Investigation of Mixed Cell Treatment via the Support Operator Method

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Introduction

- CRASH simulates radiation transport with the diffusion equation
- Multiple moving fluids create mixed cells
- Mixed cells are a source of inaccuracy in the simulations
- The support operator method (SOM) provides a conservative means to discretizes the diffusion equation
- The SOM allows for Cartesian or Non-Cartesian meshes and anisotropic or non-diagonal diffusion tensors
- Using a single code for each mixed-cell treatment allows for direct comparisons of accuracy and computational cost

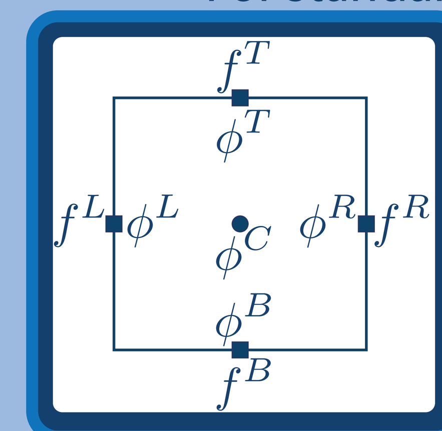
Why the SOM?

Pros

- The coefficient matrix is sparse and SPD, which can be solved efficiently
- Versatility of SOM maintains 2nd order spatial convergence in many cases:
  - Anisotropic or discontinuous diffusion tensors
  - Non-smooth or unstructured meshes
  - Cells with different angles or number of sides

Cons

- Increases number of unknowns by having both cell- and face-centered
- Difficult to implement
- For standard problems (isotropic diffusion, rectangular cells), the method is overly complicated



Mixed Cell Treatment Options

- Mean
  - $D_h = \dfrac{2D_1D_2}{D_1+D_2}$
  - $D_a = \dfrac{D_1+D_2}{2}$
  - $D_g = \sqrt{D_1D_2}$
- Choose one
  - $D_b = \max\{D_1, D_2\}$
  - $D_s = \min\{D_1, D_2\}$
- Rotate Interface
  - Simulate interface with tensor properties

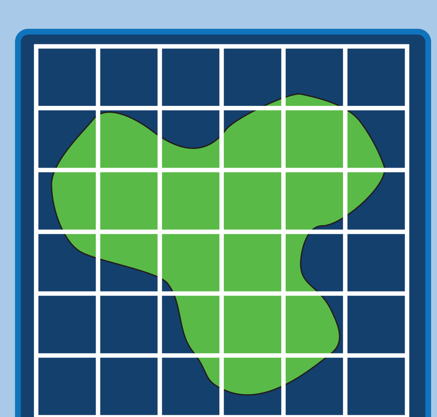
- The angle of the interface shown here is 0°
  - Flow in the x-direction needs an arithmetic mean
  - Flow in the y-direction needs a harmonic mean
    - $\overleftrightarrow{D}_r(\theta=0^\circ) = \begin{bmatrix} D_a & 0 \\ 0 & D_h \end{bmatrix}$
- A transformation with the rotation matrix allows this interface to be rotated

$$\overleftrightarrow{D}_r = \overleftrightarrow{R}\,\overleftrightarrow{D}\,\overleftrightarrow{R}^T \qquad \overleftrightarrow{R} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

$$\overleftrightarrow{D}_r = \begin{bmatrix} D_a\cos^2\theta + D_h\sin^2\theta & (D_a-D_h)\sin 2\theta \\ (D_a-D_h)\sin 2\theta & D_a\sin^2\theta + D_h\cos^2\theta \end{bmatrix}$$

Definition of a Mixed Cell

- A mixed cell is grid element containing more than one material
- A pure cell has only one material
- Mixed cells are common in Eulerian hydrodynamic codes
- Grid refinement alleviates effects of mixed-cells
- Grid refinement increases computational costs



- Figure shows a mesh with many mixed cells
- The cell boundaries are shown in white
- There are two fluids:
  - Green on the interior
  - Blue surrounding the green
- More than half of the cells are mixed

Verification of Code

Error

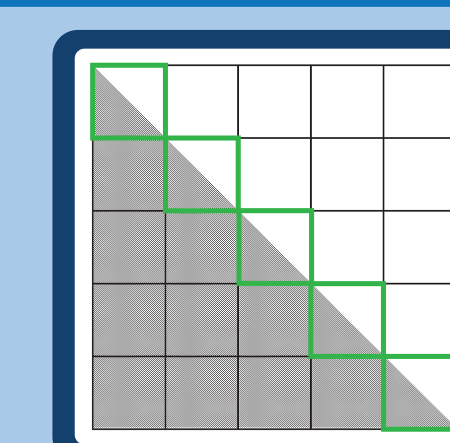
- The spatial error for a grid spacing of Δx_i has the following form
  - $E(\Delta x_i) \approx C(\Delta x_i)^m$
- One can solve for m, the convergence rate, by comparing error from different grids
  - $m \approx \dfrac{\log(E(\Delta x_1)/E(\Delta x_2))}{\log(\Delta x_1/\Delta x_2)}$
- While error can be measured in many ways, the L_2 error is used here
  - $E_{L_2}(\Delta x) = \sqrt{\sum_{i,j} (\phi_{i,j}^{calculated} - \phi_{i,j}^{exact})\Delta x\ \Delta y}$

Manufacturing a Solution

- Let ϕ^{exact} be a known solution
- Operate the diffusion equation on ϕ^{exact}
- Add this result as a source to drive the problem
- The problem is run to steady state
- Dirichlet boundary conditions are used
- The domain is $x, y \in [0, 1]$

Creating a Mixed Cell Test Problem

- Set up diffusion coefficients as pictured to the right, with the mixed cells highlighted in green
- Divides the domain into two materials
- Generates 1 mixed cell per row/column
- Each mixed cell has a -45° interface angle and equal volume fraction
- Initialize problem with concentration profile and evolution
  - $\phi(x,y) = \cos\left(\dfrac{\pi}{2}x\right)$
- Results are forthcoming



Cons of this approach

- Only a small fraction ($\frac{1}{N_x}$) of total cells are mixed
- No known solution
- Only one interface angle
- Volume fractions are equal
- Only two fluids

Details of the SOM

- The SOM discretization of the diffusion equation preserves the Gauss-Green identity:

$$\int_V \vec{H}\cdot\overleftrightarrow{D}^{-1}\vec{F}\,dV = \int_V \phi\vec{\nabla}\cdot\vec{H}\,dV - \oint_{\partial V}(\phi\vec{H})\cdot\hat{n}\,dA$$

- This embeds the relation between flux and intensity from the diffusion equation:

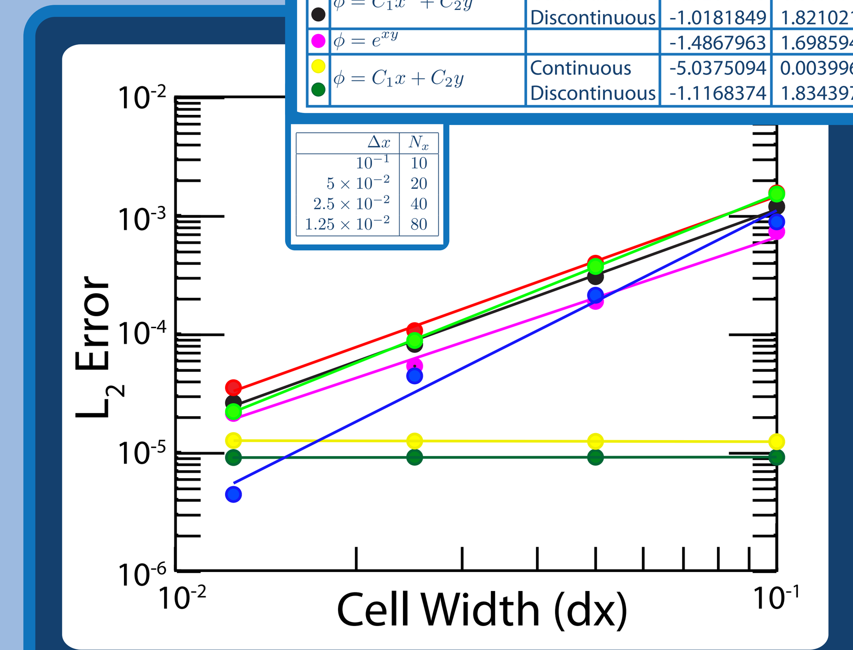
$$\frac{\partial\phi}{\partial t} + \vec{\nabla}\cdot\vec{F} = Q \qquad \vec{F} = -\overleftrightarrow{D}\vec{\nabla}\phi$$

- Similar to a finite element method, the coefficient matrix assembled is always Symmetric and Positive-Definite (SPD)

Convergence Results

- Plots for several test problems are shown
- The sin-log problem shows results for both isotropic and anisotropic diffusion tensors
- Discontinuous diffusion tensor problems are shown for both linear and quadratic solutions
- A best fit logarithmic line is calculated for each
  - Equation plotted
    $y = 10^b x^m$
  - Log of Equation
    $\log y = m\log x + b$

	Solution	Variant	b	m
blue	$\phi = \sin(\pi x)\log(y+1)$	Isotropic	-0.4101558	2.5493467
green		Anisotropic	-0.7898177	2.0337021
red	$\phi = C_1x^2 + C_2y^2$	Continuous	-4.9201138	-0.0091954
black		Discontinuous	-1.0181849	1.8210217
magenta	$\phi = e^{xy}$		-1.4867963	1.6985940
yellow	$\phi = C_1x + C_2y$	Continuous	-5.0375094	0.0039960
dark green		Discontinuous	-1.1168374	1.8343976



Δx	N_x
10^{-1}	10
5×10^{-2}	20
2.5×10^{-2}	40
1.25×10^{-2}	80

Summary & Future Work

- Use SOM to determine best mixed cell method for this test
- Implement triangular cells to cut mixed cells, generating the exact solution for test problem
- Create a more robust test problem for the mixed cells
- Implement a Multigrid pre-conditioner
- Consider partitioning the update to the cell-center for a mixed cell by a weighted volume fraction of the diffusivities
- Explore higher order time derivatives to reduce time discretization errors