Mimetic Finite Difference Methods for Diffusion Equations *

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This paper reviews and extends the theory and application of mimetic finite difference methods for the solution of diffusion problems in strongly heterogeneous non-isotropic materials. These difference operators satisfy the fundamental identities, conservation laws and theorems of vector and tensor calculus on nonorthogonal, nonsmooth, structured and unstructured computational grids. We provide explicit approximations for equations in two dimensions with discontinuous nondiagonal diffusion tensors. We mention the similarities and differences between the new methods and mixed finite element or hybrid mixed finite element methods.

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1. Introduction and Rationale

The development of high-quality finite-difference methods (FDM's) for the diffusion equation is one part of an effort to create a discrete analog of vector and tensor calculus [1]-[7] that can be used to accurately approximate continuum models for a wide range of physical processes. These FDM's are based on using discrete operators that preserve certain critical properties of the original continuum differential operators. Conservation laws, solution symmetries, and the fundamental identities and theorems of vector and tensor calculus are examples of such properties. This "mimetic" approach has been used to construct high-quality FDM's approximating the diffusion equation [6], [8]-[12], the gas dynamics equations [13], the equations of continuum mechanics [7], Maxwell's first-order curl equations [14], and the equations of magnetic diffusion [14].

This paper reviews and extends these mimetic FDMs for the solution of diffusion problems in strongly heterogeneous non-isotropic materials on nonorthogonal, nonsmooth computational grids.

The steady state solution of the diffusion equation (the pressure equation in the context of reservoir simulations) satisfies

$$-\mathbf{div}\, K\, \mathbf{grad}\, u = f \quad (x, y, z) \in V\,. \tag{1}$$

Here $u(x, y, z)$ is the pressure, $K(x, y, z)$ is a symmetric positive-definite tensor (permeability tensor) that can vary discontinuously in space, $f(x, y, x)$ is a given function, i.e., a source/sink distribution dependent on the wells, and V is, in general, a three-dimensional region. For simplicity in this paper we consider only the zero Dirichlet boundary condition

$$u(x, y, z) = 0\,, \quad (x, y, z) \in \partial V\,, \tag{2}$$

where ∂V denotes the outer surface of V. Discretizations for Neumann and general Robin boundary conditions can be found in [5], [9].

Because the mimetic FDMs are based on discrete analogs of first-order coordinate-invariant operators, it is natural to write equation (3) as a system of first order equations:

$$\mathbf{div}\, \vec{W} = f\,, \quad \vec{W} = -K\, \mathbf{grad}\, u\,, \tag{3}$$

where $\vec{W}$ is generally called the flux, in the case of reservoir simulations is the velocity vector. The first equation is called the mass balance equation because it expresses the conservation of mass. The second equation defines the flux (velocity) in terms of the diffusion tensor and the gradient of the pressure, and is called Darcy's Law. As suggested by this formulation, we use discrete analogs of both u and $\vec{W}$ as the primary variables in our FDM's.

It is convenient to introduce a new operator, $G\,u$, called the flux operator, where

$$G\,u = -K\,\mathbf{grad}\,u\,, \tag{4}$$

and write equation 3 as

$$\mathbf{div}\,\vec{W} = f\,, \quad \vec{W} = G\,u\,. \tag{5}$$

On an interface between two different materials, only the normal component of flux, $\vec{W}$, is continuous. In constructing mimetic FDM's, we define the vectors in terms of the normal flux components defined with respect to cell-face normals. This makes it easy to achieve continuity of the normal flux component at a material interface.

If zero Dirichlet boundary conditions are satisfied by the scalar functions, or if Neumann boundary conditions are satisfied by the vector functions, the operators, **div** and **grad**, satisfy the following integral identity

$$\int_V u\,\mathbf{div}\,\vec{W}\,dV + \int_V (\vec{W}, \mathbf{grad}\,u)\,dV = 0\,. \tag{6}$$

We stress that unless otherwise noted, u and $\vec{W}$ represent arbitrary scalar and vector functions, respectively. Expressing the integrand in the second integral in terms of the flux operator, G, we get

$$\int_V u\,\mathbf{div}\,\vec{W}\,dV - \int_V (K^{-1}\,\vec{W}, G\,u)\,dV = 0\,. \tag{7}$$

Here we have used the fact that K (and therefore K^{-1}) is symmetric (self-adjoint).

Introducing the following inner products in the scalar space, H, and the vector space, $\mathcal{H}$,

$$(u, v)_H = \int_V u\,v\,dV\,, \tag{8}$$

$$(\vec{A}, \vec{B})_{\mathcal{H}} = \int_V (K^{-1}\,\vec{A}, \vec{B})\,dV\,, \tag{9}$$

we can write the identity (7) as

$$(u, \mathbf{div}\,\vec{W})_H - (\vec{W}, Gu)_{\mathcal{H}} = 0\,. \tag{10}$$

This expression clearly states that the flux and divergence operators are adjoint to each other

$$G = \mathbf{div}^* \, . \tag{11}$$

This adjoint relationship between the divergence and flux operators is the constructive basis of our approach for developing mimetic FDM's for the diffusion equation. More specifically, we construct discrete analogs of the divergence and flux operators in such a way that they satisfy a discrete analog of (11).

In this approach we first define the space of discrete scalars and vectors associated with our FDM. We then construct a discrete analog of the divergence operator using the divergence theorem

$$\int_V \mathbf{div}\vec{W} \, dV = \oint_{\partial V} (\vec{W}, \vec{n}) \, dS \, , \tag{12}$$

where $\vec{n}$ is the unit outward normal for ∂V. Next, we define discrete analogs of the continuum scalar and vector inner products given in (8) and (9), respectively. Finally, the discrete analog of the flux operator is obtained by requiring it to be the adjoint of the discrete divergence. This represents a complete conceptual description of our approach. Further details follow.

Local conservation is important for geoscience applications, so a cell-centered conservative discretization for the balance equation is a natural choice. In these discretizations the scalar unknowns are located at the center of each spatial cell with one value of u per cell. We refer to this corresponding discrete space of scalars as HC. As one would expect, the discrete forcing function, f, and the range of the discrete divergence operator are also defined at the center of each cell, or equivalently, defined to be in the space HC.

For reasons previously discussed, our discrete flux unknowns are defined in terms of normal vector components. In particular, a value of the normal component of the flux is defined at the center of each cell face. This component approximates the dot product of the continuum flux vector located at the center of the cell face with a unit vector that is normal to the cell face. We stress that there is only one flux component for each cell face even though each cell face on the mesh interior is shared by two cells. The unit normal vector for each face on the mesh interior is outward-directed with respect to one cell and inward-directed with respect to the other. The particular choice of direction is arbitrary. One must simply account for the direction of the normal when forming the discrete divergence operator for any given cell. However, as is shown later, we choose a particular orientation for the face normals on a logically-rectangular grid. We refer to the discrete space of vectors as $\mathcal{HF}$.

Under the restriction that each cell contain only one material, defining a single normal flux component on each face automatically ensures the continuity of the normal flux component at material interfaces.

Because there is *only one* component of the flux on each cell face, it is not obvious as to how best construct the full flux within multidimensional cells. Interpolation schemes can be defined that yield a full flux vector at all points within the cell [6]. For simplicity, we define the full flux vectors only at the cell *corners*. A cell corner physically coincides with a cell vertex, but a corner unknown is uniquely associated with both a vertex and a cell that contains that vertex. Thus if N cells share a vertex, there are N corner unknowns defined at that vertex, i.e, one for each cell. In order to construct a full vector at a corner, we assume that each cell corner is subtended by two cell faces in 2-D and three cell faces in 3-D, and that the normal flux components are constant on each cell face. These assumptions enable a full vector to be naturally constructed at each cell corner via the normal components associated with the subtending cell faces. The assumption of two subtending faces in 2D is valid for quadrilaterals and triangles, and the assumption of three subtending faces in 3D is valid, for example, for hexahedra, wedges, and tetrahedra. It is not valid for pyramids because one vertex of a pyramid is subtended by four faces. An advantage of the face-centered normal component representation for vectors is that the divergence operator can be trivially constructed (see Sec. 2.4).

This definition of the discrete divergence operator also plays a major role in our discrete vector analysis [2].

Let us denote the discrete divergence by $\mathbf{DIV}$, and the discrete flux operator by $\mathcal{G}$. Once $\mathbf{DIV}$ and the discrete analogs of the inner products given in (8) and (9) have been defined, $\mathcal{G}$ is obtained by requiring the discrete analog of identity (10) to hold for all discrete vectors. The diffusion operator, which we denote by $\mathcal{D}$ is formally obtained simply by forming the product of the discrete divergence and gradient operators: $\mathcal{D} = \mathbf{DIV}\,\mathcal{G}$. By construction, $\mathbf{DIV} : \mathcal{HF} \to HC$. Because $\mathcal{G}$ is adjoint to $\mathbf{DIV}$, it follows that $\mathcal{G} : HC \to \mathcal{HF}$. Thus, as expected, $\mathcal{D} : HC \to HC$.

The method that we have thus far described is called the *global* method because $\mathcal{G}$ is a dense matrix. However, performing a matrix-vector multiply with $\mathcal{G}$ is not as expensive as one might expect because $\mathcal{G}$ can be expressed as a banded matrix multiplied from the left by the inverse of a banded matrix. Therefore to perform a matrix-vector multiply, e.g., to obtain the discrete fluxes given the discrete pressure, one need only perform a banded matrix-vector multiply followed by the solution of a banded system of equations that is usually well-conditioned.

There is alternative approach that results in a banded flux matrix (and consequently, a banded diffusion matrix). We call this the *local* method. A banded flux matrix is obtained at the cost of additional face-center pressure unknowns. The local approach is based upon initially viewing each cell as a separate problem domain. The integral identity given in (7) is simplified in the sense that it holds only when u or $\vec{W}\cdot\vec{n}$ is zero on the domain boundary. Because neither of these conditions will always be met on the faces of the interior-mesh cells, it follows that we must use the following general form of the identity:

$$\int_V u\,\mathbf{div}\,\vec{W}\,dV - \int_V (K^{-1}\,\vec{W}, G\,u)\,dV = \oint_{\partial V} u\,(\vec{W},\vec{n})\,dS\,. \tag{13}$$

The presence of the surface integral integral in (13) clearly suggests the need for face-center pressure unknowns in addition to face-center normal flux components. The discrete divergence operator is defined exactly as in the global method. A discrete flux operator is obtained for each cell by requiring a discrete analog of (13) to hold over the cell for all discrete vectors. The discrete analogs of the continuum inner products appearing on the left side of (13) are identical to those defined for the global method. Applying the discrete divergence operator to the discrete flux operator from the left yields a balance equation for each cell and hence, each cell-center pressure unknown. Since each cell is considered an independent domain, each cell generates its own face-center normal flux component as a function of the cell-center and face-center pressures within the cell. Thus continuity of the normal flux component across cell faces must be explicitly enforced. The equation for each face-center pressure unknown expresses the continuity of the normal flux component across the cell face. This completes our initial description of the local method.

One can show that local and global approaches are algebraically equivalent to each other if one eliminates the face-center pressure unknowns from the local system.

The review of other approaches, and in particular an analysis of similarities between our approach and mixed finite-elements methods and the connection between our method and an algebraic topology framework is done in [2], [15], [12].

Numerical examples illustrating the methods are in references [6], [8]-[12], [16].

We will first describe the mimetic FDM in two dimensions with a logically rectangular grid and a diagonal tensor $K = k(x,y)\,I$, then we describe how to extend our method to unstructured grids, three dimensions, and a general non-diagonal tensor K.

In the next section we describe the basic (*global*) FDM. In section (3) we describe the *local* modification of our method, which has additional unknowns for u on the cell faces. In section (4) we discuss possible generalizations, which include more general boundary conditions, cylindrical coordinates, unstructured grids, three dimensional methods, and so on. Finally, in the last section we summarize the main properties of the our mimetic FDM's and make recommendations for future work.

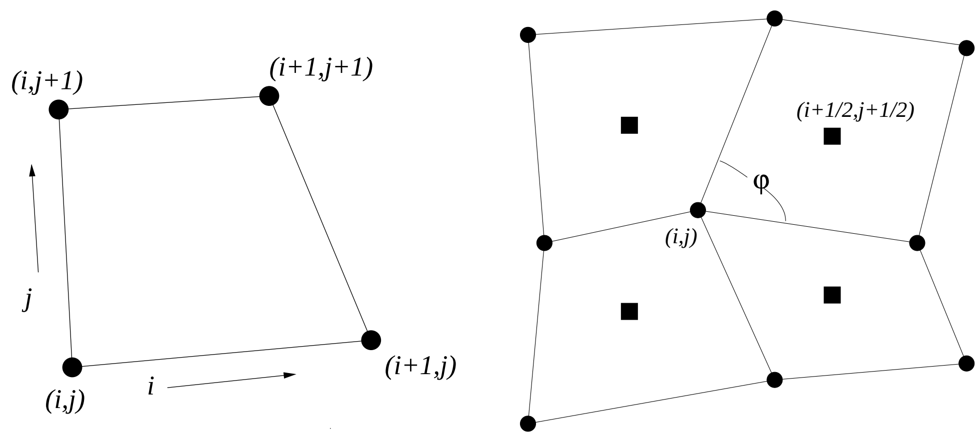
2. The 2D Global Method

We begin by deriving our mimetic FDM for logically-rectangular non-orthogonal mesh in 2D Cartesian geometry.

2.1. The Grid Notation

Consider a logically rectangular grid with quadrilateral cells, where the grid is defined in terms of vertices (nodes). Each vertex carries two indices, (i,j) : $1 \le i \le M;\ 1 \le j \le N$. This vertex indexing is illustrated in Fig. 1 a).

The grid quantities include: cells, cell volumes, cell faces, face areas, face unit normal vectors, face unit tangential vectors, corner volumes, and corner angles. The unknown variables in our method are defined at cell centers, face centers, or cell corners. Cells and cell-centered quantities carry two half-integer indices, e.g., the volume of cell $i+\frac{1}{2}, j+\frac{1}{2}$ is denoted by $V_{i+\frac{1}{2},j+\frac{1}{2}}$. Cell faces and face-centered quantities carry one integer index and one half-integer index, e.g., the areas associated with faces $i, j+\frac{1}{2}$ and $i+\frac{1}{2}, j$, are respectively denoted by $A_{i,j+\frac{1}{2}}$ and $A_{i+\frac{1}{2},j}$. Each cell corner location coincides with a vertex, but it is uniquely associated with both that vertex and a cell that contains that vertex. Thus corner quantities carry two sets of indices, e.g., the corner angle associated with vertex i,j and cell $i+\frac{1}{2}, j+\frac{1}{2}$ is denoted by $\varphi_{i,j}^{i+\frac{1}{2},j+\frac{1}{2}}$ and is illustrated in Fig. 1 b).



a) b)

Figure 1. *Geometry of the mesh: a) Mesh vertex indexing, b) The corner angle* $\varphi_{i,j}^{i+1/2,j+1/2}$ *associated with vertex* (i,j) *and cell* $(i+1/2, j+1/2)$.

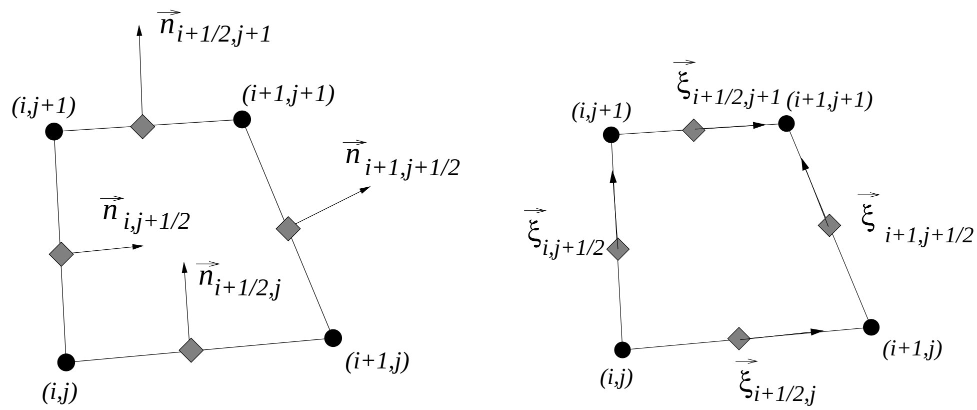
2.2. Discrete Scalar and Vector Functions

The discrete scalar unknowns are located at cell centers. A pressure unknown at the center of cell $i+\frac{1}{2}, j+\frac{1}{2}$ is denoted by $u_{i+\frac{1}{2},j+\frac{1}{2}}$. The discrete scalar space is denoted by HC. The vector unknowns are constructed at the cell corners using normal components located at the face centers. In particular, the two normal components needed to define a full vector at each vertex are obtained from the two faces that subtends that vertex. The face-normal flux component of $\vec{W}$ on face $i+\frac{1}{2}, j$ is denoted by $W_{i+\frac{1}{2},j}$, and the face-normal flux component of $\vec{W}$ on face $i, j+\frac{1}{2}$ is denoted by $W_{i,j+\frac{1}{2}}$. The unit normal for face $i+\frac{1}{2}, j$ is is denoted by $\vec{n}_{i+\frac{1}{2},j}$ and directed along increasing j. The unit normal for face $i, j+\frac{1}{2}$ is denoted by $\vec{n}_{i,j+\frac{1}{2}}$ and is directed along increasing i. The face unit normal vectors are depicted in Fig. 2 a).

The full vector, $\vec{W}$, at corner i,j of cell $i+\frac{1}{2}, j+\frac{1}{2}$ is denoted by $\vec{W}_{i,j}^{i+\frac{1}{2},j+\frac{1}{2}}$. This physical vector is expressed in terms of the two face-normal flux components, $W_{i+\frac{1}{2},j}$ and $W_{i,j+\frac{1}{2}}$, as follows

$$\vec{W}_{i,j}^{i+\frac{1}{2},j+\frac{1}{2}} = W_{i+\frac{1}{2},j} \frac{\vec{\xi}_{i,j+\frac{1}{2}}}{\sin \varphi_{i,j}^{i+\frac{1}{2},j+\frac{1}{2}}} + W_{i,j+\frac{1}{2}} \frac{\vec{\xi}_{i+\frac{1}{2},j}}{\sin \varphi_{i,j}^{i+\frac{1}{2},j+\frac{1}{2}}}\,, \tag{14}$$

where $\vec{\xi}_{i+\frac{1}{2},j}$ denotes a unit vector tangent to face $i+\frac{1}{2}, j$ that is directed along



a) b)

Figure 2. *Normal and tangential vectors: a) Face unit normal vectors. Note that these vectors are directed along increasing "i" if the j-index is half-integer, and along increasing "j" if the i-index is half-integer, b) Face unit tangent vectors. Note that these vectors are directed along increasing "i" if the i-index is half-integer, and along increasing "j" if the j-index is half-integer,*

increasing i. Similarly, $\vec{\xi}_{i,j+\frac{1}{2}}$ denotes a unit vector tangent to face $i, j+\frac{1}{2}$ that is directed along increasing j. The tangent vectors are illustrated in Fig. 2 b). The discrete vector space is denoted by $\mathcal{HF}$.

2.3. Discrete Inner Products

Defining consistent FDM's also requires deriving the appropriate discrete adjoint operators. To define the adjoint operators we must specify the inner products in the spaces of discrete scalar and vector functions. These inner products are analogs of the continuum inner products in (8) and (9):

$$[u, v]_{HC} \stackrel{def}{=} \sum_c u_c \, v_c \, V_c \,, \tag{15}$$

$$\left[\vec{A}, \vec{B}\right]_{\mathcal{HF}} \stackrel{def}{=} \sum_c \sum_{n(c)} (k_n^c)^{-1} (\vec{A}_n^c, \vec{B}_n^c) \, V_n^c \,. \tag{16}$$

Here c represents an index running over the cell centers, n denotes a running index over the vertices associated with cell center c, k_n^c is the scalar diffusion coefficient located in cell c at vertex n, u and v denote arbitrary discrete global scalar functions, V_c denotes the volume associated with cell center c, $\vec{A}$ and $\vec{B}$ denote

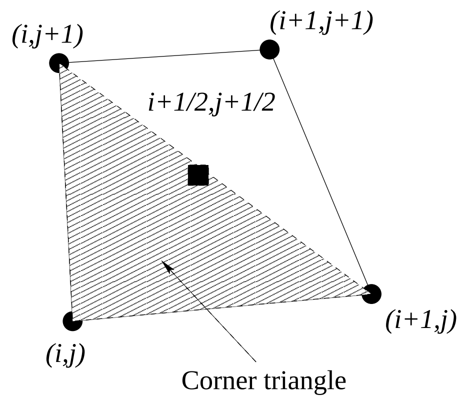


Figure 3. *Corner triangle associated with vertex* (i, j) *and cell* $(i + 1/2, j + 1/2)$.

arbitrary global discrete Cartesian vector functions, $\vec{A}_n^c$ and $\vec{B}_n^c$ denote arbitrary local Cartesian vectors located in cell c at vertex n and constructed from the fundamental face-center normal components as described in the previous section, and V_n^c denotes the corner volume (defined below) associated with cell center c and cell vertex n.

We choose each corner volume to be half of the volume of the triangle formed by the vertex associated with that corner and its two nearest-neighbor vertices within the cell. This corner triangle is illustrated in Fig. 3. We make this choice for the corner volumes because it is the only choice that results in a flux that is exact for linear scalar functions [16]. We refer to these inner products as natural inner products.

It is useful to express the discrete vector inner product directly in terms of the fundamental face-normal vector components. To this end, we to define an algebraic vector, $\hat{W}$, that consists of the face-normal components for physical vector, $\vec{W}$, i.e.,

$$\hat{W}^{i,j}_{i+\frac{1}{2},j+\frac{1}{2}} \stackrel{def}{=} (W_{i+\frac{1}{2},j}, W_{i,j+\frac{1}{2}})^t \,,$$

where the superscript "t" denotes the transpose. If the normal vectors and the tangent vectors are expressed in Cartesian coordinates, then equation (14) can be used to generate a matrix, $\mathbf{T}$, that maps each algebraic vector to its Cartesian equivalent, i.e.,

$$\vec{W} = \mathbf{T}\hat{W} \,. \tag{17}$$

There is a matrix $\mathbf{T}$ for each cell corner, so these matrices carry corner indices.

Substituting from (17) into (16), we get

$$[\hat{A}, \hat{B}]_{\mathcal{HF}} \stackrel{def}{=} \sum_{c} \sum_{n(c)} (k_n^c)^{-1} \, (\mathbf{T}_n^c \hat{A}_n^c, \, \mathbf{T}_n^c \hat{B}_n^c) \, V_n^c \, ,$$

where $\hat{A}$ and $\hat{B}$ denote arbitrary discrete global algebraic vector functions, and $\hat{A}_n^c$ and $\hat{B}_n^c$ denote arbitrary local algebraic vectors located in cell c at vertex n. Using the properties of the adjoint matrix, we re-write the above expression as

$$\left[\hat{A}, \hat{B}\right]_{\mathcal{HF}} \stackrel{def}{=} \sum_{c} \sum_{n(c)} (k_n^c)^{-1} (\hat{A}_n^c, \, \mathbf{S}_n^c \hat{B}_n^c) \, V_n^c \, , \tag{18}$$

where $\mathbf{S} = \mathbf{T}^t \mathbf{T}$. It is shown in [11] that

$$\mathbf{S} = \frac{1}{\sin^2(\varphi)} \begin{bmatrix} 1 & \cos(\varphi) \\ \cos(\varphi) & 1 \end{bmatrix} \, ,$$

where φ is the corner angle. Note that $\mathbf{S}$ is symmetric positive definite (SPD) matrix, invariant to the ordering of the face components in the algebraic vector. Furthermore $\mathbf{S}$ becomes the identity matrix on an orthogonal ($\varphi = 90$ degrees) mesh.

2.4. The Discrete Divergence Operator

To discretize $\mathbf{div}\vec{W}$ in the balance equation we use the coordinate invariant definition of the $\mathbf{div}$ operator based on Gauss' divergence theorem:

$$\mathbf{div}\, \vec{W} = \lim_{V \to 0} \frac{\oint_{\partial V} (\vec{W}, \vec{n}) \, dS}{V} \, , \tag{19}$$

where $\vec{n}$ is the unit outward normal to the boundary ∂V. In the discrete case, V is the volume of the grid cell and ∂V is the set of faces of the cell, i.e., the local discrete divergence operator for cell $i + \frac{1}{2}, j + \frac{1}{2}$ is given by

$$\begin{aligned} &(\mathbf{DIV}\, \vec{W})_{i+1/2, j+1/2} = \\ &\frac{1}{V_{i+\frac{1}{2}, j+\frac{1}{2}}} \, \Big\{ \Big(W_{i+1, j+\frac{1}{2}} \, A_{i+1, j+\frac{1}{2}} - W_{i, j+\frac{1}{2}} \, A_{i, j+\frac{1}{2}} \Big) + \\ &\Big(W_{i+\frac{1}{2}, j+1} \, A_{i+\frac{1}{2}, j+1} - W_{i+\frac{1}{2}, j} \, A_{i+\frac{1}{2}, j} \Big) \Big\} \, , \end{aligned} \tag{20}$$

where A denotes a face area (actually a length in 2D).

Note that the local divergence operator can be thought of as operating on the algebraic corner vectors rather than the Cartesian corner vectors, so one could substitute $(\mathbf{DIV}\,\hat{W})_{i+1/2,j+1/2}$ for $(\mathbf{DIV}\,\vec{W})_{i+1/2,j+1/2}$ in (20). The discrete divergence operator (global) is denoted as either $\mathbf{DIV}\,\vec{W}$ (operating on discrete global Cartesian vector functions) or $\mathbf{DIV}\,\hat{W}$ (operating on discrete global algebraic vector functions.) The natural domain for the discrete divergence operator is the space $\mathcal{HF}$ and the natural range is HC. Indeed, as can be seen from (20), ($\mathbf{DIV} : \mathcal{HF} \to HC$). One can directly prove that $\mathbf{DIV}$ is exactly zero on constant vector function [9]. This is not a trivial statement because the face-normal components of a constant vector are not constant if the cells change shape across the grid.

2.5. Discrete Flux Operator

As previously noted, we define the derived discrete analog of the flux operator G as the adjoint of $\mathbf{DIV}$

$$\mathcal{G} \stackrel{def}{=} \mathbf{DIV}^* \,. \tag{21}$$

To derive a matrix expression for this operator, we first use the natural inner products (15) and (18) to construct a discrete analog of identity (10)

$$\left[u, \mathbf{DIV}\,\hat{W}\right]_{HC} = \left[\hat{W}, \mathcal{G}\,u\right]_{\mathcal{HF}} \,. \tag{22}$$

Using the property of the adjoint operator, we rewrite the above expression as

$$\left[\hat{W}, \mathbf{DIV}^*\,u\right]_{HC} = \left[\hat{W}, \mathcal{G}\,u\right]_{\mathcal{HF}} \,. \tag{23}$$

Equation (21) follows from the requirement that (23) must hold for all $\hat{W}$.

Greater insight into the nature of $\mathcal{G}$ can be gained through the use of another set of discrete scalar and vector inner products that we refer to as the formal inner products. Specifically,

$$\langle u, v \rangle_{HC} \stackrel{def}{=} \sum_c u_c\, v_c \,, \tag{24}$$

and

$$\langle \hat{A}, \hat{B} \rangle_{\mathcal{HF}} \stackrel{def}{=} \frac{1}{2} \sum_c \sum_n \, (\hat{A}_n^c,\, \hat{B}_n^c) \equiv \sum_f \, A_f B_f \,. \tag{25}$$

Here f denotes a running index over cell faces, and A_f and B_f denote the face-normal vector components associated with the discrete global algebraic vector functions $\hat{A}$ and $\hat{B}$.

Re-expressing (22) in terms of the formal inner products (using (15) and (18)), we get

$$\langle u, \mathcal{C}\,\mathbf{DIV}\,\hat{W}\rangle_{HC} = \langle \hat{W}, \mathcal{S}\,\mathcal{G}\,u\rangle_{\mathcal{HF}}\,, \tag{26}$$

where $\mathcal{C}$ is a diagonal matrix whose elements are the cell volumes, and $\mathcal{S}$ is a banded SPD matrix arising from the diffusion coefficients, the corner **S**-matrices, and the corner volumes. A detailed description of the matrix $\mathcal{S}$ is given in [2] and [9]. It is important to note that $\mathcal{S}$ becomes diagonal on an orthogonal mesh.

Using the property of the adjoint operator, we can rewrite (26) as follows

$$\langle \hat{W}, \mathbf{DIV}^{\dagger}\,\mathcal{C}\,u\rangle_{HC} = \langle \hat{W}, \mathcal{S}\,\mathcal{G}\,u\rangle_{\mathcal{HF}}\,, \tag{27}$$

Since the above expression must hold for all $\hat{W}$, it follows that

$$\mathcal{G} = -\mathbf{DIV}^{*} = -\mathcal{S}^{-1}\,\mathbf{DIV}^{\dagger}\,\mathcal{C}\,. \tag{28}$$

where $\mathbf{DIV}^{\dagger}$ is the adjoint of $\mathbf{DIV}$ with respect to the formal inner products. Note that $\mathbf{DIV}^{\dagger}$ is a banded matrix. Because the operator $\mathcal{S}$ is non-diagonal on non-orthogonal grids, its inverse $\mathcal{S}^{-1}$ is full. Consequently, $\mathcal{G}$ has a *nonlocal* stencil and we call it a *global operator*.

The discrete flux, $\vec{W} = \mathcal{G}\,u = \mathcal{S}^{-1}\,\mathbf{DIV}^{\dagger}\,\mathcal{C}\,u$, is obtained by solving the banded linear system

$$\mathcal{S}\,\vec{W} = \vec{F} = \mathbf{DIV}^{\dagger}\,\mathcal{C}\,u\,. \tag{29}$$

On an orthogonal grid, $\mathcal{S}$ is diagonal, so $\mathcal{G}$ is banded. For instance, assuming that the diffusion coefficient is constant within a cell and that the cells are square and of length h on a side, a face-normal flux component takes the following simple form

$$W_{i,j+\frac{1}{2}} = -\frac{k_{i,j+\frac{1}{2}}}{h}(u_{i+\frac{1}{2},j+\frac{1}{2}} - u_{i-\frac{1}{2},j+\frac{1}{2}})\,, \tag{30}$$

where the effective face-diffusion coefficient is given by the harmonic mean of the adjacent cell-center diffusion coefficients

$$k_{i,j+\frac{1}{2}} = \left(\frac{1}{2k_{i-\frac{1}{2},j+\frac{1}{2}}} + \frac{1}{2k_{i+\frac{1}{2},j+\frac{1}{2}}}\right)^{-1}\,.$$

The flux component defined by formula (30) is exact for a linear u and piece-wise constant k. As previously noted, $\mathcal{G}$ is exact for linear u in the case of a general grid as well.

An important property of the continuum gradient is that $\mathbf{grad}\, u = 0$ if and only if u is a constant. It easy to show that the same is true for the discrete flux operator $\mathcal{G}$ (see [9]). It is highly desirable that the null space of the discrete gradient **GRAD** contain only constant functions. The are many discretizations that do not have this property, particularly those where vector components are co-located at the corners of cells. For such discretizations, typically the highest-frequency mode on the grid is also in the null space of the discrete gradient, and then a special procedure for filtering noise from the solution is required, as in the method of *Margolin* [17].

Our discrete equations for the continuum problem (5) are written as follows

$$\mathbf{DIV}\, \vec{W} = f\,, \quad \vec{W} = \mathcal{G}\, u = -\mathcal{S}^{-1}\, \mathbf{DIV}^{\dagger}\, \mathcal{C}\, u\,. \tag{31}$$

The flux $\vec{W}$ can be eliminated to obtain a discrete diffusion equation for u

$$\mathcal{L}\, u = \mathbf{DIV}\ \mathcal{G}\, u = -\mathbf{DIV}\ \mathcal{S}^{-1}\ \mathbf{DIV}^{\dagger}\ \mathcal{C}\, u\,, \tag{32}$$

where the matrix $\mathcal{L}$ is SPD. The matrix $\mathcal{L}$ is full because $\mathcal{S}^{-1}$ is full. Consequently, we refer to our method as the *global* method.

One approach to solve these discrete equations is based directly on its saddle point form

$$\begin{pmatrix} 0 & \mathcal{C}\,\mathbf{DIV} \\ \mathbf{DIV}^{\dagger}\,\mathcal{C} & S \end{pmatrix} \begin{pmatrix} u \\ \vec{W} \end{pmatrix} = \begin{pmatrix} C\, f \\ 0 \end{pmatrix}\,, \tag{33}$$

which is obtained from equations 31 by applying the operator $\mathcal{C}$ to the first equation and the operator S to the second equation. For recent advances and a review of existing methods for solving saddle point problems see for example [18].

Another approach is based on directly solving the system (32) and using iterative methods, which do not require an explicit expression for the operator matrix, but rather need a procedure to compute the action of the operator matrix on vector functions. For example, in the conjugate gradients method one must compute $\mathcal{L}\, u^{\ell}$, where u^{ℓ} is a solution vector iterate. For our method it is done in two steps. First, one solves the system

$$\mathcal{S}\hat{W}^{\ell} = -\mathbf{DIV}^{\dagger}\, \mathcal{C}\, u^{\ell}\,, \tag{34}$$

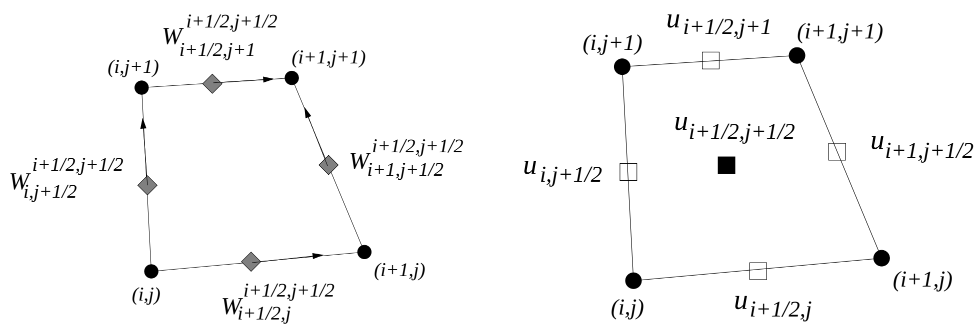


Figure 4. *Scalar and vector unknowns for local method: a) Scalar unknowns for local method. Note that the face pressures are shared by adjacent cells, b) Face-normal vector components for local method. Note that these unknowns are not shared by adjacent cell. Hence, the carry face and cell indices.*

to find the flux which corresponds to u^ℓ. Second, one explicitly applies **DIV** to compute $\mathcal{L}\, u^\ell$

$$\mathcal{L}\, u^\ell = \mathbf{DIV}\, \hat{W}^\ell\,. \tag{35}$$

This approach requires solving the system, (34), on each iteration. Note that the operator for (34) is the same for all iterations, and that $\mathcal{S}$ is symmetric positive-definite and becomes diagonal when the mesh is orthogonal. These properties allow effective preconditioning such as multigrid method.

We stress that in the case of orthogonal grids the operator $\mathcal{L}$ reduces to the standard five-point discretization with face-center diffusion coefficients obtained by harmonically averaging adjacent cell-center diffusion coefficients.

3. The Local Method

In the local version of our method we first apply a variant of the global method to a single cell to obtain a flux operator matrix. As shown in Fig. (4), additional scalar unknowns are placed at the face centers. While the global method has a single face-normal flux component for each face, the local method has two such components - one for each cell sharing the face. Thus each face-normal vector component carries a superscript cell index in addition to a subscript face index. This is illustrated in Fig. 4.

A discrete version of the continuum identity, (13), is used to define the discrete flux operator. In particular, this discrete identity takes the following form for cell $i+\frac{1}{2}, j+\frac{1}{2}$

$$u_{i+\frac{1}{2},j+\frac{1}{2}} \Big[-A_{i,j+\frac{1}{2}} W_{i,j+\frac{1}{2}} + A_{i+\frac{1}{2},j+1} W_{i+\frac{1}{2},j+1}$$

$$A_{i+1,j+\frac{1}{2}} W_{i+1,j+\frac{1}{2}} - A_{i+\frac{1}{2},j} W_{i+\frac{1}{2},j} \Big] -$$

$$\left(\hat{W}_{i,j}\,,\,\mathbf{S}_{i,j}\hat{F}_{i,j}\right) V_{i,j} - \left(\hat{W}_{i,j+1}\,,\,\mathbf{S}_{i,j+1}\hat{F}_{i,j+1}\right) V_{i,j+1} -$$
$$\left(\hat{W}_{i+1,j+1}\,,\,\mathbf{S}_{i+1,j+1}\hat{F}_{i+1,j+1}\right) V_{i+1,j+1} - \left(\hat{W}_{i+1,j}\,,\,\mathbf{S}_{i+1,j}\hat{F}_{i+1,j}\right) V_{i+1,j} =$$

$$-A_{i,j+\frac{1}{2}} u_{i,j+\frac{1}{2}} W_{i,j+\frac{1}{2}} + A_{i+\frac{1}{2},j+1} u_{i+\frac{1}{2},j+1} W_{i+\frac{1}{2},j+1} +$$

$$A_{i+1,j+\frac{1}{2}} u_{i+1,j+\frac{1}{2}} W_{i+1,j+\frac{1}{2}} - A_{i+\frac{1}{2},j} u_{i+\frac{1}{2},j} W_{i+\frac{1}{2},j}\,, \tag{36}$$

where $\hat{F}_{i,j}$ denotes an algebraic flux vector located at corner i, j of the cell with face-normal components $F_{i,j+\frac{1}{2}}$ and $F_{i+\frac{1}{2},j}$. Note that the superscript index $i+\frac{1}{2}, j+\frac{1}{2}$ has been suppressed for the face-normal vector components, the corner algebraic vectors, the corner S-matrices, and the corner volumes. Also note that the volumetric integral terms on the left side of (36) are discretized exactly as in the global method. In particular, the local discrete divergence operator for cell $i+\frac{1}{2}, j+\frac{1}{2}$ is given by

$$\left(\mathbf{DIV}\,\hat{W}\right)_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{1}{V_{i+\frac{1}{2},j+\frac{1}{2}}} \Big[-A_{i,j+\frac{1}{2}} W_{i,j+\frac{1}{2}} + A_{i+\frac{1}{2},j+1} W_{i+\frac{1}{2},j+1} +$$
$$A_{i+1,j+\frac{1}{2}} W_{i+1,j+\frac{1}{2}} - A_{i+\frac{1}{2},j} W_{i+\frac{1}{2},j} \Big]\,, \tag{37}$$

where the superscript index $i+\frac{1}{2}, j+\frac{1}{2}$ has been suppressed for the face-normal vector components. The discretization of the surface integral term on the right side of (36) is a direct generalization of the divergence discretization.

A 4×4 system of linear equations for the face-normal components of the fluxes is obtained from identity (36) by requiring the identity hold for all $\hat{W}$. For instance, the equation for $F_{i,j+\frac{1}{2}}$ is obtained by setting $W_{i,j+\frac{1}{2}}$ to 1 and the remaining three face-normal vector components of $\vec{W}$ to zero. Equations for the other flux components are obtained analogously. The resulting 4×4 linear system is solved numerically to obtain the local discrete flux operator, $\mathcal{G}_{i+\frac{1}{2},j+\frac{1}{2}}$, that relates the flux components in the cell to differences between the face-center and cell-center pressures

$$\bar{G}_{i+\frac{1}{2},j+\frac{1}{2}} = \mathcal{G}_{i+\frac{1}{2},j+\frac{1}{2}} \, (\Delta\bar{u})_{i+\frac{1}{2},j+\frac{1}{2}} \ , \tag{38}$$

where

$$\bar{G}_{i+1,j+\frac{1}{2}} = \left(G^{i+\frac{1}{2},j+\frac{1}{2}}_{i,j+\frac{1}{2}}, G^{i+\frac{1}{2},j+\frac{1}{2}}_{i+\frac{1}{2},j+1}, G^{i+\frac{1}{2},j+\frac{1}{2}}_{i+1,j+\frac{1}{2}}, G^{i+\frac{1}{2},j+\frac{1}{2}}_{i+\frac{1}{2},j} \right)^t \ , \tag{39}$$

and

$$(\Delta\bar{u})_{i+\frac{1}{2},j+\frac{1}{2}} = \tag{40}$$
$$\left(u_{i,j+\frac{1}{2}} - u_{i+\frac{1}{2},j+\frac{1}{2}}, u_{i+\frac{1}{2},j+1} - u_{i+\frac{1}{2},j+\frac{1}{2}}, u_{i+1,j+\frac{1}{2}} - u_{i+\frac{1}{2},j+\frac{1}{2}}, u_{i+\frac{1}{2},j} - u_{i+\frac{1}{2},j+\frac{1}{2}} \right)^t .$$

The local discrete diffusion operator for the cell, $\mathcal{L}_{i+\frac{1}{2},j+\frac{1}{2}}$, is obtained by applying the local divergence operator to the local discrete flux operator,

$$\mathcal{L}_{i+\frac{1}{2},j+\frac{1}{2}} \Delta\bar{u} = \mathbf{DIV}_{i+\frac{1}{2},j+\frac{1}{2}} \, \mathcal{G}_{i+\frac{1}{2},j+\frac{1}{2}} \, (\Delta\bar{u})_{i+\frac{1}{2},j+\frac{1}{2}} \ . \tag{41}$$

The local discrete diffusion operator is used to construct the balance equation for each cell. This balance equation serves as the equation for the cell-center pressure unknown in the cell.

Thus the first step in the local method can be thought of as independently applying the global method (albeit with an additional surface integral term in the integral identity that necessitates additional surface pressure unknowns) to obtain a discrete diffusion equation for the cell. Next the cells are "connected" to satisfy a global version of (36). This is achieved by requiring continuity of the face-normal components on the mesh interior, i.e.,

$$+W^{i+\frac{1}{2},j+\frac{1}{2}}_{i,j+\frac{1}{2}} - W^{i-\frac{1}{2},j+\frac{1}{2}}_{i,j+\frac{1}{2}} = 0 \, , \tag{42}$$

$$+W^{i+\frac{1}{2},j+\frac{1}{2}}_{i+\frac{1}{2},j} - W^{i+\frac{1}{2},j-\frac{1}{2}}_{i+\frac{1}{2},j} = 0 \, , \tag{43}$$

where the face indices are restricted to those on the interior mesh.

These continuity-of-flow equations serve as the equations for the face-center pressure unknowns on the mesh interior, e.g., (42) is the equation for $u_{i,j+\frac{1}{2}}$. It is important to note that the sign of each face-normal flux component appearing in Eqs. (42) and (43) must be preserved to achieve a symmetric positive-definite coefficient matrix, e.g., see [11], [12]. Equations are not needed for the pressure unknowns on the outer boundary faces because they are explicitly set to zero,

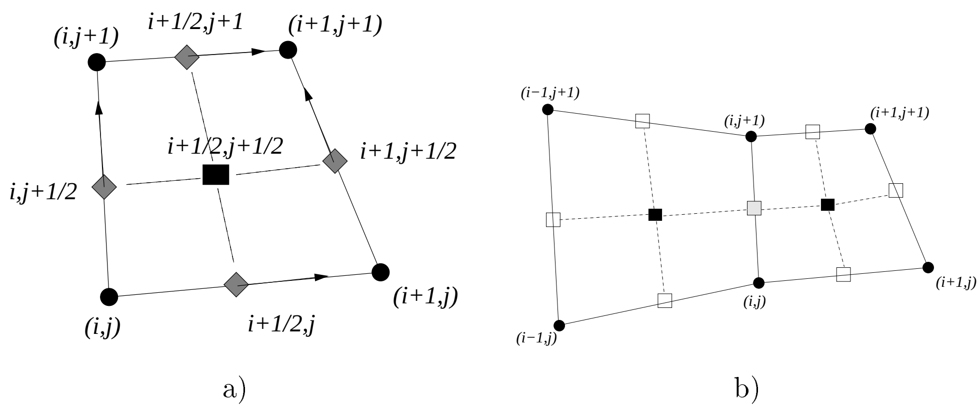


Figure 5. *Stencils: a) Five-point stencil for balance equation associated with* $u_{i+1/2,j+1/2}$*, b) Nine-point stencil for continuity-of-flux equation associated with* $u_{i+1/2,j}$*.*

thereby satisfying the Dirichlet condition. The coefficient matrix for the cell-center pressure unknowns and the interior-mesh face-center pressure unknowns is both sparse and SPD [11]. The cell-center equations have five non-zero matrix elements, and the face-center equations have nine non-zero elements. These stencils are illustrated in Fig. 5 a), and Fig. 5 b). The vector unknowns are constructed at the cell corners using normal components located at the face centers.

It is possible to use the cell-center equations to eliminate the cell-center fluxes from the system, leaving only face-center pressure unknowns. However, testing of the method has thus far been limited to the full cell-center/face-center system. A pure cell-center multigrid preconditioner has been developed for the full system that is quite effective on meshes that are not too skewed [11], [12], [19].

The local and and global approaches are equivalent in the sense that they produce the same normal flux components and cell-centered pressures. Thus these methods represent the same discrete operator and differ only in the choice of independent variables.

4. Generalizations

4.1. Other Coordinate Systems

All of our mimetic FDMs are formulated in terms coordinate-invariant geometrical elements: volumes, areas, and, angles. If it is more convenient to use another coordinate system, then one simply needs to know how to compute these geometrical quantities in that coordinate system. An example of our local method in 2D cylindrical coordinates is presented in [11].

4.2. More Accurate Discretizations

Our discretization for the integral over a cell of a dot product of two vectors is based upon constructing the full vectors at the cell corners. This approach can be thought of as using a quadrature formula for the integral with points at the cell corners. More accuracy could obviously be achieved by using quadrature formulae with points on the interior of the cell. However, this requires a vector interpolation scheme on the cell interior consistent with our face-normal component representation. More accurate approximations for the dot product integral have been derived in [6] using an interpolation scheme that is exact for both constant vector functions and a class of vector functions obtained via the so-called Piola transform [20], [21]. For these functions the interpolated integrand can be integrated exactly using symbolic manipulations [6]. The resulting expression for dot product integral is more accurate then the one described here, but it has the same order of convergence. However, the interpolated dot product method requires wider stencil for certain of the discrete equations, and the coefficient matrix is more poorly conditioned than that of the method described in this paper. Moreover, the interpolated dot product method is less robust on non-smooth grids and cannot be used on degenerate quadrilaterals.

4.3. General Non-Diagonal Tensor K

The global and local methods described here can be easily extended to accommodate general non-diagonal symmetric positive-definite tensors, K, [10]. For this case the vector inner product definition given in (18) is modified by removing factor of k^{-1} from (18) and redefining the $\mathbf{S}$-matrices from $\mathbf{S} = \mathbf{T}^t\mathbf{T}$ to $\mathbf{S} = \mathbf{T}^t\,\mathbf{K}^{-1}\,\mathbf{T}$. The S-matrices remain SPD under this new definition, but they reduce to K^{-1} rather than the identity on an orthogonal mesh. Thus, with a general tensor diffusion tensor, the global method yields dense flux and diffusion matrices even when the mesh is orthogonal.

4.4. General Robin Boundary Condition

The diffusion problem with general Robin boundary conditions can be written as first-order system

$$\vec{w} = G\,u\,, \quad D\,\vec{w} + \Omega\,u = F\,, \tag{44}$$

where G is the flux operator, and

$$D\vec{w} = \begin{cases} \mathbf{div}\,\vec{w}\,, \text{on } V, \\ -(\vec{w},\vec{n})\,, \text{on } \partial V, \end{cases} ,\Omega u = \begin{cases} 0\,\text{on } V, \\ \alpha\,u\,, \text{on } \partial V, \end{cases} , \quad F = \begin{cases} f \text{ on } V\,, \\ \psi\,, \text{on } \partial V\,. \end{cases} \tag{45}$$

We will call D the *extended* divergence operator.

If we modify the scalar inner product by including the boundary term to give

$$(u,\,v)_H = \int_V u\,v\,dV + \oint_{\partial V} u\,v\,dS\,, \quad u,v \in H\,, \tag{46}$$

and use the inner product for vector functions defined in (16), then the flux operator and the extended divergence operator are adjoint to each other. The presence of the boundary term in (46) necessitates adding face-center scalar unknowns on the outer boundary faces. The construction of our mimetic FDM follows the same path as it does with Dirichlet boundary conditions.

We first construct discrete analog, $\mathcal{D}$, of the extended divergence D. the extended divergence operator is the standard divergence in the interior, so we use the discretization given in (20). On the outer boundary, the discretization of D is trivial because it produces the normal components of the flux, which are our primary vector unknowns. The discrete analog of G is defined as the adjoint of the discrete extended divergence operator

$$\mathcal{G} = \mathcal{D}^* \tag{47}$$

and the discrete diffusion operator (including discretization of boundary conditions), $\mathcal{L}$ is defined as the product of $\mathcal{D}$ and $\mathcal{G}$

$$\mathcal{L} = \mathcal{D}\,\mathcal{G}\,. \tag{48}$$

One can easily prove that because of (47), the discrete diffusion matrix has the same desirable properties as those obtained with Dirichlet boundary conditions, [5], [9].

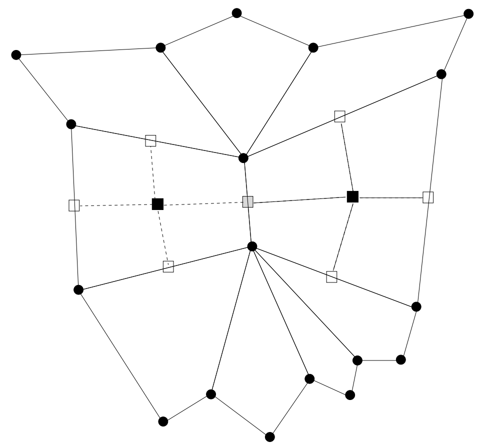


Figure 6. *Stencil for continuity-of-flow equation on unstructured quad grid.*

4.5. Numerical Accuracy

The numerical results presented in [8]-[12], [16] demonstrate second-order convergence of our FDMs for scalar unknown (pressure) on both smooth and non-smooth (randomly perturbed) grids and with both scalar and tensor diffusion. The fluxes have a second-order convergence rate on smooth and piece-wise smooth grids, but have a first-order convergence rate on non-smooth (randomly perturbed) grids,[6].

4.6. Unstructured Meshes

It is straight forward to extend these FDM's to unstructured meshes composed of quads and triangles or hexahedra, tetrahedra and any cell type having three faces subtending each vertex. Since these FDM's are cell-centered, and couple to other cells only through the faces, the methods can be directly applied to unstructured meshes. For instance, in the local method, the stencils for each balance equation and each continuity-of-flow equation are invariant to the number of cells that subtends a vertex. This can readily be seen from Fig. 6.

4.7. Three Dimensions

The construction of FDM's in 3D is completely analogous to the construction of 2D schemes as long as the cell volumes, face areas, and face unit normals are well defined. This is clearly the case for tetrahedral meshes. For general hexahedral grids, the volumes and face areas are well-defined using trilinear and bilinear finite-element mappings, but the unit normal vector varies across each cell face. This problem can be dealt with by defining an "average" unit normal [12]. In 3D one also has the problem that more than three faces may subtend a vertex, thereby making it unclear as to how to define a full vector at that vertex. This problem has not yet been adequately addressed. Possible choices for constructing finite difference methods on hexahedral meshes are considered in [12]. In addition, a detailed description of our 3D hexahedral-mesh method is presented along with numerical results.

5. Summary and Future Work

In this section we give a summary of the properties of our FDM's and describe some of our current research, and research we intend to do in the near future.

5.1. Summary

There are two basic methods: the global method and the local method. The global method has cell-center scalar unknowns and flux unknowns that take the form of face-normal components. The global method has a dense flux matrix and a dense diffusion matrix, but both of these matrices are the product of sparse matrices and the inverse of a sparse SPD matrix. Furthermore, this inverse degenerates to the identity when the mesh is orthogonal. This makes it much less expensive to perform a dense matrix-vector multiply then would otherwise be the case. The local method has sparse flux and diffusion matrices at the cost of additional face-center scalar unknowns. The local and global methods give identical solutions for the cell-center scalar unknowns and the fluxes. Thus they represent the same basic approximation with different independent variables.

Both the local and global methods have the following properties:

1. The coefficient matrix for the scalar unknowns is symmetric positive-definite.

2. Computational testing indicates that second-order convergence is achieved for the scalar unknowns on both smooth and non-smooth meshes with material discontinuities. Similar convergence rates are achieved for the flux unknowns except that non-smooth meshes yield a first-order convergence rate.

3. When the mesh is orthogonal, the method is equivalent to the standard 5-point (in 2D) and 7-point (in 3D) cell-centered diffusion discretizations.

4. The null space of the discrete flux operator contains only constant functions.

5.2. Future Work

The best preconditioners currently available for our global and local methods are based upon approximate diagonalization of the corner **S** matrices. When this is done, the global method no longer produces dense flux and diffusion matrices, but rather produces a pure cell-center (only cell-center scalar unknowns) 5-point scheme in 2D [11] and a pure cell-center 7-point scheme in 3D [12] that is SPD and completely equivalent to the full system when the mesh is orthogonal.

Diagonalization of the **S** matrices in the local scheme enables each face-center scalar unknown to be eliminated from the full face-center/cell-center scalar system, leaving the same cell-center scheme directly produced by the global method. Because this approximate cell-center scheme is exact when the mesh is orthogonal, it is extremely effective as a preconditioner when the mesh is mildly skewed. However, its effectiveness rapidly degrades with increasing mesh skewness. This is not particularly surprising because the approximate method is non-convergent, i.e., gives zeroth order accuracy, on non-orthogonal meshes.

We are investigating a 2D method that has two normal flux components per face rather than one. This FDM (whether in local or global form) produces a pure cell-center 9-point SPD diffusion discretization method on logically-rectangular meshes that converges with second-order accuracy on smooth meshes, but does not converge on non-smooth meshes. Because of its convergence properties, we expect this FDM to be a good preconditioner for both our global and local schemes when the mesh is significantly skewed.

Another important property of both the existing 5-point preconditioner and the proposed 9-point preconditioner is that each of them can be very efficiently preconditioned using the black-box multigrid scheme [22]. Thus, rather than fully solve the approximate pure cell-center preconditioning system, we simply perform a fixed number of multigrid V-cycles on it. This results in a true multilevel solution technique that has been shown to be very efficient for the case of the 5-point preconditioner. We not only intend to extend this approach to the 9-point preconditioner on logically-rectangular meshes, but we also intend to investigate an unstructured-mesh variant using algebraic multigrid [23].

There is a strong connection between our FDMs and the mixed finite-element methods. In fact, our global scheme is akin to mixed finite-elements and our local scheme is akin to hybrid mixed finite-elements. We have not previously been able to theoretically prove the convergence of our methods on non-orthogonal meshes. In the future, we intend to exploit the connection between finite-element methods and our FDMs (see [12]) to prove the convergence of our methods.

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