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

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

The formal inner product in HC corresponds to the usual dot product of two vectors in $\Re^m$, where m is the total number of unknowns. The formal inner product in $\mathcal{HS}$ corresponds to the usual dot product of two vectors from the direct sum of the two spaces $HS\xi$ and $HS\eta$,

$$\mathcal{HS} = HS\xi \oplus HS\eta. \tag{3.9}$$

Here, the spaces $HS\xi$ and $HS\eta$ are defined as follows:

$$\begin{aligned}
HS\xi &\stackrel{\text{def}}{=} \left\{WS\xi_{i,j+1/2};\ i=1,\ldots,M;\ j=1,\ldots,N-1\right\},\\
HS\eta &\stackrel{\text{def}}{=} \left\{WS\eta_{i+1/2,j};\ i=1,\ldots,M-1;\ j=1,\ldots,N\right\}.
\end{aligned}$$

This connection with usual linear algebra dot products is useful for deriving the matrix form of the finite-difference equations.

The natural and formal inner products satisfy the relationships

$$(U,V)_{HC} = [\mathcal{C}U,V]_{HC} \quad \text{and} \quad \left(\vec{A},\vec{B}\right)_{\mathcal{HS}} = \left[\mathcal{S}\vec{A},\vec{B}\right]_{\mathcal{HS}}, \tag{3.10}$$

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

$$[\mathcal{C}U,V]_{HC} = [U,\mathcal{C}V]_{HC} \quad \text{and} \quad [\mathcal{C}U,U]_{HC} > 0, \tag{3.11}$$

and therefore,

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

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

$$\mathcal{S}\vec{A} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}\begin{pmatrix} AS\xi \\ AS\eta \end{pmatrix} = \begin{pmatrix} S_{11}AS\xi + S_{12}AS\eta \\ S_{21}AS\xi + S_{22}AS\eta \end{pmatrix}, \tag{3.12}$$

and is symmetric and positive in the formal inner product

$$\left[\mathcal{S}\vec{A},\vec{B}\right]_{\mathcal{HS}} = \left[\vec{A},\mathcal{S}\vec{B}\right]_{\mathcal{HS}}, \qquad \left[\mathcal{S}\vec{A},\vec{A}\right]_{\mathcal{HS}} > 0. \tag{3.13}$$

By comparing the formal and natural inner products, that is,

$$\begin{aligned}
\left(\vec{A},\vec{B}\right)_{\mathcal{HS}} &= \left[\mathcal{S}\vec{A},\vec{B}\right]_{\mathcal{HS}}\\
&= \sum_{i=1}^{M}\sum_{j=1}^{N-1}\left[(S_{11}AS\xi)_{(i,j+1/2)} + (S_{12}AS\eta)_{(i,j+1/2)}\right] BS\xi_{(i,j+1/2)}\\
&\quad + \sum_{i=1}^{M-1}\sum_{j=1}^{N}\left[(S_{21}AS\xi)_{(i+1/2,j)} + (S_{22}AS\eta)_{(i+1/2,j)}\right] BS\eta_{(i+1/2,j)},
\end{aligned} \tag{3.14}$$

we can derive the explicit formulas for S:

$$
\begin{aligned}
(S_{11}AS\xi)_{(i,j+1/2)} &= \left(\sum_{k=\pm 1/2; l=0,1} \frac{V_{(i,j+l)}^{(i+k,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i+k,j+1/2)}} \right) AS\xi_{(i,j+1/2)}, \\
(S_{12}AS\eta)_{(i,j+1/2)} &= \sum_{k=\pm 1/2; l=0,1} (-1)^{k+1/2+l} \frac{V_{(i,j+l)}^{(i+k,j+1/2)}}{\sin^2 \varphi_{(i,j+l)}^{(i+k,j+1/2)}} \cos \varphi_{(i,j+l)}^{(i+k,j+1/2)} AS\eta_{(i+k,j+l)}, \\
(S_{21}AS\xi)_{(i+1/2,j)} &= \sum_{k=\pm 1/2; l=0,1} (-1)^{k+1/2+l} \frac{V_{(i+l,j)}^{(i+1/2,j+k)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j+k)}} \cos \varphi_{(i+l,j)}^{(i+1/2,j+k)} AS\xi_{(i+l,j+k)}, \\
(S_{22}AS\eta)_{(i+1/2,j)} &= \left(\sum_{k=\pm 1/2; l=0,1} \frac{V_{(i+l,j)}^{(i+1/2,j+k)}}{\sin^2 \varphi_{(i+l,j)}^{(i+1/2,j+k)}} \right) AS\eta_{(i+1/2,j)}.
\end{aligned}
\tag{3.15}
$$

The operators S_{11} and S_{22} are diagonal, and the stencils for the operators S_{12} and S_{21} are shown in Figure 5. These formulas are valid only for the sides of the grid cells interior to the domain. They can be applied at 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.

These discrete inner products satisfy axioms of inner products,

- $(A, B)_{H_h} = (B, A)_{H_h}$,
- $(\lambda A, B)_{H_h} = \lambda (A, B)_{H_h}$ (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, as well as approximations for continuous inner products and the discrete spaces are Euclidean spaces.

4. DISCRETE ANALOGS OF div AND grad

4.1. Natural Operator DIV

The coordinate invariant definition of the **div** operator is based on Gauss' divergence theorem

$$
\mathbf{div}\, \vec{W} = \lim_{V \to 0} \frac{\oint_{\partial V} \left(\vec{W}, \vec{n} \right) dS}{V}, \tag{4.1}
$$

where $\vec{n}$ is a unit outward normal to boundary ∂V.

The natural definition of the discrete divergence operator is

$$
\mathbf{DIV} : \mathcal{H}S \to HC, \tag{4.2}
$$

where

$$
\begin{aligned}
\left(\mathbf{DIV}\, \vec{W} \right)_{(i+1/2,j+1/2)} = \frac{1}{VC_{(i,j)}} \{ & \left(WS\xi_{(i+1,j+1/2)} S\xi_{(i+1,j+1/2)} - WS\xi_{(i,j+1/2)} S\xi_{(i,j+1/2)} \right) \\
& + \left(WS\eta_{(i+1/2,j+1)} S\eta_{(i+1/2,j+1)} - WS\eta_{(i+1/2,j)} S\eta_{(i+1/2,j)} \right) \}.
\end{aligned}
\tag{4.3}
$$

The extended divergence operator $\mathbf{d}$ defined by (2.23) is approximated by the discrete operator $\mathbf{D}$ coinciding with $\mathbf{DIV}$ on the internal cells $(\mathbf{D}\vec{W})_{(i+1/2,j+1/2)} = (\mathbf{DIV}\, \vec{W})_{(i+1/2,j+1/2)}$, and is defined by

$$
\begin{aligned}
\left(\mathbf{D}\vec{W}\right)_{(i+1/2,1)} &= -WS\eta_{(i+1/2,1)}, & i &= 1,\ldots,M-1,\\
\left(\mathbf{D}\vec{W}\right)_{(i+1/2,N)} &= +WS\eta_{(i+1/2,N)}, & i &= 1,\ldots,M-1,\\
\left(\mathbf{D}\vec{W}\right)_{(1,j+1/2)} &= -WS\xi_{(1,j+1/2)}, & j &= 1,\ldots,N-1,\\
\left(\mathbf{D}\vec{W}\right)_{(M,j+1/2)} &= +WS\xi_{(M,j+1/2)}, & j &= 1,\ldots,N-1,
\end{aligned}
\tag{4.4}
$$

on the boundary.

4.2. Adjoint Operator $\overline{\mathbf{GRAD}}$

Operator **grad** is the negative adjoint of **d**, in inner products (2.21) and (2.12);

$$\mathbf{grad} = -\mathbf{d}^*, \tag{4.5}$$

that follows from the identity (2.8)

$$
\begin{aligned}
(\vec{w}, \mathbf{grad}\, u)_{\mathcal{H}} &= \int_V (\vec{w}, \mathbf{grad}\, u)\; dV\\
&= -\left(\int_V u\; \mathbf{div}\,\vec{w}\, dV - \oint_{\partial V} u\,(\vec{w},\vec{n})\; dS\right)\\
&= (-\mathbf{d}\vec{w}, u)_H\,.
\end{aligned}
\tag{4.6}
$$

We define the derived discrete operator $\overline{\mathbf{GRAD}}$ as the negative adjoint of $\mathbf{D}$

$$\overline{\mathbf{GRAD}} \stackrel{\text{def}}{=} -\mathbf{D}^*. \tag{4.7}$$

Because $\mathbf{D} : \mathcal{H}S \to HC$, the adjoint operator $\overline{\mathbf{GRAD}} : HC \to \mathcal{H}S$ is defined in terms of the inner products

$$\left(\mathbf{D}\vec{W}, U\right)_{HC} = \left(\vec{W}, \mathbf{D}^* U\right)_{\mathcal{H}S}, \tag{4.8}$$

which translates to the formal inner products as

$$\left[\mathbf{D}\vec{W}, \mathcal{C}U\right]_{HC} = \left[\vec{W}, \mathcal{S}\mathbf{D}^* U\right]_{\mathcal{H}S}. \tag{4.9}$$

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

$$\left[\vec{W}, \mathbf{D}^\dagger \mathcal{C}U\right]_{\mathcal{H}S} = \left[\vec{W}, \mathcal{S}\mathbf{D}^* U\right]_{\mathcal{H}S}. \tag{4.10}$$

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

$$\overline{\mathbf{GRAD}} = -\mathbf{D}^* = -\mathcal{S}^{-1}\mathbf{D}^\dagger\mathcal{C}. \tag{4.11}$$

Because the operator $\mathcal{S}$ is banded on nonorthogonal grids, its inverse $\mathcal{S}^{-1}$ is full; consequently, $\overline{\mathbf{GRAD}}$ has a *nonlocal* stencil.

The discrete flux,

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

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

$$\mathcal{S}\vec{W} = \mathbf{D}^\dagger\mathcal{C}U, \tag{4.12}$$

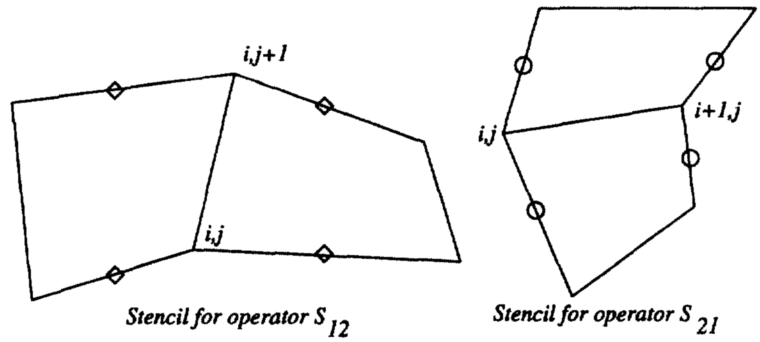


Figure 5. The stencils of the components S_{12} and S_{21} of the symmetric positive operator $\mathcal{S}$ that connects the natural and formal inner products $(\vec{A}, \vec{B})_{\mathcal{H}S} = [\mathcal{S}\vec{A}, \vec{B}]_{\mathcal{H}S}$.

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

$$\begin{aligned} FS\xi_{i,j+1/2} &= -S\xi_{i,j+1/2}\left(U_{i+1/2,j+1/2} - U_{i-1/2,j+1/2}\right), \\ FS\eta_{i+1/2,j} &= -S\eta_{i+1/2,j}\left(U_{i+1/2,j+1/2} - U_{i+1/2,j-1/2}\right). \end{aligned} \tag{4.13}$$

The discrete operator $\mathcal{S}$ is symmetric positive definite and can be represented as the matrix with five nonzero elements in each row (see (3.15) and Figure 5).

5. DISCRETE DIRICHLET BOUNDARY VALUE PROBLEM

5.1. Finite-Difference Method in Operator Form

The discrete problem for Dirichlet boundary conditions is formulated as

$$\begin{gathered} \mathbf{DIV}\,\vec{W} = F, \\ \vec{W} = -\overline{\mathbf{GRAD}}U, \\ U_{1,j+1/2} = \psi_{1,j+1/2}, \quad U_{M,j+1/2} = \psi_{M,j+1/2}, \qquad j = 1, \dots, N-1, \\ U_{i+1/2,1} = \psi_{i+1/2,1}, \quad U_{i+1/2,N} = \psi_{i+1/2,N}, \qquad i = 1, \dots, M-1, \end{gathered} \tag{5.1}$$

where $F = \{f_{i+1/2,j+1/2};\ i = 1, \dots, M-1;\ j = 1, \dots, N-1\}$ and $f_{i+1/2,j+1/2}$ is an approximation of $f(x,y)$ in the cell. The function $\psi_{k,l}$ approximates $\psi(x,y)$, determining Dirichlet boundary conditions.

To transform (5.1) into a problem with zero Dirichlet boundary conditions, we introduce the discrete function $\Psi \in HC$, which is equal to zero in interior cells and which has values on the boundary that coincide with corresponding values of ψ and defines a new unknown function $\tilde{U}$ as

$$\tilde{U} = U - \Psi,$$

satisfying the equations

$$\begin{gathered} \mathbf{DIV}\,\tilde{\vec{W}} = \tilde{F}, \qquad \tilde{F} = F + \mathbf{DIV}\,\overline{\mathbf{GRAD}}\Psi, \\ \tilde{\vec{W}} = -\overline{\mathbf{GRAD}}\tilde{U}, \\ \tilde{U}_{1,j+1/2} = 0, \quad \tilde{U}_{M,j+1/2} = 0, \qquad j = 1, \dots, N-1; \\ \tilde{U}_{i+1/2,1} = 0, \quad \tilde{U}_{i+1/2,N} = 0, \qquad i = 1, \dots, M-1. \end{gathered} \tag{5.2}$$

We use the "$\sim$" notations to denote functions and operators that are defined in $\overset{0}{H}$. Therefore, we define the operator $\widetilde{\overline{\mathbf{GRAD}}}$ as a restriction of $\overline{\mathbf{GRAD}}$ to subspace $\overset{0}{H}$ by dropping terms in

$\overline{\mathbf{GRAD}}$ that vanish on the boundary. Problem (5.2) can now be stated as

$$\mathbf{DIV}\,\tilde{\vec{W}} = \tilde{F}, \tag{5.3a}$$

$$\tilde{\vec{W}} = -\widetilde{\overline{\mathbf{GRAD}}}\tilde{U}. \tag{5.3b}$$

By definition, the operators **DIV** and $-\widetilde{\overline{\mathbf{GRAD}}}$ are adjoint to each other in the inner products $(\vec{A}, \vec{B})_{\mathcal{HS}}$ and $(U, V)_{\overset{\circ}{H}}$;

$$-\widetilde{\overline{\mathbf{GRAD}}} = \mathbf{DIV}^* = \mathbf{DIV}^\dagger \cdot \mathcal{C}. \tag{5.4}$$

Also, in the subspace $\overset{0}{H}$, the operator $\mathbf{DIV}^\dagger \cdot \mathcal{C}$ simplifies on the boundary. For example, for $i = 1$, we get

$$\left(\left(\mathbf{DIV}_\xi^\dagger \mathcal{C}\right) U\right)_{(1,j+1/2)} = -\mathcal{S}\xi_{1,j+1/2}U_{1,j+1/2}. \tag{5.5}$$

The flux $\tilde{\vec{W}}$ can be eliminated in (5.3a) to give the explicit operator form of (5.3b);

$$\tilde{A}U = \mathbf{DIV} \cdot \mathcal{S}^{-1} \cdot \mathbf{DIV}^\dagger \mathcal{C}\tilde{U} = \tilde{F}. \tag{5.6}$$

The operator $\tilde{A}$ is symmetric and positive definite in the space $\overset{0}{H}C$;

$$\left(\tilde{A}U, V\right)_{\overset{\circ}{H}C} = \left(U, \tilde{A}V\right)_{\overset{\circ}{H}C}, \qquad \left(\tilde{A}U, U\right)_{\overset{\circ}{H}C} > 0. \tag{5.7}$$

In terms of the formal inner products, we have

$$\left[\mathcal{C}\tilde{A}U, V\right]_{\overset{\circ}{H}C} = \left[U, \mathcal{C}\tilde{A}V\right]_{\overset{\circ}{H}C}, \qquad \left[\mathcal{C}\tilde{A}U, U\right]_{\overset{\circ}{H}C} > 0. \tag{5.8}$$

Therefore, the discrete operator $A = \mathcal{C} \cdot \tilde{A}$ will be symmetric and positive definite in the formal inner product.

To obtain the corresponding system of linear equations with a symmetric positive discrete operator, we apply $\mathcal{C}$ to both sides of (5.6):

$$AU = \mathcal{C}\,\mathbf{DIV} \cdot \mathcal{S}^{-1} \cdot \mathbf{DIV}^\dagger \mathcal{C}\tilde{U} = \mathcal{C}\tilde{F}. \tag{5.9}$$

Because the operator $\mathcal{S}^{-1}$ has a nonlocal stencil for general grids, equation (5.9) is interesting primarily from a theoretical point of view and is not explicitly constructed when we define the finite-difference method. Further in this section, we explain how to formulate these equations so that they can be effectively solved.

5.2. Solving a System of Equations with Nonlocal Stencil

In this section, we describe an approach to solving (5.6), where the operator $\mathcal{S}$ is local, but where the operator $\mathcal{S}^{-1}$ has a nonlocal stencil. The equations are formulated so that algorithms, such as preconditioned conjugate gradient methods, requiring only a multiplication of a vector by A can be used. Given U, AU can be computed efficiently by solving $\mathcal{S}\vec{W} = \mathbf{DIV}^\dagger \mathcal{C}U$, for $\vec{W}$ and evaluating $AU = \mathbf{DIV}\,\vec{W}$. When solving the system $\mathcal{S}\vec{W} = \mathbf{DIV}^\dagger \mathcal{C}U$, we need to use the appropriate formulas like (5.5) on the boundary. Because $\mathcal{S}$ is a positive-definite symmetric local operator, the equation for $\vec{W}$ can be solved efficiently with iterative methods.

Other efficient algorithms to solve this system include the family of two-level gradient methods, such as the minimal residual method, the minimal correction method, and the minimal error method. All these methods can be written as

$$BU^{(s+1)} = BU^{(s)} + \tau_s \left(F - AU^{(s)}\right), \tag{5.10}$$

where $U^{(s)}$ is an approximate solution to U on iteration number s, τ_s is some iteration parameter, and the operator B is a preconditioner.

A family of three-level iteration methods, which require only the computation of AU, includes the three-level conjugate-direction methods, like the conjugate gradient method. All these methods can be written as

$$BU^{(s+1)} = \alpha_{s+1}\left(B - \tau_{s+1}A\right)U^{(s)} + \left(1 - \alpha_{s+1}\right)BU^{(s-1)} + \alpha_{s+1}\tau_{s+1}F,$$
$$BU^{(1)} = (B - \tau_1 A)U^{(0)} + \tau_1 F.$$

The appropriate inner product with which to compute the parameters α_s, τ_s is the natural inner product, where operator A is symmetric and positive-definite.

The effectiveness of these methods strongly depends on the choice of the preconditioner. The simplest Jacobi-type preconditioner approximates S by its diagonal blocks. This preconditioner is exact for orthogonal grids and produces a five-cell symmetric, positive-definite operator corresponding to removing the mixed derivatives from the variable-coefficient Laplacian on nonorthogonal grids. Some details can be found in [11,13].

6. DISCRETE NEUMANN BOUNDARY VALUE PROBLEM

Following the continuous case in Section 2.2, we consider both the modified inner product and flux form approaches. The discrete analog of (2.18) is

$$\mathcal{A}U = -\mathbf{D}\cdot\overline{\mathbf{GRAD}}U = \mathcal{F}, \tag{6.1}$$

where the operator $\overline{\mathbf{GRAD}}$ is defined on the space HC including the boundary faces, $\mathcal{F}$ includes the approximation of ψ on the boundary and is defined similarly to $\mathbf{F}$ in (2.18). The operator $\overline{\mathbf{GRAD}} = -\mathbf{D}^*$ in the HC inner product (which includes boundary terms), and therefore,

$$\mathcal{A} = \mathbf{D}\cdot\mathbf{D}^*, \qquad \mathcal{A} = \mathcal{A}^* \geq 0.$$

In [3], we proved that the solution of this problem is unique up to a constant if the compatibility condition

$$\sum_{i=1}^{M-1}\sum_{j=1}^{N-1} f_{i+1/2,j+1/2}VC_{i+1/2,j+1/2} = \sum_{i=1}^{M-1}\left(\psi_{M,j+1/2}S\xi_{M,j+1/2} - \psi_{1,j+1/2}S\xi_{1,j+1/2}\right)$$
$$+\sum_{j=1}^{N-1}\left(\psi_{i+1/2,N}S\eta_{i+1/2,N} - \psi_{i+1/2,0}S\eta_{i+1/2,1}\right)$$

is satisfied.

The explicit operator form of (6.1) is similar to (5.9) and can be written as

$$\mathcal{C}\mathbf{D}S^{-1}\mathbf{D}^{\dagger}\mathcal{C}U = \mathcal{F}. \tag{6.2}$$

The flux form of (6.1) is

$$\mathbf{DIV}\,\vec{G} = f_{i,j}, \qquad \text{for all cells}, \tag{6.3a}$$

$$\vec{G} = \begin{pmatrix} GS\xi \\ GS\eta \end{pmatrix} = -\overline{\mathbf{GRAD}}U, \qquad \text{for all faces}, \tag{6.3b}$$

$$\begin{aligned} GS\xi_{1,j+1/2} &= \psi_{1,j+1/2}, \quad GS\xi_{M,j+1/2} = \psi_{M,j+1/2}, \qquad j = 1,\ldots,N-1, \\ GS\eta_{i+1/2,1} &= \psi_{i+1/2,1}, \quad GS\eta_{i+1/2,N} = \psi_{i+1/2,N}, \qquad i = 1,\ldots,M-1. \end{aligned} \tag{6.3c}$$

To construct the discrete analog of the flux form expressed in (2.31a) to (2.31c), we start with a discrete analog of (2.29a)

$$\left(\mathbf{DIV}\vec{W}\right)_{i+1/2,j+1/2}$$
$$\frac{[WS\xi_{i+1,j+1/2}S\xi_{i+1,j+1/2} - WS\xi_{i,j+1/2}S\xi_{i,j+1/2}WS\eta_{i+1/2,j+1}S\eta_{i+1/2,j+1} - WS\eta_{i+1/2,j}S\eta_{i+1/2,j}]}{VC_{i+1/2,j+1/2} = f_{i+1/2,j+1/2}}, \quad (6.4)$$

and a discrete analog of the boundary conditions in (2.29c):

$$\begin{aligned} &WS\xi_{1,j+1/2} = \psi_{1,j+1/2}, \quad WS\xi_{M,j+1/2} = \psi_{M,j+1/2}, \quad && j = 1, \ldots, N-1, \\ &WS\eta_{i+1/2,1} = \psi_{i+1/2,1}, \quad WS\eta_{i+1/2,N} = \psi_{i+1/2,N}, \quad && i = 1, \ldots, M-1. \end{aligned} \quad (6.5)$$

If we eliminate the known boundary fluxes from (6.4), we obtain equations defining the discrete operator $\widetilde{\mathbf{DIV}}$, which is the restriction of **DIV**, on the subspace of vector functions with zero normal components on the boundary. Also, the right-hand side of these equations has to be modified. In the interior, the operator $\widetilde{\mathbf{DIV}}$ and modified right-hand side $\tilde{f}$ coincide with **DIV** and f, respectively. The formulas for the modified discrete divergence, and $\tilde{f}$ in the left-bottom corner cell and in the bottom row of cells are

$$\begin{aligned} \left(\widetilde{\mathbf{DIV}}\vec{W}\right)_{3/2,3/2} &= \frac{WS\xi_{2,3/2}S\xi_{2,3/2} + WS\eta_{3/2,2}S\eta_{3/2,2}}{VC_{3/2,3/2}} \\ &= \tilde{f}_{3/2,3/2} = f_{3/2,3/2} + \frac{\psi_{1,3/2}S\xi_{1,3/2}}{VC_{3/2,3/2}} + \frac{\psi_{3/2,1}S\eta_{3/2,1}}{VC_{3/2,3/2}}, \\ \left(\widetilde{\mathbf{DIV}}\vec{W}\right)_{3/2,j+1/2} &= \frac{WS\xi_{2,j+1/2}S\xi_{2,j+1/2} + WS\eta_{3/2,j+1}S\eta_{3/2,j+1} - WS\eta_{3/2,j}S\eta_{3/2,j}}{VC_{3/2,j+1/2}} \\ &= \tilde{f}_{3/2,j+1/2} = f_{3/2,j+1/2} + \frac{\psi_{1,j+1/2}S\xi_{1,j+1/2}}{VC_{3/2,j+1/2}}, \qquad j = 2, \ldots, N-2. \end{aligned} \quad (6.6)$$

The formulas in the other corner cells and the cells adjacent to the boundary are similar.

We define the discrete analog of the operator **grad** as the negative adjoint of $\widetilde{\mathbf{DIV}}$, using the relationship that the operator **grad** is adjoint to the restriction of **div** defined on vector functions with zero normal components on the boundary. In the discrete case, this means that the inner product for the space of scalar functions does not include boundary terms. Therefore, we define $\overline{\mathbf{GRAD}}$ only on the interior faces, and this definition does not include the values of U on the boundary.

The discrete analog of (2.31a) and (2.31b) is

$$\left(\widetilde{\mathbf{DIV}}\vec{W}\right) = \tilde{f}, \qquad \text{in all cells}, \quad (6.7)$$

$$\vec{W} = -\overline{\mathbf{GRAD}}U, \qquad \text{in internal faces}, \quad (6.8)$$

where all the values of the scalar function U are unknown in the cells and where the components of $\vec{W} = \{WS\xi, WS\eta\}$ are unknown only on the internal faces. The known boundary values of $WS\xi$, $WS\eta$ have been taken into account in the definition of $\tilde{f}$.

Equation (6.8) is defined only for internal faces and does not contain U on the boundary. Furthermore, the right-hand sides of these equations contain only the differences of U in the cells. Therefore, the values of U on the boundary do not participate in equations (6.7) and (6.8). This is the main difference between the approach based on flux formulation and the modified inner-product approach.

The values of U on the boundary can be found in terms of the internal values of U and the fluxes by using equations like (6.3b) and (6.3c), written in the form

$$\mathcal{S}\vec{G} = \mathbf{D}^{\dagger} \cdot \mathcal{C}U, \quad (6.9)$$

after solving the system expressed in (6.7) and (6.8). The relations in (6.9) are explicit because the right-hand side of each equation expressed as (6.9) contains only differences between one value of U in the internal cell and one value of U on the boundary.

7. DISCRETE ROBIN BOUNDARY VALUE PROBLEM

We follow the approach used in the continuous case to define discrete analogs of the operators **d**, **grad**, and Ω for Robin boundary conditions. The discrete analogs of the first two operators are defined by (4.3), (4.4), and (4.11). The discrete analog of Ω (2.40) is defined by

$$(\Omega U)_{(k,l)} = \begin{cases} 0, & \text{in the interior,} \\ \alpha_{(k,l)} U_{(k,l)}, & \text{on the boundary,} \end{cases} \tag{7.1}$$

where k and l are corresponding indices. The discrete analog of the continuum system (2.42) is

$$\Omega U + \mathcal{D}\vec{W} = F, \qquad \vec{W} = \mathcal{G}U. \tag{7.2}$$

The operator equation (2.39) is given by

$$\mathcal{A}\, U = (\Omega + \mathcal{D}\mathcal{G})\, U = F, \tag{7.3}$$

and the explicit form of (7.2) is

$$\mathbf{DIV}\, \vec{G} = f_{i,j}, \qquad \text{for all cells,} \tag{7.4a}$$

$$\vec{G} = \begin{pmatrix} GS\xi \\ GS\eta \end{pmatrix} = -\overline{\mathbf{GRAD}}U, \qquad \text{for all faces,} \tag{7.4b}$$

$$\begin{aligned}
-GS\xi_{1,j+1/2} + \alpha_{1,j+1/2} U_{1,j+1/2} &= \psi_{1,j+1/2}, & j &= 1, \dots, N-1, \\
+GS\xi_{M,j+1/2} + \alpha_{M,j+1/2} U_{M,j+1/2} &= \psi_{M,j+1/2}, & j &= 1, \dots, N-1, \\
-GS\eta_{i+1/2,1} + \alpha_{i+1/2,1} U_{i+1/2,1} &= \psi_{i+1/2,1}, & i &= 1, \dots, M-1, \\
+GS\eta_{i+1/2,N} + \alpha_{i+1/2,N} U_{i+1/2,N} &= \psi_{i+1/2,N}, & i &= 1, \dots, M-1.
\end{aligned}$$

In this system, the fluxes are defined on all the faces and unknown values of U include the values on the boundary faces. These equations are formally equivalent to (7.3), which contains only U. By construction, the operator of this equation is self-adjoint and positive definite.

8. SUMMARY

The goal of mimetic finite-difference methods is to retain crucial properties of the continuum problem. This approach has proven effective in practical applications in fluid dynamics [7], including the flow through strongly heterogeneous, nonisotropic materials [7,13].

We have described an approach for embedding Dirichlet, Neumann, and Robin boundary conditions into a finite-difference approximation for Poisson's equation and proved that the resulting model is self-adjoint and positive-definite on nonsmooth logically rectangular grids.

The two key ideas in these proofs are to define an appropriate discrete inner product and to exploit the fact that the SOM discrete gradient is the negative adjoint of the SOM divergence operator on arbitrary nonuniform grids and preserve this property when incorporating the boundary conditions. Then, forming the Laplacian **div grad** as the composition of these operators guarantees the resulting discrete operator to be self-adjoint. Once the symmetry properties for the discrete operators is established, the proofs for the discrete approximations follows the same logic as that for the continuum equations.

The Dirichlet boundary condition is an essential boundary condition and has to be explicitly imposed on function space where we are looking for the solution. To prove the result for Dirichlet boundary conditions, we transformed the problem into an equivalent problem with zero boundary conditions and then accounted for in the class of discrete functions that vanish on the boundary.

We took the Neumann and Robin boundary conditions into account by changing the definition of the inner product in the functional spaces without imposing the boundary conditions on the solution. We proved that the discrete approximation of the Neumann boundary value problem is self-adjoint and positive when the equations are solved as a second-order system and the boundary conditions are incorporated directly into the inner product and when the equations are written in flux form and solved as a first-order system. We proved the result for the Robin boundary conditions by defining an inner product in the space of discrete scalar functions, which includes a discrete analog of the boundary integral for the boundary conditions.

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