A Local Support-Operators Diffusion Discretization Scheme for Hexahedral Meshes

by

Jim Morel and Michael Hall
Transport Methods Group, X-6
and
Mikhail J. Shashkov
Mathematical Modeling and Analysis Group, T-7

Los Alamos National Laboratory
Los Alamos NM, 87545

Overview

- Introduction
- Properties of the Scheme
- The Support Operator Method
- Derivation of the Discretization
- Solution of the Equations
- Computational Results
- Future Work

Introduction

- The purpose of this paper is to present a local support-operators diffusion discretization for arbitrary 3-D hexahedral meshes.

- We use the standard finite-element definition for hexahedra [1].

- The method that we present is a generalization of a similar scheme for 2-D $r-z$ quadrilateral meshes that was developed by Morel, Roberts, and Shashkov [2].

- We assume a logically-rectangular mesh in our derivation for convenience, but the scheme can also be applied to unstructured meshes.

Introduction (Cont.)

- The diffusion equation that we seek to solve can be expressed in the following general form:

$$\frac{\partial \phi}{\partial t} - \overrightarrow{\nabla} \cdot D \overrightarrow{\nabla} \phi = Q \quad , \tag{1}$$

where t denotes the time variable, ϕ denotes a scalar function that we refer to as the intensity, D denotes the diffusion coefficient, and Q denotes the source or driving function. It is sometimes useful to express Eq. (1) in terms of a vector function, $\overrightarrow{F}$, that we refer to as the flux:

$$\overrightarrow{F} = -D \overrightarrow{\nabla} \phi \quad .$$

Properties of the Scheme

1. It is a cell-centered discretization for arbitrary hexahedral meshes but has both cell-center and face-center intensities.

2. It gives second-order convergence of the intensity on both smooth and non-smooth meshes both with and without material discontinuities.

3. It generates a sparse SPD coefficient matrix.

4. It is equivalent to the standard 7-point cell-center diffusion discretization scheme when the mesh is orthogonal.

The Support-Operators Method

We next describe the support-operators method. It is convenient at this point to define a flux operator given by $-D\overrightarrow{\nabla}$. The diffusion operator of interest is given by the product of the divergence operator and the flux operator: $-\overrightarrow{\nabla}\cdot D\overrightarrow{\nabla}$. The support-operator method is based upon the following three facts:

- Given appropriately defined scalar and vector inner products, the divergence and flux operators are adjoint to one another.

- The adjoint of an operator varies with the definition of its associated inner products, but is unique for fixed inner products.

- The product of an operator and its adjoint is a self-adjoint positive-definite operator.

The Support-Operators Method (Cont.)

The adjoint relationship between the flux and divergence operators is embodied in the following integral identity:

$$\oint_{\partial V} \phi \overrightarrow{H} \cdot \overrightarrow{n} \, dA - \int_V D^{-1} \overrightarrow{H} \cdot D \overrightarrow{\nabla} \phi \, dV =$$

$$\int_V \phi \overrightarrow{\nabla} \cdot \overrightarrow{H} \, dV \quad ,$$

where ϕ is an arbitrary scalar function, $\overrightarrow{H}$ is an arbitrary vector function, V denotes a volume, ∂V denotes its surface, and $\overrightarrow{n}$ denotes the outward-directed unit normal associated with that surface.

The Support-Operators Method (Cont.)

Our support-operator method can be described in the simplest terms as follows:

1. Define discrete scalar and vector spaces to be used in a discretization of the integral identity.

2. Fully discretize all but the flux operator in the identity over a single arbitrary cell. The flux operator is left in the general form of a discrete vector as defined in Step 1.

3. Solve for the discrete flux operator (i.e., for its vector components) on a single arbitrary cell by requiring that the discrete version of the identity hold for all elements of the discrete scalar and vector spaces defined in Step 1.

The Support-Operators Method (Cont.)

4. Obtain the interior-mesh discretization of the identity by connecting adjacent mesh cells in such a way as to ensure that the identity is satisfied over the whole grid. This simply amounts to enforcing continuity of intensity and normal-component flux at the cell interfaces.

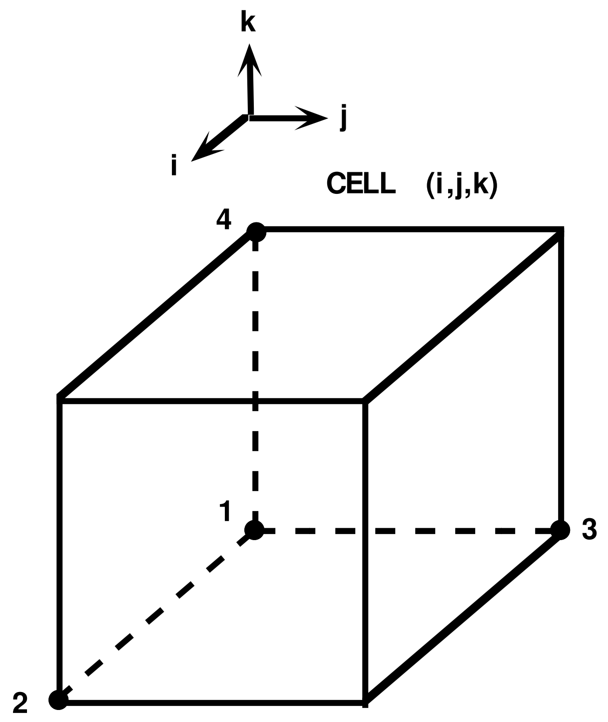
5. Change the flux operator at those cell faces on the exterior mesh boundary so as to satisfy the appropriate boundary conditions.

6. Combine the global divergence matrix and the global flux matrix to obtain the global diffusion matrix.

Derivation of the Discretization

- We begin by defining our mesh indexing.
- We use both global and local indexing.
- Local indices enable us to uniquely define certain quantities that are associated with a vertex or face center *and* a cell.
- The following figures illustrate the indexing.

Figure 1: Global indexes for four vertices associated with cell (i, j, k).



1 - (i-1/2 , j-1/ 2, k-1/2)

2 - (i+1/2 , j-1/2, k-1/2)

3 - (i-1/2 , j+1/2, k-1/2)

4 - (i-1/2 , j-1/ 2, k+1/2)

Figure 2: Local and global indices for three of six face centers associated with cell (i, j, k).

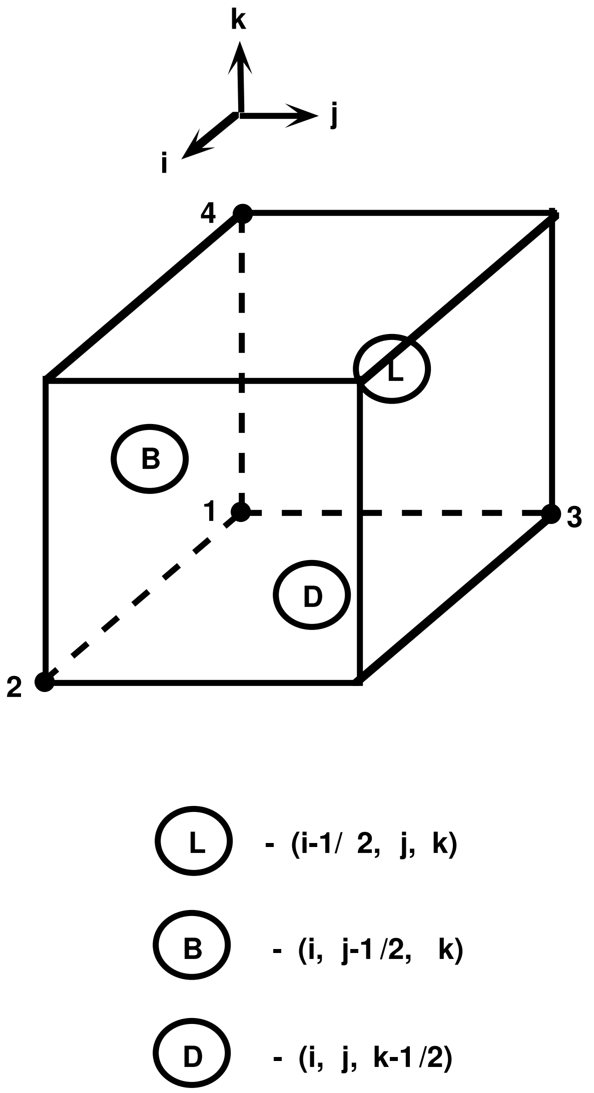


Figure 3: Local and global indices for three of six face centers associated with cell (i, j, k).

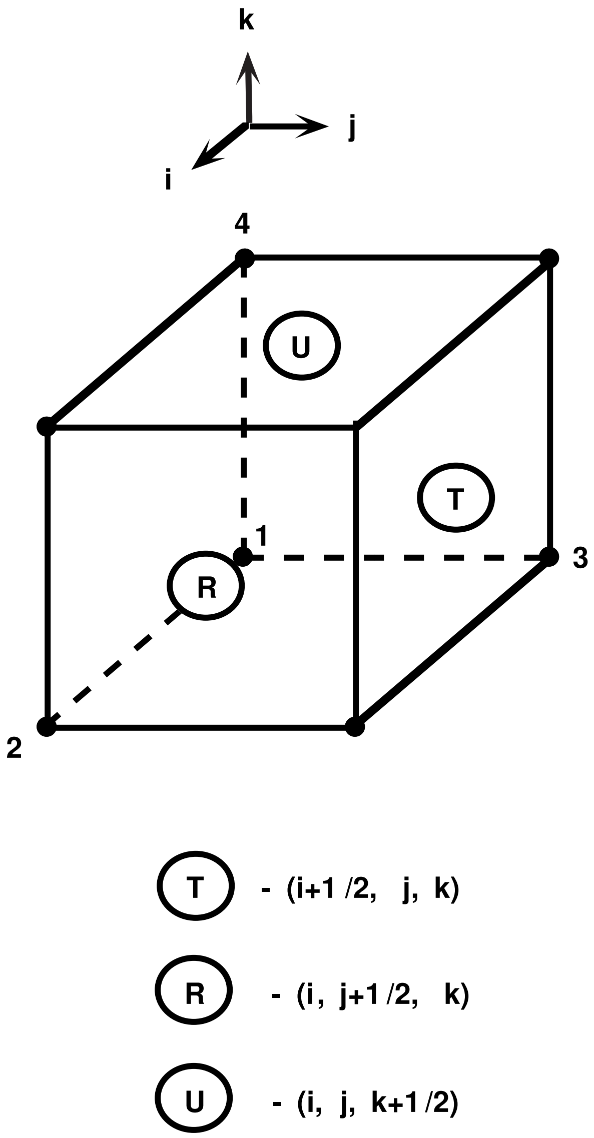
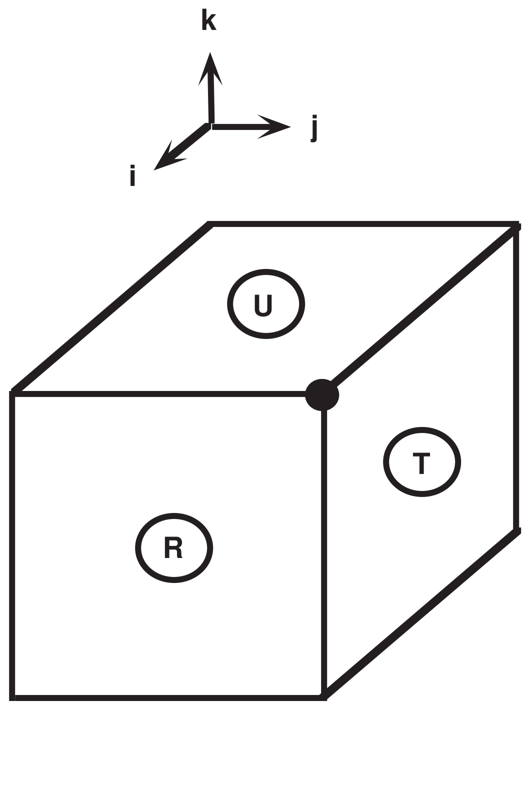


Figure 4: Vertex shared by the Right, Top, and Up faces having local index RTU.



Derivation of the Discretization (Cont.)

- The intensities (scalars) are defined to exist at both cell center: $\phi^C_{i,j,k}$, and on the face centers: $\phi^L_{i,j,k}$, $\phi^R_{i,j,k}$, $\phi^B_{i,j,k}$, $\phi^T_{i,j,k}$, $\phi^D_{i,j,k}$, $\phi^U_{i,j,k}$.

- As previously noted, the use of local indices implies that a quantity is uniquely associated with a single cell. For instance, unless it is otherwise stated, one should assume that $\phi^R_{i,j,k} \neq \phi^L_{i+1,j,k}$.

- Vectors are defined in terms of face-area components located at the face centers: $f^L_{i,j,k}$, $f^R_{i,j,k}$, $f^B_{i,j,k}$, $f^T_{i,j,k}$,$f^D_{i,j,k}$, $f^U_{i,j,k}$, where $f^L_{i,j,k}$ denotes the dot product of $\overrightarrow{F}$ with the outward-directed area vector located at the center of the left face of cell i, j, k. The other face-area components are defined analogously.

Derivation of the Discretization (Cont.)

- The area vector is defined as the integral of the outward-directed unit normal vector over the face, i.e.,

$$\overrightarrow{A} = \oint \overrightarrow{n}\, dA \quad ,$$

where $\overrightarrow{n}$ is a unit vector that is normal to the face at each point on the face.

- The average outward-directed unit normal vector for the face is defined as follows:

$$\left\langle \overrightarrow{n} \right\rangle = \frac{\overrightarrow{A}}{\| \overrightarrow{A} \|} \quad ,$$

where $\| \overrightarrow{A} \|$ denotes the magnitude (standard Euclidian norm) of $\overrightarrow{A}$.

Derivation of the Discretization (Cont.)

- This definition can be used to convert face-area flux components to face-normal components if desired, e.g.

$$
\begin{aligned}
\overrightarrow{F} \cdot \left\langle \overrightarrow{n} \right\rangle &= \overrightarrow{F} \cdot \frac{\overrightarrow{A}}{\| \overrightarrow{A} \|} \quad , \\
&= \frac{f}{\| \overrightarrow{A} \|} \quad .
\end{aligned}
$$

- Note that $\| \overrightarrow{A} \|$ is equal to the face area only when the face is flat.

- Interestingly, the true face areas never arise in our discretization scheme.

Derivation of the Discretization (Cont.)

- Since it takes three components to define a full vector, the full vectors are considered to be located at the cell vertices: $\overrightarrow{F}^{LBD}_{i,j,k}$, $\overrightarrow{F}^{RBD}_{i,j,k}$, $\overrightarrow{F}^{LTD}_{i,j,k}$, $\overrightarrow{F}^{RTD}_{i,j,k}$, $\overrightarrow{F}^{LBU}_{i,j,k}$, $\overrightarrow{F}^{RBU}_{i,j,k}$, $\overrightarrow{F}^{LTU}_{i,j,k}$, $\overrightarrow{F}^{RTU}_{i,j,k}$.

- Each vertex vector is constructed using the face-area components and area vectors associated with the three faces that share that vertex. For instance,

$$\overrightarrow{F}^{LBD}_{i,j,k} = \frac{f^L\left(\overrightarrow{A}^B \times \overrightarrow{A}^D\right)}{\overrightarrow{A}^L \cdot \left(\overrightarrow{A}^B \times \overrightarrow{A}^D\right)} +$$

$$\frac{f^B\left(\overrightarrow{A}^D \times \overrightarrow{A}^L\right)}{\overrightarrow{A}^L \cdot \left(\overrightarrow{A}^D \times \overrightarrow{A}^L\right)} + \frac{f^D\left(\overrightarrow{A}^L \times \overrightarrow{A}^B\right)}{\overrightarrow{A}^D \cdot \left(\overrightarrow{A}^L \times \overrightarrow{A}^B\right)} .$$

Derivation of the Discretization (Cont.)

- It is convenient for our purposes to define an algebraic flux vector, $\hat{F}$, consisting of the three face-area components associated with the physical vector, $\overrightarrow{F}$, e.g.,

$$\hat{F}_{LBD} = \left(f^{L}_{i,j,k},\ f^{B}_{i,j,k},\ f^{D}_{i,j,k} \right)^{t} \quad ,$$

where a superscript "t" denotes "transpose." The three face-area components associated with the Right-Top-Up vertex are illustrated in Fig.4. The algebraic flux vectors for the other vertices are defined analogously.

Derivation of the Discretization (Cont.)

- Our next step is to discretize the integral identity over a single cell.

- We first discretize the surface integral:

$$\oint_{\partial V} \phi \overrightarrow{H} \cdot \overrightarrow{n} \, dA \approx \sum_{f} \phi^{f} h^{f} \quad ,$$

where f is the face index and the sum is taken over all faces.

- Next we approximate the flux volumetric integral:

$$\int_{V} -D^{-1} \overrightarrow{H} \cdot D \overrightarrow{\nabla} \phi \, dV \approx$$

$$\sum_{v} D^{-1} \left(\overrightarrow{H}^{v} \cdot \overrightarrow{F}^{v} \right) V^{v} ,$$

where v is the vertex index, and V^{v} denotes the volumetric weight associated with vertex v.

Derivation of the Discretization (Cont.)

- The vertex volumetric weight is a free parameter in the support-operators method. We have tried several different weight definitions.

- The best choice appears to be one-eighth the triple product of the three edge vectors that share the vertex. For instance, the volumetric weight for the Left-Bottom-Down vertex can be expressed as follows using the point numbering shown in Fig.2:

$$V^{LBD} = \frac{1}{8} \overrightarrow{R}_{1,2} \times \overrightarrow{R}_{1,3} \cdot \overrightarrow{R}_{1,4} \quad ,$$

  where $\overrightarrow{R}_{i,j}$ denotes the vector from vertex i to vertex j.

- Since these weights do not necessarily sum to the total hexahedral volume, we normalize them to do so.

Derivation of the Discretization (Cont.)

- Although the expression given previously for the physical flux vector can be used to evaluate the dot products in the flux volumetric integral, we find it preferable to evaluate them in terms of the algebraic face-area flux vectors.

- This is achieved by transforming the face-area vectors to Cartesian vectors and then taking the dot product.

- There is a separate transformation matrix for each vertex. Let us denote this matrix for the Left-Bottom-Down vertex by $\mathbf{A}^{LBD}$. Although we cannot explicitly define this matrix, we can explicitly define its inverse.

Derivation of the Discretization (Cont.)

- This inverse matrix transforms Cartesian vectors to face-area vectors:

$$\left[\mathbf{A}^{LBD}\right]^{-1} \overrightarrow{H}^{LBD} = \hat{H}^{LBD} \quad ,$$

where $\overrightarrow{H}$ denotes a Left-Bottom-Down Cartesian flux vector,

$$\overrightarrow{H} = (h^x, h^y, h^z)^t \quad ,$$

$\hat{H}$ denotes a Left-Bottom-Down face-area flux vector,

$$\hat{H} = \left(h^L, h^B, h^D\right)^t \quad ,$$

and

$$\left[\mathbf{A}^{LBD}\right]^{-1} = \begin{bmatrix} a_x^L & a_y^L & a_z^L \\ a_x^B & a_y^B & a_z^B \\ a_x^D & a_y^D & a_z^D \end{bmatrix} \quad ,$$

where a_x^L denotes the x-component of the area vector associated with the left face. The remaining components of the matrix are defined analogously.

Derivation of the Discretization (Cont.)

- To obtain $\mathbf{A}$, we numerically invert $\mathbf{A}^{-1}$.

- We can now rewrite the approximation to the flux volumetric integral in terms of the face-area flux vectors as follows:

$$\int_V -D^{-1}\overrightarrow{H} \cdot \overrightarrow{F} \, dV \approx$$

$$\sum_v D^{-1}\left(\hat{H}^v \cdot \mathbf{S}^v \hat{F}^v\right) V^v ,$$

where

$$\mathbf{S} = \mathbf{A}^t \mathbf{A} \quad ,$$

and the dot product is taken in the usual way.

- Finally, we approximate the divergence volumetric integral:

$$\int_V \phi \, \overrightarrow{\nabla} \cdot \overrightarrow{H} \, dV \approx \phi^C \sum_f h^f \quad ,$$

where the sum is taken over all faces.

Derivation of the Discretization (Cont.)

- Putting all of the pieces together, we obtain obtain the discretized integral identity:

$$\sum_f \phi^f h^f + \sum_v D^{-1} \left(\hat{H}^v \cdot \mathbf{S}^v \hat{F}^v \right) V^v = \phi^C \sum_f h^f \ .$$

- This identity must hold for all $\hat{H}$. This requirement uniquely determines the six face-area components of the flux operator in terms of the cell-center and face-center intensities. In particular the equation for a given flux component is obtained by setting that component to unity while setting the remaining five components to zero. A matrix equation of the following form is obtained:

$$\mathbf{W}^{-1} \hat{\mathcal{F}} = \Delta \hat{\Phi} \quad ,$$

where

$$\hat{\mathcal{F}} = \left(f^L, f^R, f^B, f^T, f^D, f^U \right)^t \quad ,$$

and

$$\Delta \hat{\Phi} = \left(\phi^C - \phi^L, \phi^C - \phi^R, \ldots, \phi^C - \phi^U \right)^t \ .$$

Derivation of the Discretization (Cont.)

- Numerically inverting the 6×6 matrix, $\mathbf{W}^{-1}$, we obtain the desired expressions for the six face-area flux components associated with the cell:

$$\hat{\mathcal{F}} = \mathbf{W} \Delta \hat{\Phi} \ .$$

- Having enforced the discrete identity over each single cell, we next enforce it over the entire mesh simply by requiring continuity of the intensity and the flow at each cell face on the mesh interior. For instance, at the interior face $(i + \frac{1}{2}, j, k)$, requiring continuity of the intensity yields:

$$\phi^R_{i,j,k} = \phi^L_{i+1,j,k} = \phi_{i+\frac{1}{2},j,k} \ ,$$

while requiring continuity of the flow yields:

$$-f^R_{i,j,k} - f^L_{i+1,j,k} = 0 \ ,$$

Derivation of the Discretization (Cont.)

- Eliminating the fluxes via the **W**-matrices and eliminating half of the face-center intensities via the continuity requirement, we are left with one intensity unknown at each cell center, and one intensity unknown with a unique global index at each face center.

- The equation for the intensity at the center of cell (i, j, k) is the balance equation for cell (i, j, k):

  $$\frac{\partial \phi^C}{\partial t} V + f^L + f^R + f^B + f^T + f^D + f^U = Q^C V \quad ,$$

  where V denotes the total cell volume, Q_C denotes the cell-center inhomogeneous source, and the cell index (i, j, k) has been supressed for simplicity.

- The equation for each face-center intensity on the mesh interior is a continuity-of-flow equation. For instance, the equation for $\phi_{i+\frac{1}{2},j,k}$ is:

  $$-f^R_{i,j,k} - f^L_{i+1,j,k} = 0 \ .$$

Derivation of the Discretization (Cont.)

- The equation for each face-center intensities on the outer mesh boundary is also a continuity-of-flux equation, but an extrapolated boundary condition is used to define the face-area flux component in the "ghost cell" adjacent to each boundary cell. For instance, the equation for $\phi_{\frac{1}{2},j,k}$ takes the following form with a Marshak-type extrapolated boundary condition:

$$-f^R_{0,j,k} - f^L_{1,j,k} = 0 \ ,$$

where

$$-f^R_{0,j,k} = \frac{1}{2} \| \overrightarrow{A} \|^L_{1,j,k} \left(\phi_{\frac{1}{2},j,k} - \phi^e_{\frac{1}{2},j,k} \right) \ ,$$

where $\overrightarrow{A}^L_{1,j,k}$ is the Left area vector associated with cell $(1, j, k)$, and $\phi^e_{\frac{1}{2},j,k}$ is the extrapolated intensity associated with the boundary face.

- This completes the derivation of our discretization scheme.

Solution of the Equations

- We use preconditioned conjugate-gradient method to solve our equations on an unstructured hexahedral mesh.

- The operator used for preconditioning is a 7-point pure cell-centered discretization that results from our full scheme when the off-diagonal components of the matrices are set to zero. This is completely analogous to the preconditioner used in [2].

- The conjugate-gradient method is also be used to solve the preconditioning equations.

Computational Results

- We have performed a set of calculations intended to demonstrate that our support-operators method converges with second-order accuracy for a problem with a material discontinuity and a non-smooth mesh.

- There are two types of meshes used in all of the calculations: orthogonal and random.

- Every mesh geometrically models a unit cube, and the outer surface of each mesh conforms exactly to the outer surface of that cube.

- Each orthogonal mesh is composed of uniform cubic cells having a characteristic length, l_c.

Computational Results (Cont.)

- The random meshes represent randomly distorted orthogonal grids. In particular, each vertex on the mesh interior is randomly relocated within a sphere of radius r_0, where $r_0 = 0.25 l_c$. These random meshes are both non-smooth and skewed, but these properties are approximately constant independent of the mesh size.

- The problem associated with the first set of calculations can be described as follows:

$$-D(z)\frac{\partial \phi}{\partial z} = Qz^2 \quad ,$$

for $z \in [0, 1]$, where

$$\begin{aligned} D(z) &= D_1 \quad , \text{for } z \in [0, 0.5], \\ &= D_2 \quad , \text{for } z \in [0.5, 1], \end{aligned}$$

with an extrapolated zero intensity at $z = 1 + 2D$ and $z = -2D$, and where $D_1 = \frac{1}{30}$, $D_2 = \frac{1}{30}$, and $Q = 1$.

Computational Results (Cont.)

- The exact solution to this two-material problem is:

$$\begin{aligned}\phi &= a + bz + c_1 z^4 \quad \text{, for } z \in [0, 0.5], \\ &= a + c_2 z^4 \quad \text{, for } z \in [0.5, 1.0],\end{aligned}$$

where

$$a = \frac{Q(1 + 8D_2)}{12D_2} \quad , b = \frac{Q\,(D_2 - D_1)}{192 D_1 D_2} \quad ,$$

$$c_1 = -\frac{Q}{12D_1} \quad , c_2 = -\frac{Q}{12D_2} \quad .$$

- This problem is solved in 3-D on a unit cube having the extrapolated condition on one side of the cube together with reflecting conditions on the remaining five sides.

- We have performed several calculations for the two-material problem with meshes of various sizes.

- Each calculation uses a mesh with an average cell width that is half that of the preceeding calculation.

Computational Results (Cont.)

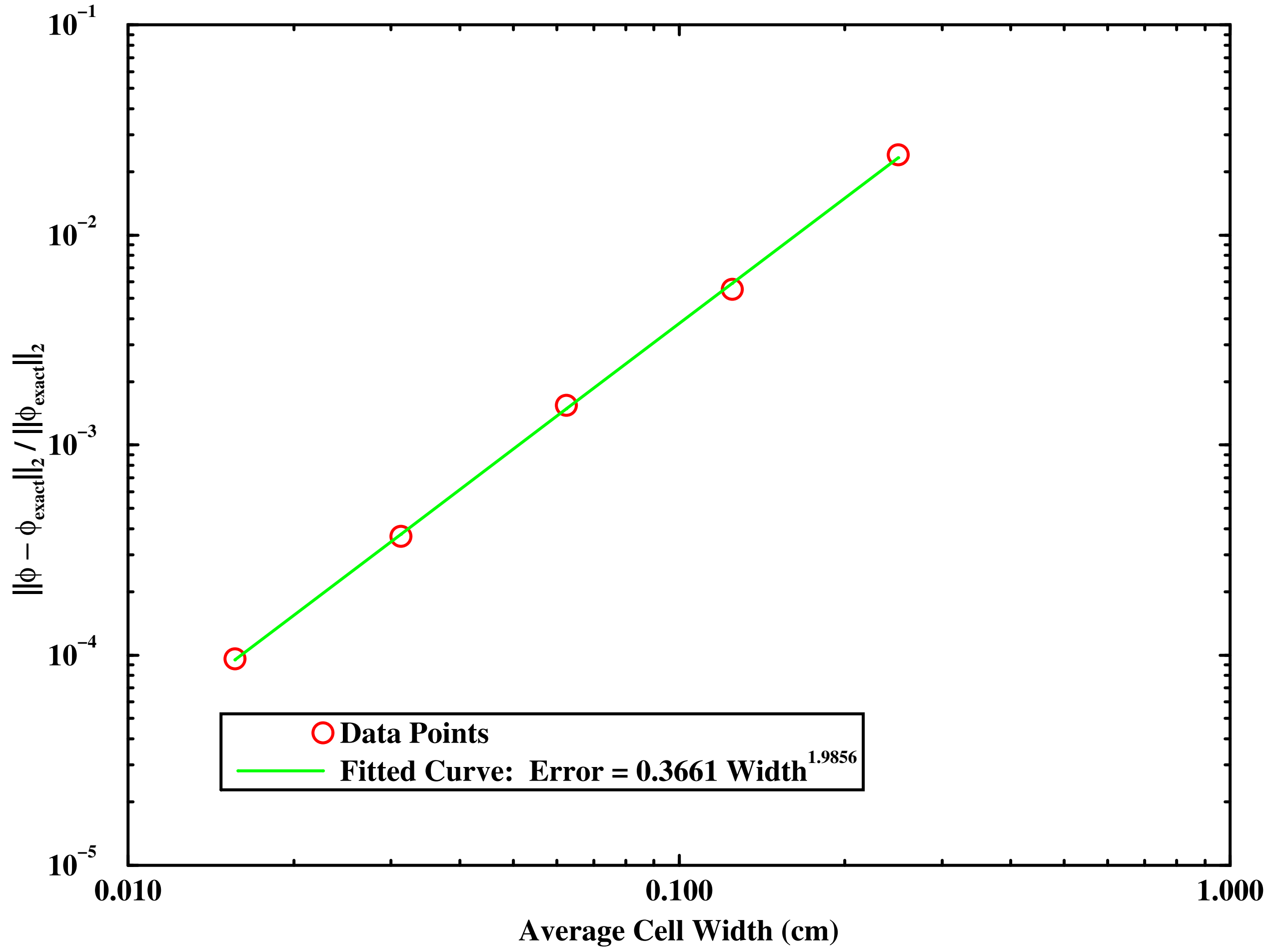
- The relative L_2 intensity error was computed for each calculation and is plotted as a function of average cell length in Fig.5 together with a linear fit to the logarithm of the error as a function of the logarithm of the average cell length.

- The slope of this linear function is 1.98.

- Perfect second-order convergence corresponds to a slope of 2.0.

- Thus we conclude that our support operators diffusion scheme converges with second-order accuracy for the two-material problem on random meshes.

Figure 5: Logarithmic Plot of Error Versus Cell Width



Future Work

- We intend to investigate algebraic multigrid methods for solving our preconditioning equations on unstructured grids.

- We intend to look at a more sophisticated 9-point pure cell-centered preconditioner.

- We intend to investigate the performance of our scheme on highly non-linear problems.

References

1. O. C. Zienkiewicz, *The Finite Element Method*, McGraw-Hill, London, 3rd Edition (1977).

2. J. E. Morel, Randy M. Roberts, and Mihkail J. Shashkov, "A Local Support-Operators Diffusion Discretization Scheme for Quadrilateral $r-z$ Meshes," *J. Comput. Phys.*, **144**, 17 (1998).

3. J. E. Morel, Michael L. Hall, and Mihkail J. Shashkov, "A Local Support-Operators Diffusion Discretization Scheme for Hexahedral Meshes," submitted to *J. Comput. Phys.*, (1999). Available on X-6 website: http://www-xdiv.lanl.gov/XTM/