Shashkov's Method Retaining Cell-Edge
Unknowns

Randy M. Roberts

January 5, 1996

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1 Preliminaries

In deriving Shashkov's method (SM) scalar cell-edge and cell-center variables will be defined from a scalar quantity, ϕ , as

$$\Phi = \begin{bmatrix} \phi_l \\ \phi_t \\ \phi_r \\ \phi_b \\ \phi_c \end{bmatrix}. \quad (1)$$

Vector quantities will be defined from a vector quantity, $\vec{a}$, by the normal component of the vector for each edge of the cell,

$$\mathbf{a} = \begin{bmatrix} a_l \\ a_t \\ a_r \\ a_b \end{bmatrix}, \quad (2)$$

where $a_l = \vec{a} \cdot \hat{n}_l$, and similarly for the other components of $\mathbf{a}$.

2 Dot Product of Cell-Edge Vectors

Consider the dot product of two vectors, $\vec{a}$ and $\vec{b}$, represented as in Equation 2 by $\mathbf{a}$ and $\mathbf{b}$, respectively, evaluated at one corner of a cell. We shall choose the upper-left corner as an example, and call this corner, corner 1. At this corner the left and top components of $\mathbf{a}$ are related to $\vec{a}$ by

$$\begin{bmatrix} a_l \\ a_t \end{bmatrix} = \begin{bmatrix} n_{lx} & n_{ly} \\ n_{tx} & n_{ty} \end{bmatrix} \begin{bmatrix} a_x \\ a_y \end{bmatrix}, \quad (3)$$

or

$$\mathbf{P}_1 \mathbf{a} = \mathbf{N}_1 \vec{a}, \quad (4)$$

where $\mathbf{N}_1$ represents the cell-edge normal vector matrix for corner 1, and $\mathbf{P}_1$ is the operator that projects out the upper-left components of $\mathbf{a}$, i.e.,

$$\mathbf{P}_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}. \quad (5)$$

The next step is to evaluate $\vec{a} \cdot \vec{b}$ at corner 1,

$$\vec{a} \cdot \vec{b} \Big|_1 = \vec{a}^T \vec{b} \Big|_1 \quad (6)$$

$$= \mathbf{a}^T \mathbf{P}_1^T \mathbf{N}_1^{-T} \mathbf{N}_1^{-1} \mathbf{P}_1 \mathbf{b} \quad (7)$$

$$= \mathbf{a}^T \mathbf{S}_1 \mathbf{b}, \quad (8)$$

where

$$\mathbf{S}_1 = \mathbf{P}_1^T (\mathbf{N}_1 \mathbf{N}_1^T)^{-1} \mathbf{P}_1 \quad (9)$$

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is a 4 by 4 real matrix.

We can evaluate $\mathbf{S}_1$ from θ_1 , the angle formed at corner 1.

$$(\mathbf{N}_1 \mathbf{N}_1^T)^{-1} = \left(\begin{bmatrix} n_{lx} & n_{ly} \\ n_{tx} & n_{ty} \end{bmatrix} \begin{bmatrix} n_{lx} & n_{tx} \\ n_{ly} & n_{ty} \end{bmatrix} \right)^{-1} \quad (10)$$

$$= \begin{bmatrix} 1 & -\cos \theta_1 \\ -\cos \theta_1 & 1 \end{bmatrix}^{-1} \quad (11)$$

$$= \frac{1}{\sin^2 \theta_1} \begin{bmatrix} 1 & \cos \theta_1 \\ \cos \theta_1 & 1 \end{bmatrix}, \quad (12)$$

$$\mathbf{S}_1 = \frac{1}{\sin^2 \theta_1} \begin{bmatrix} 1 & \cos \theta_1 & 0 & 0 \\ \cos \theta_1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (13)$$

It is important to notice that $\mathbf{S}_1^T = \mathbf{S}_1$. Since the dot product of a non-zero vector with itself is always positive, $\mathbf{S}_1$ is symmetric positive definite (SPD).

Similar results may be found for the other three corners; therefore, the dot product of $\vec{a}$ and $\vec{b}$ evaluated at the i 'th corner may now be represented by $\vec{a}^T \mathbf{S}_i \vec{b}$.

3 Discretized Divergence and Gradient

In this section we will choose a discretization for the divergence and derive a discretization for the gradient, and therefore, for the diffusion operator, consistent with our choice of divergence discretization.

We shall start with a simple calculus relation for the divergence of a scalar, ϕ , multiplied by a vector, $\vec{w}$,

$$\vec{\nabla} \cdot (\phi \vec{w}) = \phi \vec{\nabla} \cdot \vec{w} + \vec{\nabla} \phi \cdot \vec{w}. \quad (14)$$

We will integrate this expression over the volume of the cell, and then, by invoking the divergence theorem, express the volume integral of the divergence as a surface integral.

$$-D^{-1} \int \vec{f} \cdot \vec{w} dV = \int \vec{\nabla} \phi \cdot \vec{w} dV \quad (15)$$

$$= \int \vec{\nabla} \cdot (\phi \vec{w}) dV - \int \phi \vec{\nabla} \cdot \vec{w} dV \quad (16)$$

$$= \oint \phi \vec{w} \cdot \hat{n} dA - \int \phi \vec{\nabla} \cdot \vec{w} dV, \quad (17)$$

where

$$\vec{f} = -D \vec{\nabla} \phi. \quad (18)$$

The first term on the right hand side of Equation 17 may be approximated by the sum of the cell-edge values of $\phi \vec{w} \cdot \hat{n}$ multiplied by the cell-edge areas.

$$\oint \phi \vec{w} \cdot \hat{n} dA \approx \phi_l w_l A_l + \phi_t w_t A_t + \phi_r w_r A_r + \phi_b w_b A_b. \quad (19)$$

The second term on the right hand side of Equation 17 may be approximated by the pulling out the cell centered value of ϕ from the integral, and then using the same approximation for the area integral as above,

$$\int \phi \vec{\nabla} \cdot \vec{w} dV \approx \phi_c \int \vec{\nabla} \cdot \vec{w} dV \quad (20)$$

$$= \phi_c \oint \vec{w} \cdot \hat{n} dA \quad (21)$$

$$\approx \phi_c (w_l A_l + w_t A_t + w_r A_r + w_b A_b). \quad (22)$$

Combining Equations 19 and 22, the right hand side of Equation 17 becomes

$$w_l A_l (\phi_l - \phi_c) + w_t A_t (\phi_t - \phi_c) + w_r A_r (\phi_r - \phi_c) + w_b A_b (\phi_b - \phi_c) = \mathbf{w}^T \mathbf{M}_0 \Phi, \quad (23)$$

where

$$\mathbf{M}_0 = \begin{bmatrix} A_l & 0 & 0 & 0 & -A_l \\ 0 & A_t & 0 & 0 & -A_t \\ 0 & 0 & A_r & 0 & -A_r \\ 0 & 0 & 0 & A_b & -A_b \end{bmatrix}. \quad (24)$$

The volume integral on the left hand side of Equation 17 is to be approximated by a weighted sum of dot products evaluated at each of the corners, with the weights summed to the total volume of the cell,

$$-D^{-1} \int \vec{f} \cdot \vec{w} dV \approx -D^{-1} \sum_{i=1}^4 V_i \vec{f} \cdot \vec{w} \Big|_i \quad (25)$$

$$= -D^{-1} \sum_{i=1}^4 V_i \mathbf{w}^T \mathbf{S}_i \mathbf{f} \quad (26)$$

$$= -D^{-1} \mathbf{w}^T \mathbf{S} \mathbf{f}, \quad (27)$$

where

$$\mathbf{S} = \sum_{i=1}^4 V_i \mathbf{S}_i. \quad (28)$$

If all of the V_i 's are positive then $\mathbf{S}$ and $\mathbf{S}^{-1}$ are guaranteed to be SPD matrices.

Setting Equation 27 equal to Equation 23, and recalling that Equation 14 holds for any vector, $\vec{w}$, we obtain the following expression for the discretization of $\vec{f} = -D \vec{\nabla} \phi$,

$$\mathbf{S} \mathbf{f} = -D \mathbf{M}_0 \Phi \quad (29)$$

$$\mathbf{f} = -D \mathbf{S}^{-1} \mathbf{M}_0 \Phi. \quad (30)$$

4 Diffusion Equation with Cell-Edge Continuity and Boundary Conditions

We will use the results of the previous section to solve the diffusion equation.

$$\int_{\text{cell}} \vec{\nabla} \cdot \vec{f} dV = Q, \quad (31)$$

for each cell. This equation can be rewritten using the divergence theorem,

$$\int_{\text{cell}} \vec{\nabla} \cdot \vec{f} dV = \oint_{\text{cell}} \vec{f} \cdot \hat{n} dA \quad (32)$$

$$= \mathbf{M}_1^T \mathbf{f} \quad (33)$$

$$= -D\mathbf{M}_1^T \mathbf{S}^{-1} \mathbf{M}_0 \Phi, \quad (34)$$

with

$$\mathbf{M}_1 = \begin{bmatrix} A_l \\ A_t \\ A_r \\ A_b \end{bmatrix}. \quad (35)$$

We have also used Equation 30 to express the equation in terms of the ϕ unknowns. The expression $\mathbf{M}_1^T \mathbf{S}^{-1} \mathbf{M}_0$ is a 1 by 5 real matrix.

The diffusion equation is subject to cell-edge continuity and boundary conditions of the following form,

$$A_l(\lambda_l \phi_l - f_l) = j_l \quad (36)$$

$$A_t(\lambda_t \phi_t - f_t) = j_t \quad (37)$$

$$A_r(\lambda_r \phi_r - f_r) = j_r \quad (38)$$

$$A_b(\lambda_b \phi_b - f_b) = j_b, \quad (39)$$

or

$$\mathbf{j} = \mathbf{M}_2(\Lambda \Phi - \mathbf{f}) \quad (40)$$

$$= \mathbf{M}_2(\Lambda + D\mathbf{S}^{-1} \mathbf{M}_0) \Phi, \quad (41)$$

with

$$\mathbf{M}_2 = \begin{bmatrix} A_l & 0 & 0 & 0 \\ 0 & A_t & 0 & 0 \\ 0 & 0 & A_r & 0 \\ 0 & 0 & 0 & A_b \end{bmatrix}, \quad (42)$$

and

$$\Lambda = \begin{bmatrix} \lambda_l & 0 & 0 & 0 & 0 \\ 0 & \lambda_t & 0 & 0 & 0 \\ 0 & 0 & \lambda_r & 0 & 0 \\ 0 & 0 & 0 & \lambda_b & 0 \end{bmatrix}. \quad (43)$$

The expression $\mathbf{M}_2(\mathbf{A} - D\mathbf{S}^{-1}\mathbf{M}_0)$ is a 4 by 5 real matrix.

The Q represents source terms that do not depend on the ϕ unknowns, the j 's represent system boundary conditions or current continuity conditions from neighboring cells, not involving the ϕ for that cell-edge, and the λ 's represent coefficients for mixed boundary conditions, e.g. Marshak boundary conditions set $\lambda = 1/2$, or the cell-edge contribution from the neighbor cell.

Each cell will have 5 equations associated with its 5 ϕ unknowns. These equations (Equations 34 and 41) can be combined into one set of simultaneous equations, expressed as a 5 by 5 matrix-vector multiplication,

$$\begin{bmatrix} j \\ Q \end{bmatrix} = \begin{bmatrix} \mathbf{M}_2(\mathbf{A} + D\mathbf{S}^{-1}\mathbf{M}_0) \\ -D\mathbf{M}_1^T\mathbf{S}^{-1}\mathbf{M}_0 \end{bmatrix} \Phi \quad (44)$$

$$= \left(\begin{bmatrix} \mathbf{M}_2\mathbf{A} \\ 0 \end{bmatrix} + D \begin{bmatrix} \mathbf{M}_2\mathbf{S}^{-1}\mathbf{M}_0 \\ -\mathbf{M}_1^T\mathbf{S}^{-1}\mathbf{M}_0 \end{bmatrix} \right) \Phi \quad (45)$$

$$= \mathbf{A}\Phi. \quad (46)$$

It is this 5 by 5 cell matrix that is assembled into a global matrix, that when solved will determine the values of the ϕ unknowns.

5 Symmetric Positive Definite Solution Matrix

We shall now show that $\mathbf{A}$ is a symmetric positive definite 5 by 5 matrix. It is evident that the first term in Equation 45 represents a diagonal matrix; therefore, we need only look at the remaining term,

$$\begin{bmatrix} \mathbf{M}_2\mathbf{S}^{-1}\mathbf{M}_0 \\ -\mathbf{M}_1^T\mathbf{S}^{-1}\mathbf{M}_0 \end{bmatrix}, \quad (47)$$

to determine whether $\mathbf{A}$ is symmetric. We can rewrite $\mathbf{M}_0$ as,

$$\mathbf{M}_0 = [\mathbf{M}_2 \quad -\mathbf{M}_1]. \quad (48)$$

We may express the remaining term using $\mathbf{M}_2$ and $\mathbf{M}_1$,

$$\begin{bmatrix} \mathbf{M}_2\mathbf{S}^{-1}\mathbf{M}_0 \\ -\mathbf{M}_1^T\mathbf{S}^{-1}\mathbf{M}_0 \end{bmatrix} = \begin{bmatrix} \mathbf{M}_2\mathbf{S}^{-1}\mathbf{M}_2 & -\mathbf{M}_2\mathbf{S}^{-1}\mathbf{M}_1 \\ -\mathbf{M}_1^T\mathbf{S}^{-1}\mathbf{M}_2 & \mathbf{M}_1^T\mathbf{S}^{-1}\mathbf{M}_1 \end{bmatrix}. \quad (49)$$

Since both $\mathbf{M}_2$ and $\mathbf{S}^{-1}$ are symmetric matrices it is evident that the above matrix is also symmetric, and therefore, that matrix $\mathbf{A}$ is symmetric.

To prove that second term in $\mathbf{A}$, $\mathbf{A}'$, is SPD, we can show that $\mathbf{A}'$ has a Cholesky decomposition,

$$\mathbf{A}' = \mathbf{L}_A \mathbf{L}_A^T, \quad (50)$$

where $\mathbf{L}_A$ is a real lower-triangular matrix with positive diagonals.

Since $\mathbf{S}^{-1}$ is SPD it can be written as

$$\mathbf{S}^{-1} = \mathbf{L}_S \mathbf{L}_S^T, \quad (51)$$

where $\mathbf{L}_S$ is a real lower-triangular matrix with positive diagonals.

During this proof we must keep in mind that $\mathbf{M}_2$ is a positive diagonal 4 by 4 matrix, and $\mathbf{M}_1$ is a positive 4 by 1 matrix. We may rewrite $\mathbf{A}'$ as

$$\mathbf{A}' = \begin{bmatrix} \mathbf{M}_2 \mathbf{L}_S \mathbf{L}_S^T \mathbf{M}_2 & -\mathbf{M}_2 \mathbf{L}_S \mathbf{L}_S^T \mathbf{M}_1 \\ -\mathbf{M}_1^T \mathbf{L}_S \mathbf{L}_S^T \mathbf{M}_2 & \mathbf{M}_1^T \mathbf{L}_S \mathbf{L}_S^T \mathbf{M}_1 \end{bmatrix}. \quad (52)$$

Consider the following matrix for $\mathbf{L}_A$ in block matrix form.

$$\mathbf{L}_A = \begin{bmatrix} \mathbf{M}_2 \mathbf{L}_S & \mathbf{0} \\ -l_{22}^{-1} \mathbf{M}_1^T \mathbf{L}_S \mathbf{L}_S^T \mathbf{M}_2 & l_{22} \end{bmatrix}, \quad (53)$$

with

$$l_{22} = (\mathbf{M}_1^T \mathbf{L}_S \mathbf{L}_S^T \mathbf{M}_1)^{\frac{1}{2}}. \quad (54)$$

It is not hard to show that $\mathbf{A}' = \mathbf{L}_A \mathbf{L}_A^T$ for this choice of $\mathbf{L}_A$. We now need to show that $\mathbf{L}_A$ is indeed a real lower-triangular matrix with positive diagonals. Since $\mathbf{M}_2$ is real positive diagonal, $\mathbf{M}_2 \mathbf{L}_S$ is real lower-triangular with positive diagonals; therefore, we need only prove that l_{22} is real and positive. The only way for l_{22} not to be real and positive is if $\mathbf{M}_1^T \mathbf{L}_S \mathbf{L}_S^T \mathbf{M}_1$ is less than or equal to 0. By defining the column vector, $\mathbf{x}$, as

$$\mathbf{x} = \mathbf{L}_S^T \mathbf{M}_1, \quad (55)$$

we can write

$$l_{22} = (\mathbf{x}^T \mathbf{x})^{\frac{1}{2}}, \quad (56)$$

which is a real quantity. To prove that l_{22} is non-zero it is only necessary, from Equation 55, to show that the determinant of $\mathbf{L}_S$ is non-zero. Since $\mathbf{L}_S$ has positive diagonal elements its determinant must be positive; therefore, $\mathbf{x}$ cannot be the zero column vector and l_{22} is real and positive.

We have now shown that $\mathbf{A}'$ is the product of a real lower-triangular matrix with positive diagonals and its transpose; therefore, $\mathbf{A}'$ is an SPD matrix. We must now turn to the the $\mathbf{A}$ contribution to $\mathbf{A}$.

If all of the λ 's turn out to be positive it seems that $\mathbf{A}$ is an SPD matrix. For Marshak boundary conditions, $\lambda = 1/2$, it is the case that λ is positive. For current continuity conditions, λ_l is derived from the ϕ_r term of the neighbor cell to the left. The value for λ_l becomes,

$$\lambda_l = D^{(l)} (\mathbf{S}^{(l)-1} \mathbf{M}_0^{(l)})_{rr} \quad (57)$$

$$= D^{(l)} (\mathbf{S}^{(l)-1} \mathbf{M}_2^{(l)})_{rr}, \quad (58)$$

where (l) refers to the neighbor cell to the left. The diagonal of $\mathbf{S}^{-1} \mathbf{M}_2$ should be a positive value, since $\mathbf{S}^{-1}$ is SPD, and $\mathbf{M}_2$ is a positive diagonal matrix, and, therefore, the product $\mathbf{S}^{-1} \mathbf{M}_2$ is SPD. We would then conclude that $\mathbf{A}$ is an SPD matrix.