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Problems with Heterogeneous and Non-Isotropic Media or Distorted Grids

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ABSTRACT *In this paper we define discretizations of the divergence and flux operators that produce symmetric, positive-definite, and accurate approximations to steady-state diffusion problems. Because discontinuous material properties and highly distorted grids are allowed, the flux operator, rather than the gradient, is used as a fundamental operator to be discretized. The resulting finite-difference scheme is similar to those obtained from the mixed finite-element method.*

Key Words: diffusion equation, heterogeneous, non-isotropic, distorted grid, finite-difference, support-operators.

1 The Continuum Problem

Many practical steady-state diffusion problems can be described using the operator $\triangle = \nabla\cdot\mathcal{K}\nabla$, where $\nabla\cdot$ is the divergence operator, ∇ is the gradient operator, and $\mathcal{K}$ is a symmetric tensor describing the material properties of some physical model, then If the tensor $\mathcal{K}$ is symmetric and bounded below, then this operator is symmetric and elliptic. The goal is to find discretizations of the divergence, gradient, and the material tensor so that the induced discretization of $\triangle$ is symmetric, positive-definite, and accurate. In fact, this is done by finding a discretization of the divergence $\nabla\cdot$ and the flux operator $\mathbf{G} = \mathcal{K}\nabla$ that involves a generalization of the usual harmonic averaging on an orthogonal grid to a general multi-dimensional harmonic averaging.

There are two critical points here: it is not assumed that $\mathcal{K}$ is continuous; and the grids used in the discretization will not be assumed smooth.

If V is some region, the boundary-value problem to be discretized is

$$-\nabla\cdot\mathcal{K}\nabla u = f \quad \text{in } V\,, \quad (\mathcal{K}\nabla u, \vec{n}) + \alpha u = \psi \quad \text{in } \partial V\,, \tag{1}$$

where u is the function to be solved for, f is a given forcing function, $\vec{n}$ is the unit outward normal to the boundary ∂V, and α and ψ are functions given on ∂V. It is helpful to write problem (1) in terms of first-order operators:

$$\nabla\cdot\vec{w} = f \quad \text{in } V, \quad \vec{w} = -\mathcal{K}\nabla u \quad \text{in } V, \quad -(\vec{w},\vec{n}) + \alpha u = \psi \quad \text{in } \partial V. \tag{2}$$

The algorithm is constructed using a nontrivial generalization of the method of *support operators* which is described in detail in the book [SHA 96] by Shashkov and in series of papers [HYM 9-], [SHA 95] and [SHA 9-] by the authors. The paper [HYM 9-] contains a far more detailed account of some of the ideas presented in this paper. If u and $\vec{w}$ are smooth scalar and vector functions on V, then the support-operators idea is to discretize the operators $\nabla\cdot$, ∇, $\mathcal{K}$, and the integrals in the integral identity

$$\int_V u\,\nabla\cdot\vec{w}\,dV + \int_V (\vec{w},\nabla u)\,dV = \oint_{\partial V} u\,(\vec{w},\vec{n})\,dS\,, \tag{3}$$

so that a discrete analog of this identity holds exactly. To do this for a $\mathcal{K}$ that is not continuous, we introduce an inner product of vectors weighted by the inverse of $\mathcal{K}$.

To this end, define the space H to be the smooth scalar functions on the union of V and ∂V and the space $\mathbf{H}$ to be the smooth vector functions on V, and then define the inner products

$$\langle u, v\rangle_H = \int_V u\,v\,dV + \oint_{\partial V} u\,v\,dS\,, \quad \langle \vec{A}, \vec{B}\rangle_{\mathbf{H}} = \int_V (\mathcal{K}^{-1}\vec{A}, \vec{B})\,dV\,, \tag{4}$$

where $u, v \in H$ and $\vec{A}, \vec{B} \in \mathbf{H}$. Because the matrix $\mathcal{K}$ is symmetric and positive definite, the inner product of vectors is symmetric and positive definite. There are two important points about these inner products: the inner products for scalars provides a natural implementation of the boundary conditions; and the inner-products of vectors takes advantage of the fact that, at discontinuities of the material properties tensor $\mathcal{K}$, the normal component of the flux $\mathcal{K}\,\nabla u$ is continuous while the normal component of ∇u is not.

Now define the operators

$$\mathbf{G} : H \rightarrow \mathbf{H}\,; \quad \mathbf{D} : \mathbf{H} \rightarrow H\,; \quad \boldsymbol{\Omega} : H \rightarrow H\,; \quad \triangle : H \rightarrow H\,;$$

by

$$\begin{aligned}
\mathbf{G}u &= -\mathcal{K}\,\nabla u \quad \text{in}\, V\,, \\
\mathbf{D}\vec{w} &= \begin{cases} +\nabla\cdot\vec{w} & \text{in}\, V\,, \\ -(\vec{w}, \vec{n}) & \text{in}\, \partial V\,, \end{cases} \\
\boldsymbol{\Omega}u &= \begin{cases} 0 & \text{in}\, V\,, \\ \alpha\, u & \text{in}\, \partial V\,. \end{cases} \\
\triangle u &= \begin{cases} -\nabla\cdot\mathcal{K}\,\nabla u & \text{in}\, V \\ (\mathcal{K}\,\nabla u, \vec{n}) + \alpha\, u & \text{in}\, \partial V \end{cases}
\end{aligned}$$

The right-hand side of (1) has the form

$$\mathbf{F} = \begin{cases} f & \text{in}\, V \\ \psi & \text{in}\, \partial V \end{cases}.$$

and then problem (1) can be written as

$$\triangle\, u = \mathbf{F}\,.$$

and the first-order problem (2) can be written as

$$\boldsymbol{\Omega}\, u + \mathbf{D}\,\vec{w} = F\,, \quad \vec{w} = \mathbf{G}\, u\,.$$

The crucial result about the inner products and operators is that the integral relationship (3) can be written as

$$\langle \mathbf{D}\,\vec{w}, u\rangle_H = \langle \vec{w}, \mathbf{G}\, u\rangle_{\mathbf{H}}\,,$$

that is, the operators have the properties

$$\mathbf{D} = \mathbf{G}^*\,, \quad \boldsymbol{\Omega} = \boldsymbol{\Omega}^* \geq 0\,.$$

and because

$$\triangle = \boldsymbol{\Omega} + \mathbf{D}\cdot\mathbf{G}\,, \tag{5}$$

$\triangle$ is symmetric and positive:

$$\triangle = \triangle^* \geq 0\,.$$

So, the goal is to discretize the operators $\nabla\cdot$ and $\mathbf{G}$ so that the above properties hold exactly.

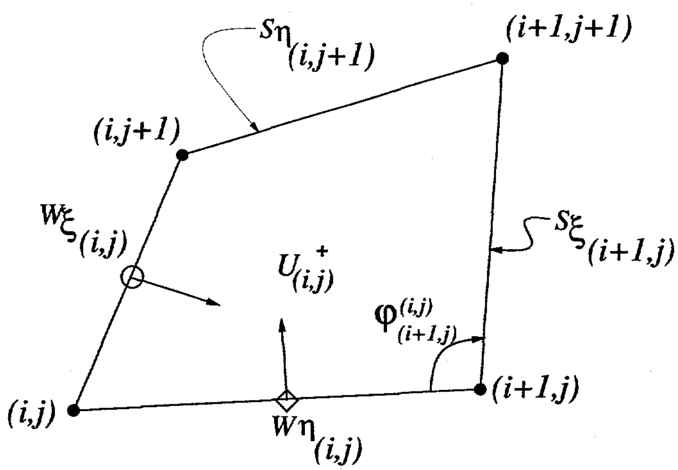

Figure 1: *The Surface Discretization of a Vector*

2 The Discretization

A standard logically-rectangular grid [KNU 93] that is made up of cells is used to discretize the problem described in the previous section. Scalars are discretized as cell-centered data except that the treatment of the boundary conditions requires the introduction of the values of the scalar function on the centers of the boundary segments. The components of **K** are discretized in the same way as u and the scalar functions α and ψ are discretized in the same way as u is on the boundary. Vectors are discretized using their orthogonal projections onto the direction which is perpendicular to the the cell edges, as shown in Figure 1. The use of the normal component is natural for discontinuous $\mathcal{K}$ because the normal flux is continuous at and discontinuity of $\mathcal{K}$.

The space of discrete scalar functions HC has the inner product $\langle\cdot,\,\cdot\rangle_{HC}$, which is a natural discretization of the inner product of scalars given in (4). The space of discrete vector functions $\mathcal{HS}$ has inner product $\langle\cdot,\,\cdot\rangle_{\mathcal{HS}}$ and is an analog of the inner product given in (4), but the fact that the components of the vectors are not defined at the cell centers where **K** is defined makes the definition of this inner product complicated. The details can be found in [HYM 9-].

To compute the adjoint relationships, it is helpful to introduce the *formal* inner product $[\cdot,\,\cdot]_{HC}$ in the spaces of scalar functions HC and the formal inner product $[\cdot,\,\cdot]_{\mathcal{HS}}$ in the space of vector functions. The formal inner products are simply the standard inner product on sequences. Then the relationships between the natural inner products and the formal inner products are:

$$\langle U,\,V\rangle_{HC} = [\mathcal{M}\,U,\,V]_{HC}\,, \qquad \langle\vec{A},\,\vec{B}\rangle_{\mathcal{HS}} = [\mathcal{S}\,\vec{A},\,\vec{B}]_{\mathcal{HS}}\,,$$

where $\mathcal{M}$ and $\mathcal{S}$ are matrices that can be easily computed. The operator $\mathcal{M}$ is a diagonal operator that is multiplication by the volumes of cells in the interior, and multiplication by the lengths of cell sides on the boundary. The operator $\mathcal{S}$ is a block matrix and, for example, in the case that $\mathcal{K}$ is the scalar k times the identity,

$$(S_{11}\,A\xi)_{(i,j)} = \left(\sum_{k,l=0}^{1} \frac{1}{k_{(i-k,j)}} \cdot \frac{V_{(i,j+l)}^{(i-k,j)}}{\sin^2(\varphi_{(i,j+l)}^{(i-k,j)})}\right) A\xi_{(i,j)}\,,$$

$$(S_{12}\,A\eta)_{(i,j)} = \sum_{k,l=0}^{1} \left(\frac{(-1)^{k+l}}{k_{(i-k,j)}} \cdot \frac{V_{(i,j+l)}^{(i-k,j)}}{\sin^2(\varphi_{(i,j+l)}^{(i-k,j)})} \cos(\varphi_{(i,j+l)}^{(i-k,j)})\right) A\eta_{(i-k,j+l)}\,,$$

where the ϕ's are the angles between two consecutive pairs of sides of the cell and the V's are the areas of the triangles formed by the consecutive pairs of side of the a cell (see Figure 1). The formulas for S_{21} and S_{22} are similar. The formulas show that these operators are symmetric and positive definite in the formal inner products provided that the volumes V are all positive.

3 The Support Operators Method

First, the divergence is discretized using an natural analog of the Gauss theorem. Next the discretization of the flux operator is derived using the fact that it must be the adjoint of the divergence in the previously defined previously. Then both the second-order equation (1) and the first-order system (2) are discretized using these operators. As these discretizations contain some non-local operators (un-banded matrices), some care must be used in solving the resulting equations.

3.1 The Prime Operator

The natural conservative invariant definition of the divergence operator is

$$\nabla \cdot \vec{w} = \lim_{V \to 0} \frac{1}{V} \oint_V (\vec{w}, \vec{n})\, dV\,,$$

and thus a natural discrete divergence is

$$(\mathbf{DIV}\, \vec{W})_{(i,j)} = \frac{\left(W\xi_{(i+1,j)}\, S\xi_{(i+1,j)} - W\xi_{(i,j)}\, S\xi_{(i,j)}\right) + \left(W\eta_{(i,j+1)}\, S\eta_{(i,j+1)} - W\eta_{(i,j)}\, S\eta_{(i,j)}\right)}{VC_{(i,j)}}\,. \tag{6}$$

In the interior, the discrete analog $\mathcal{D}$ of the operator $\mathbf{D}$ is the discrete divergence while on the boundary $\mathcal{D}$ is the normal component the discrete vector.

3.2 The Derived Operator

The derived operator $\mathcal{G}$ is the discrete analog of the flux operator $\mathbf{G}$ and is defined by $\mathcal{G} = \mathcal{D}^*$. On arbitrary grids, it is not possible to write a explicit formula for the components of the operator $\mathcal{G}$. However, it is possible to express $\mathcal{G}$ in terms of $\mathcal{M}$, $\mathcal{S}$, and $\mathcal{D}$:

$$\mathcal{G} = \mathcal{D}^* = \mathcal{S}^{-1}\, \mathcal{D}^\dagger\, \mathcal{M}\,. \tag{7}$$

Because $\mathcal{S}$ is banded, $\mathcal{S}^{-1}$ is likely to be full (unless $\mathcal{S}$ is diagonal). Hence, $\mathcal{G}$ is full, that is, it has a *non-local* stencil. This is not a serious problem, because we do not need to explicitly form $\mathcal{G}$.

The discrete fluxes are

$$\vec{W} = \mathcal{G}\, U = \mathcal{S}^{-1}\, \mathcal{D}^\dagger\, \mathcal{M}\, U\,,$$

and if the operator $\mathcal{S}$ is applied to both sides of this equation, then

$$\mathcal{S}\, \vec{W} = \mathcal{D}^\dagger\, \mathcal{M}\, U\,. \tag{8}$$

The operators on both sides of this equation have a local stencils. The finite element and compact finite difference methods that can be expressed in the form (8) with local stencils (see, for example, [LEL 92]).

The relationship $(\mathcal{D}\, \vec{W},\, U)_{HC} = (\vec{W},\, \mathcal{D}^*\, U)_{\mathcal{H}S}$ implies that

$$[\vec{W},\, \mathcal{D}^\dagger\, \mathcal{M}\, U]_{\mathcal{H}S} = [\mathcal{D}\, \vec{W},\, \mathcal{M}\, U]_{HS}\,.$$

The right-hand side of this formula can be evaluated using (6) for $\mathcal{D}$ and summation by parts to give:

$$-\left(\mathcal{D}^\dagger\, \mathcal{M}\, U\right)_{(i,j)} = \begin{pmatrix} S\xi_{(i,j)}\left(U_{(i,j)} - U_{(i-1,j)}\right) \\ S\eta_{(i,j)}\left(U_{(i,j)} - U_{(i,j-1)}\right) \end{pmatrix}. \tag{9}$$

To find the fluxes for given temperature, equation (8) must solved for $\vec{W}$. The discrete operator $\mathcal{S}$ is symmetric positive-definite and with five non-zero elements in each row, so there are many strategies for doing this (see [HYM 9-]).

3.3 The Discrete Operator Equations

The finite difference approximation of the first-order system (2) is

$$\Omega U + \mathcal{D}\vec{W} = F, \quad \vec{W} = \mathcal{G}\,U, \tag{10}$$

and then the approximation of the second-order equation (1), which is an analog of the operator equation (5), is

$$\mathcal{A}\,U = (\Omega + \mathcal{D}\,\mathcal{G})\,U = F. \tag{11}$$

In the interior of the cells, Equation (11) is

$$\left(\mathcal{D}\vec{W}\right)_{(i,j)} = \mathbf{DIV}\,\vec{W}_{(i,j)} = f_{(i,j)},$$

while the approximation of the boundary conditions is

$$\left(\mathcal{D}\vec{W}\right)_{(i,j)} + \alpha_{(i,j)}\,U_{(i,j)} = \psi_{(i,j)}.$$

where, on the boundary, the operator $\mathcal{D}$ gives the normal component of the vector.

3.4 Theoretical Properties of the Algorithms

The properties for the operators $\nabla\cdot$ and ∇ were investigated in *Shashkov and Steinberg* [SHA 9-], where it was shown that the divergence of a constant vector is zero, that for smooth grids the point truncation errors for the divergence **DIV** and for the gradient **GRAD** are second order, and for general grids, **DIV** and **GRAD** are first-order accurate, and that the **DIV** is exact for integral truncation error. A a rather lengthy geometric calculation shows that for piecewise constant **K**, the discrete analog of $\mathbf{K}\,\nabla$ is exact on piecewise linear functions.

We now prove that the null space of the operator $\mathcal{G}$ contains only constants, that is $\mathcal{G}U$ is zero if and only if U is constant. Formula (7) gives

$$\mathcal{G}\,U = \mathcal{S}^{-1}\mathcal{D}^{\dagger}\,\mathcal{M}\,U, \tag{12}$$

and then, if U is a constant, (9) shows that $\mathcal{D}^{\dagger}\,\mathcal{M}\,U = 0$, so $\mathcal{G}\,U = 0$.

Conversely, assume that $\mathcal{G}\,U = 0$. Formula (12) and the fact that operator $\mathcal{S}$ is positive definite gives

$$\mathcal{D}^{\dagger}\,\mathcal{M}\,U = 0.$$

This and Formula (9) then gives:

$$\begin{aligned} U_{(i,j)} - U_{(i-1,j)} = 0; \quad i = 1,\ldots,M; \quad j = 1,\ldots,N-1; \\ U_{(i,j)} - U_{(i,j-1)} = 0; \quad i = 1,\ldots,M-1; \quad j = 1,\ldots,N; \end{aligned}$$

which implies that U is a constant. Therefore the null space of the discrete operator $\mathcal{G}$ is the constant functions, exactly as for the differential operator $\mathcal{K}\,\nabla$.

3.5 Solving the System of Linear Equations

The discrete equations the cell-surface discretization have the form (10):

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

The fluxes can be eliminated from this system to obtain an equation for U:

$$\mathcal{A}U = \Omega\,U + \mathcal{D}\,\mathcal{G}\,U = F,$$

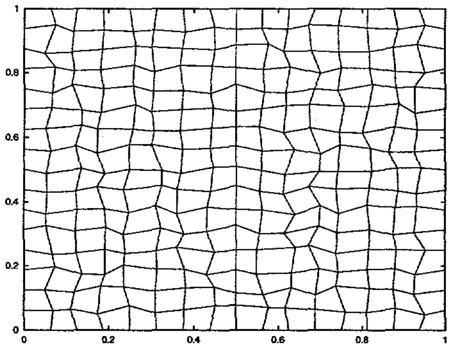

Figure 2: *Grid for the MacKinnon and Carey Problem,* $M = N = 17$

where $\mathcal{A}$ is symmetric and positive definite. The operators $\mathcal{G}$ and $\mathcal{A}$ are *non-local* and, therefore, algorithms that require explicit expressions for them are impractical for large problems. These equations can be formulated so that algorithms, such as preconditioned conjugate gradient methods, requiring only a multiplication of a vector by $\mathcal{A}$ can be used. Given U, $\mathcal{A}\,U$ can be computed efficiently by solving (8) for $\vec{W}$ and the evaluating $\mathcal{A}\,U = \Omega\,U + \mathcal{D}\vec{W}$. All operators in this formulation are explicitly known and local. Moreover, because $\mathcal{S}$ is a positive definite symmetric local operator, the equation for $\vec{W}$ can be solved efficiently using iterative methods. Note that on orthogonal grids, $\mathcal{S}$ is diagonal.

Other efficient algorithms to solve this system include the family of two-level gradient methods, including the minimal residual method, the minimal correction method, and the minimal error method. The effectiveness of these methods strongly depends on the choice of a preconditioner. The simplest Jacobi type preconditioner approximates $\mathcal{S}$ by its diagonal blocks. This 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 non-orthogonal grids.

4 Examples

We present two examples, there are many more in [HYM 9-], [SHA 95], and [SHA 9-].

4.1 MacKinnon and Carey Example

This test problem is from *MacKinnon and Carey* [MAC 88] and has a discontinuous piecewise-constant diffusion coefficient:

$$D = \begin{cases} D_1\,, & 0 < x < 0.5 \\ D_2\,, & 0.5 < x < 1 \end{cases},$$

and the exact solution is the piecewise-quadratic function

$$u(x) = \begin{cases} a_1\,\frac{x^2}{2} + b_1\,x\,, & 0 \le x \le \frac{1}{2}\,, \\ a_2\,\frac{x^2}{2} + b_2\,x + c_2\,, & \frac{1}{2} \le x \le 1\,, \end{cases}$$

where

$$a_i = \frac{-1}{D_i}\,, \quad b_1 = -\frac{3\,a_2 + a_1}{4}\,\frac{D_2}{D_1 + D_2}\,, \quad b_2 = \frac{D_2}{D_1}\,b_1\,, \quad c_2 = -(b_2 + 0.5\,a_2)\,.$$

This problem was solved on the 2-D random grid shown in Figure 2, where the discontinuity coincides, with a grid line, so the line with $x = 1/2$ is fixed, but the y coordinates of points on this line are changed randomly. The convergence analysis shows that the support-operators method is second-order accurate in both the max and L_2 norms.

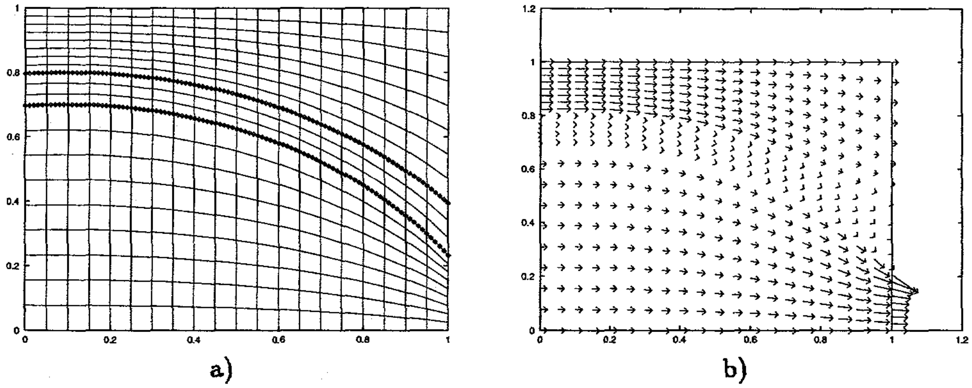

Figure 3: *a) The Geometry and the Grid for the Streak, b) Velocity Field for Cell-Node Discretization*

4.2 Flow Through a System Containing an Impermeable Streak

This example, similar to one in *Durlofsky* [DUR 94], uses the logically rectangular grid shown Figure 3 a). The top curve is chosen to be an arc of a circle with the center at $(0.1, -0.4)$ and radius equal to 1.2. The bottom curve an arc of a circle with the same center and with radius equal to 1.1.

The permeability throughout the domain is uniform and isotropic ($\mathbf{K} = \mathbf{I}$), except in the low-permeability streak where the permeability is set such that the component parallel to the local streak orientation ($k_{\|}$) is equal to 0.1 and the component perpendicular to the streak orientation ($k_{\perp}$) is equal to 0.001. In the streak, the tensor $\mathbf{K}$ is a full tensor, in terms of its Cartesian components, which vary with (x, y) and are readily determined from the knowledge of $k_{\|}$ and $k_{\perp}$. For the Cartesian components K_{xx}, K_{xy}, K_{yy}, which are used in cell-node discretization, the transformation formulas are:

$$\begin{aligned} K_{xx} &= k_{\|} \cos^2 \varphi + k_{\perp} \sin^2 \varphi \,, \\ K_{xy} &= (k_{\|} - k_{\perp}) \cos \varphi \sin \varphi \,, \\ K_{yy} &= k_{\|} \sin^2 \varphi + k_{\perp} \cos^2 \varphi \,, \end{aligned}$$

where $\varphi = \varphi(x, y)$ is the angle of rotation of the orthogonal coordinate system where the tensor $\mathbf{K}$ is diagonal and has components $k_{\|}$ and $k_{\perp}$. In our case

$$\sin \varphi = -\frac{x'}{\sqrt{(x')^2 + (y')^2)}} \,, \quad \cos \varphi = \frac{y'}{\sqrt{(x')^2 + (y')^2)}} \,,$$

where $x' = x - 0.1$ and $y' = y + 0.4$.

Figure 3 b) displays the velocity field for case of the cell-node discretization (the length of arrows are proportional to module of the vectors). The results of the cell-surface discretization will be similar. As expected physically, almost no flow enters the streak, so these results are qualitatively similar to the best results in *Durlofsky* [DUR 94].

5 Conclusion

The support-operators method can be used to produce accurate schemes for for problems with either rough coefficients or rough grids. Both non-diagonal material tensor (see [HYM 9-]) and general Robin boundary conditions are allowed. In all cases, the matrices involved in the discrete problem are symmetric and positive definite. The method is exact on problems with piece-wise linear solutions even for very rough grids. On rough grids the scheme is first-order accurate, but when the grid and the material properties are smooth, the scheme is second-order accurate.

It is clear that the results of this paper can be extended to 3-D. Because the support-operators method does not use any facts about the structure of the grid (just the structure of the cells) this method can also be extended to unstructured grids.

The support-operators method is invariantly defined, so it can be used in any coordinate system. It is very easy to transform the formulas in this paper to any other coordinate system. In particular, one only needs to use the appropriate formulas for length, areas, and volumes and then the formulas for the discrete operators in the new coordinates are the same as in the case of Cartesian coordinates.

The support-operators method, using natural discretizations for the magnetic and electric fields that involve the normal components of the magnetic field and the tangential component of an electrical field, can be used to solve Maxwell's equations and, in particular, solve the equations for the diffusion of magnetic fields, which is the natural generalization of the results of this paper to diffusion of vector fields. In this case, the derivation of the finite-difference scheme involves the construction of two different analogs of the curl operator.

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