Spartan/Augustus Overview: Simplified Spherical Harmonics and Diffusion for Unstructured Hexahedral Lagrangian Meshes

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4 / 22 / 98

Available on-line at
http://www.lanl.gov/Spartan/

Outline

- Code Package Description
- Method Overview, Mesh Description
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  - Equation Set
  - Properties
  - Solution Strategy
- Diffusion Results
- Future Work

Spartan/Augustus Code Package Description

Spartan:	SP_N, 2 T + Multi-Group, Even-Parity Photon Transport Package with v/c corrections
Augustus:	P_1 (Diffusion) Package
JTpack:	Krylov Subspace Iterative Solver Package (by John Turner, ex-LANL)
UMFPACK:	Unstructured Multifrontal Solver Package (an Incomplete Direct Method by Tim Davis, U of FL)
LINPACK:	Direct Dense Linear Equation Solver Package
BLAS:	Basic Linear Algebra Subprograms

Spartan/Augustus Code Size

Included files counted only once:

Spartan:	10213 lines, 57% comments
Augustus:	12872 lines, 60% comments
JTpack:	14167 lines, 54% comments
UMFPACK:	15393 lines, 58% comments
BLAS:	7467 lines, 48% comments
LINPACK:	6926 lines, 52% comments
Total	67038 lines, 56% comments

With includes:

Spartan:	14080 lines, 71% comments
Augustus:	31595 lines, 78% comments
JTpack:	36009 lines, 73% comments
UMFPACK:	15393 lines, 58% comments
BLAS:	7467 lines, 48% comments
LINPACK:	6926 lines, 52% comments
Total	111470 lines, 73% comments

Method Overview: Spartan

- Energy/Temperature Discretization
  - Solves 2 T + Multi-Group Even-Parity Equations
  - Can yoke T_e and T_i together to make 1 T
  - Can use a single-group radiation treatment to make 3 T
- Angular Discretization
  - Uses Simplified Spherical Harmonics — SP_N
  - Can do a P_1 (diffusion-like) solution
- Spatial Discretization
  - SP_N decouples equations into many diffusion equations
  - Diffusion equations are solved by Augustus
- Temporal Discretization
  - Linearized implicit discretization
  - Equivalent to one pass of a Newton solve
  - Iteration strategy:
    - Source iteration
    - DSA acceleration
    - LMFG acceleration

Method Overview: Augustus

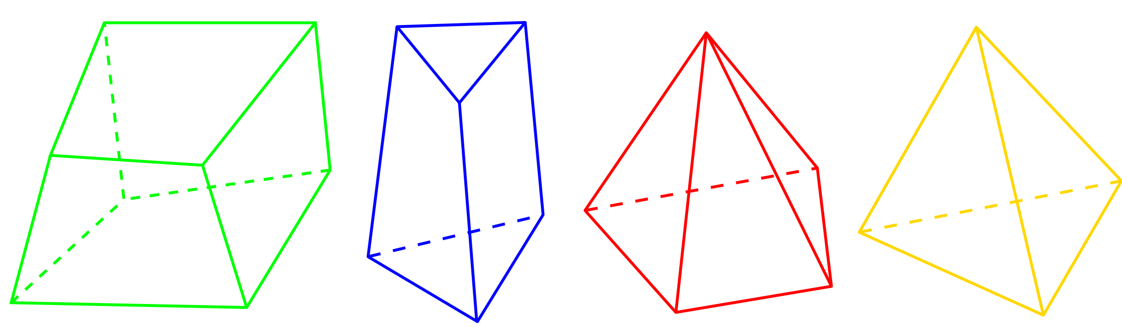
- Spatial Discretization
  - Morel-Hall asymmetric diffusion discretization
  - Support Operator symmetric diffusion discretization
  - Hall symmetric diffusion discretization (2-D, x-y only)
- Temporal Discretization
  - Backwards Euler implicit discretization
- Matrix Solution
  - Krylov Subspace Iterative Methods
    - JTpack: GMRES, BCGS, TFQMR
    - Preconditioners:
      - JTpack: Jacobi, SSOR, ILU
      - Low-order version of Morel-Hall discretization that is a smaller, symmetric system and is solved by CG with SSOR (from JTpack)
  - Incomplete Direct Method - UMFPACK

Mesh Description

Multi-Dimensional Mesh:

Dimension	Geometries	Type of Elements
1-D	spherical, cylindrical or cartesian	line segments
2-D	cylindrical or cartesian	quadrilaterals or triangles
3-D	cartesian	hexahedra or degenerate hexahedra (tetrahedra, prisms, pyramids)

all with an unstructured (arbitrarily connected) format.



This presentation will assume a 3-D mesh.

Simplified Spherical Harmonics (SP_N) Even-Parity Equation Set

Radiation transport equations:

$$\frac{1}{c}\frac{\partial}{\partial t}\xi_{m,g} + \overrightarrow{\nabla} \cdot \overrightarrow{\Gamma}_{m,g} + \sigma_g^t \xi_{m,g} = \sigma_g^s \phi_g + \sigma_g^e B_g + \mathcal{C}_g^s \ ,$$

$$\frac{1}{c}\frac{\partial}{\partial t}\overrightarrow{\Gamma}_{m,g} + \mu_m^2 \overrightarrow{\nabla} \xi_{m,g} + \sigma_g^t \overrightarrow{\Gamma}_{m,g} = \overrightarrow{\mathcal{C}}_{m,g}^{v}$$

for $m = 1, M$, and $g = 1, G$.

Temperature equations:

$$\begin{aligned} C_{vi}\frac{\partial T_i}{\partial t} &= \alpha\left(T_e - T_i\right) + Q_i \ , \\ C_{ve}\frac{\partial T_e}{\partial t} &= \alpha\left(T_i - T_e\right) + Q_e + \sum_{g=1}^{G}\left(\sigma_g^a \phi_g^{(0)} - \sigma_g^e B_g\right) \ , \end{aligned}$$

where

$$\begin{aligned} \xi_{m,g} &= \text{Even-parity pseudo-angular energy intensity,} \\ \overrightarrow{\Gamma}_{m,g} &= \text{Even-parity pseudo-angular energy current,} \end{aligned}$$

Simplified Spherical Harmonics (SP_N) Even-Parity Equation Set (cont)

$$
\begin{aligned}
\mathcal{C}_g^s &= \left(\sigma_g^a - \sigma_g^s\right) \overrightarrow{F}_g^{(0)} \cdot \frac{\overrightarrow{v}}{c} \,, \\
\overrightarrow{\mathcal{C}}_{m,g}^{v} &= 3\mu_m^2 \sigma_g^t \left(P_g + \phi_g\right) \frac{\overrightarrow{v}}{c} \,, \\
\phi_g &= \sum_{m=1}^{M} \xi_{m,g}\, w_m \,, \\
P_g &= \sum_{m=1}^{M} \xi_{m,g}\, \mu_m^2\, w_m \,, \\
\overrightarrow{F}_g &= \sum_{m=1}^{M} \overrightarrow{\Gamma}_{m,g}\, w_m \,, \\
\phi_g^{(0)} &= \phi_g - 2\, \overrightarrow{F}_g^{(0)} \cdot \frac{\overrightarrow{v}}{c} \,, \\
\overrightarrow{F}_g^{(0)} &= \overrightarrow{F}_g - \left(P_g + \phi_g\right) \frac{\overrightarrow{v}}{c} \,, \\
M &= \left(N + 1\right)/2 \,.
\end{aligned}
$$

Simplified Spherical Harmonics (SP_N) Properties

- SP_1 and P_1 equations are identical.

- SP_N and P_N equations are identical in 1-D slab geometry.

- Rotationally invariant $\longrightarrow$ no ray effects.

- SP_N is a non-convergent method. It is an asymptotic approximation associated with the diffusion limit. As $N \longrightarrow \infty$, the solution doesn't necessarily converge to the true answer.

- SP_N has almost the same accuracy for lower orders as S_N if the solution is approximately locally 1-D, but is much cheaper.

Simplified Spherical Harmonics (SP_N) Properties (cont)

- With DSA and LMFG acceleration, SP_N costs $MG + G + 1$ diffusion solutions for every outer iteration.

- Unlike the diffusion equation, the SP_N equations propagate information at a finite speed. For radiation, this speed approaches $\boldsymbol{c}$ from below as the order of approximation is increased.

- Order N unknowns for SP_N, vs. order N^2 unknowns for P_N and S_N.

- In a homogeneous region, SP_N and P_N scalar flux solutions satisfy same equation, except with different boundary conditions.

Simplified Spherical Harmonics (SP_N) Temporal Discretization

Radiation transport equations:

$$\frac{1}{c}\frac{\partial}{\partial t}\xi_{m,g} + \overrightarrow{\nabla}\cdot\overrightarrow{\Gamma}_{m,g} + \sigma_g^t \xi_{m,g} = \sigma_g^s \phi_g + \sigma_g^e B_g + \mathcal{C}_g^s \ ,$$

$$\frac{1}{c}\frac{\partial}{\partial t}\overrightarrow{\Gamma}_{m,g} + \mu_m^2 \overrightarrow{\nabla}\xi_{m,g} + \sigma_g^t \overrightarrow{\Gamma}_{m,g} = \overrightarrow{\mathcal{C}}^{v}_{m,g}$$

for $m = 1, M$, and $g = 1, G$.

Temperature equations:

$$\begin{aligned} C_{vi}\frac{\partial T_i}{\partial t} &= \alpha\left(T_e - T_i\right) + Q_i \ , \\ C_{ve}\frac{\partial T_e}{\partial t} &= \alpha\left(T_i - T_e\right) + Q_e + \sum_{g=1}^{G}\left(\sigma_g^a \phi_g^{(0)} - \sigma_g^e B_g\right) , \end{aligned}$$

where

Blue	=	Implicit or backwards Euler terms,
Magenta	=	Explicit or extrapolated implicit terms,
Red	=	Implicit terms accelerated by DSA,
Green	=	Linearized implicit terms accelerated by LMFG.

This is not quite accurate — it's actually more complicated than this — but this captures the flavor of the temporal discretization.

Simplified Spherical Harmonics (SP_N) Source Iteration Strategy

- SP_N Equations: Red and Green terms are treated explicitly, equations decouple into $M \times G$ separate diffusion equations

- DSA Equations: summing over angle and treating Red terms implicitly leads to G separate diffusion equations, which provide an angle-constant update

- LMFG Equation: summing over group and treating Green terms implicitly leads to a single diffusion equation, which provides a spectrum-scaled update

- These equations are solved repeatedly until the Red and Green terms converge

Diffusion (P_1) Equation Set:

$$\alpha \frac{\partial \Phi}{\partial t} - \overrightarrow{\nabla} \cdot D \overrightarrow{\nabla} \Phi + \overrightarrow{\nabla} \cdot \overrightarrow{J} + \sigma \Phi = S$$

Which can be written

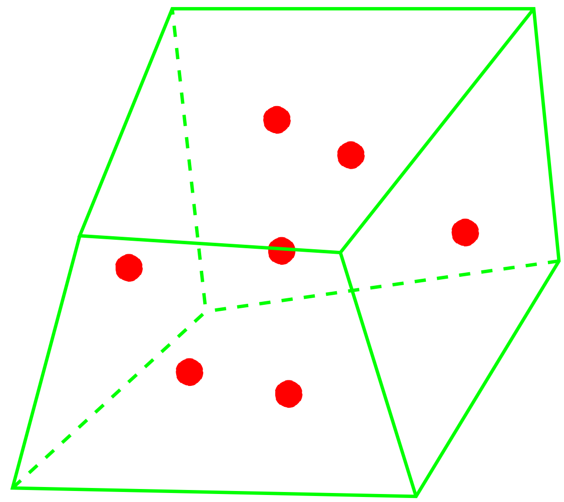
$$\alpha \frac{\partial \Phi}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{F} + \sigma \Phi = S$$

$$\overrightarrow{F} = -D \overrightarrow{\nabla} \Phi + \overrightarrow{J}$$

Where

Φ	$=$	Intensity
$\overrightarrow{F}$	$=$	Flux
D	$=$	Diffusion Coefficient
α	$=$	Time Derivative Coefficient
σ	$=$	Removal Coefficient
S	$=$	Intensity Source Term
$\overrightarrow{J}$	$=$	Flux Source Term

Diffusion Discretization Method Properties



All three methods:

- Are cell-centered – balance equations are done over a cell
- Require cell-centered and face-centered unknowns to rigorously treat material discontinuities
- Preserve the homogeneous linear solution, and are second-order accurate
- Reduce to the standard cell-centered operator for an orthogonal mesh
- Maintain local energy conservation

Diffusion Discretization Method Properties (cont)

- Morel-Hall Asymmetric Method
  - Described in

    Michael L. Hall, and Jim E. Morel. A Second-Order Cell-Centered Diffusion Differencing Scheme for Unstructured Hexahedral Lagrangian Meshes. In *Proceedings of the 1996 Nuclear Explosives Code Developers Conference (NECDC), UCRL-MI-124790*, pages 359–375, San Diego, CA, October 21–25 1996. LA-UR-97-8.

    which is an extension of

    J. E. Morel, J. E. Dendy, Jr., Michael L. Hall, and Stephen W. White. A Cell-Centered Lagrangian-Mesh Diffusion Differencing Scheme. Journal of Computational Physics, 103(2):286-299, December 1992.

    to 3-D unstructured meshes, with an alternate derivation.

- Hall Symmetric Method:
  - Based on the above method, but only applicable in 2-D x-y.

- Support Operator Symmetric Method:
  - Extension of the method described in

    Mikhail Shashkov and Stanly Steinberg. Solving Diffusion Equations with Rough Coefficients in Rough Grids. Journal of Computational Physics, 129:383-405, 1996.

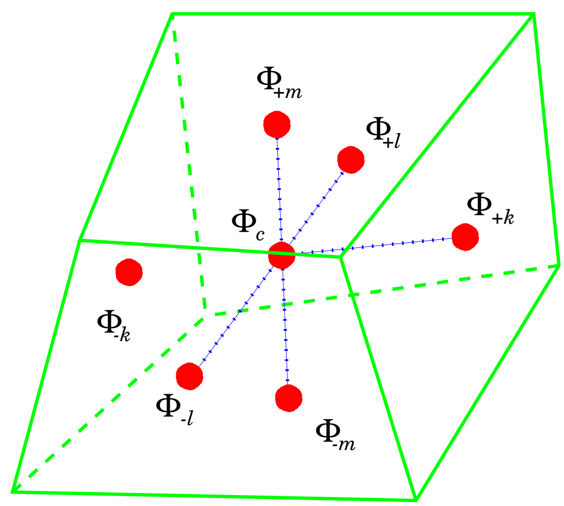
    to 3-D unstructured meshes, with an alternate derivation.

Diffusion Discretization Stencil

The flux at a given face, for example the $+\boldsymbol{k}$-face,

$$\overrightarrow{F}^{n+1}_{+k} = -D_{c,+k}\,\overrightarrow{\nabla}\,\Phi^{n+1} + \overrightarrow{J_{+k}}$$

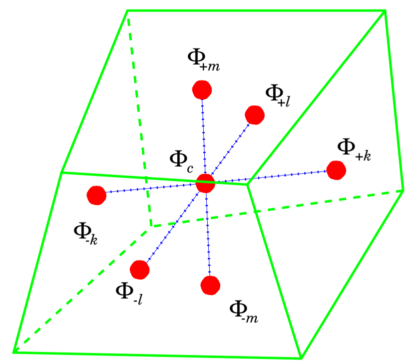
is defined using this stencil:



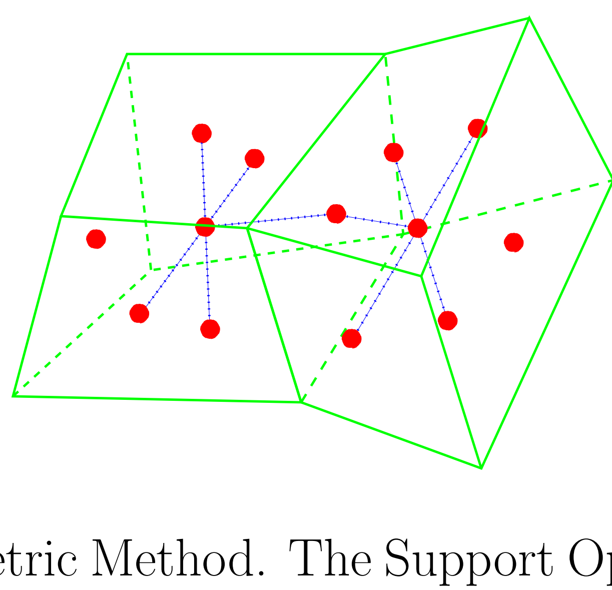
in the Asymmetric Method. The Support Operator Method uses all seven unknowns within a cell to define the face flux.

Diffusion Discretization Stencil (cont)

Each cell has a cell-centered conservation equation which involves all six face fluxes, and gives a stencil which includes all seven unknowns within the cell (in both methods).



To close the system, an equation relating the fluxes on each side of a face is added for every face in the problem. This gives the following stencil:



in the Asymmetric Method. The Support Operator Method uses all thirteen unknowns within a cell-cell pair to define the face equation.

Algebraic Solution

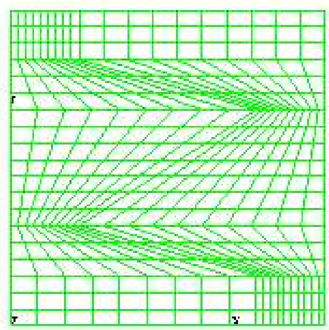
- Main Matrix System (Asymmetric Method):
  - Asymmetric – must use an asymmetric solver like GMRES, BCGS or TFQMR
  - Size is $(4n_c + n_b/2)$ squared
  - Maximum of 11 non-zero elements per row
- Main Matrix System (Support Operator Method):
  - Symmetric – can use CG to solve
  - Size is $(4n_c + n_b/2)$ squared
  - Maximum of 13 non-zero elements per row
- Preconditioner for Krylov Space methods is a Low-Order Matrix System:
  - Assume orthogonal: drop out minor directions in flux terms
  - Symmetric – can use standard CG solver
  - Size is n_c squared
  - Maximum of 7 non-zero elements per row

Results: Sample Augustus Problem

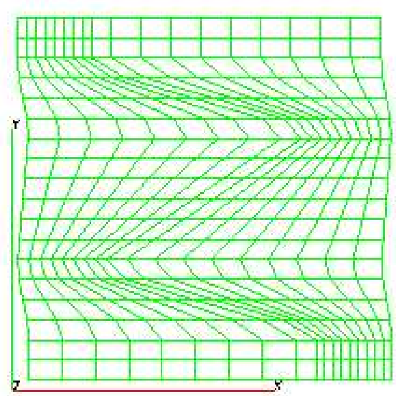
- 3-D Kershaw-Squared Mesh
- Constant properties
- No removal or sources
- Reflective boundaries on 4 sides
- Source and vacuum boundary conditions on opposite sides
- Analytic solution - linear
- Grid size - $20 \times 20 \times 20 = 8000$ nodes, 6859 cells
- 50 time steps, 15 s / time step on IBM RS/6000 Scalable POWERparallel System, SP2

Results: Sample Problem

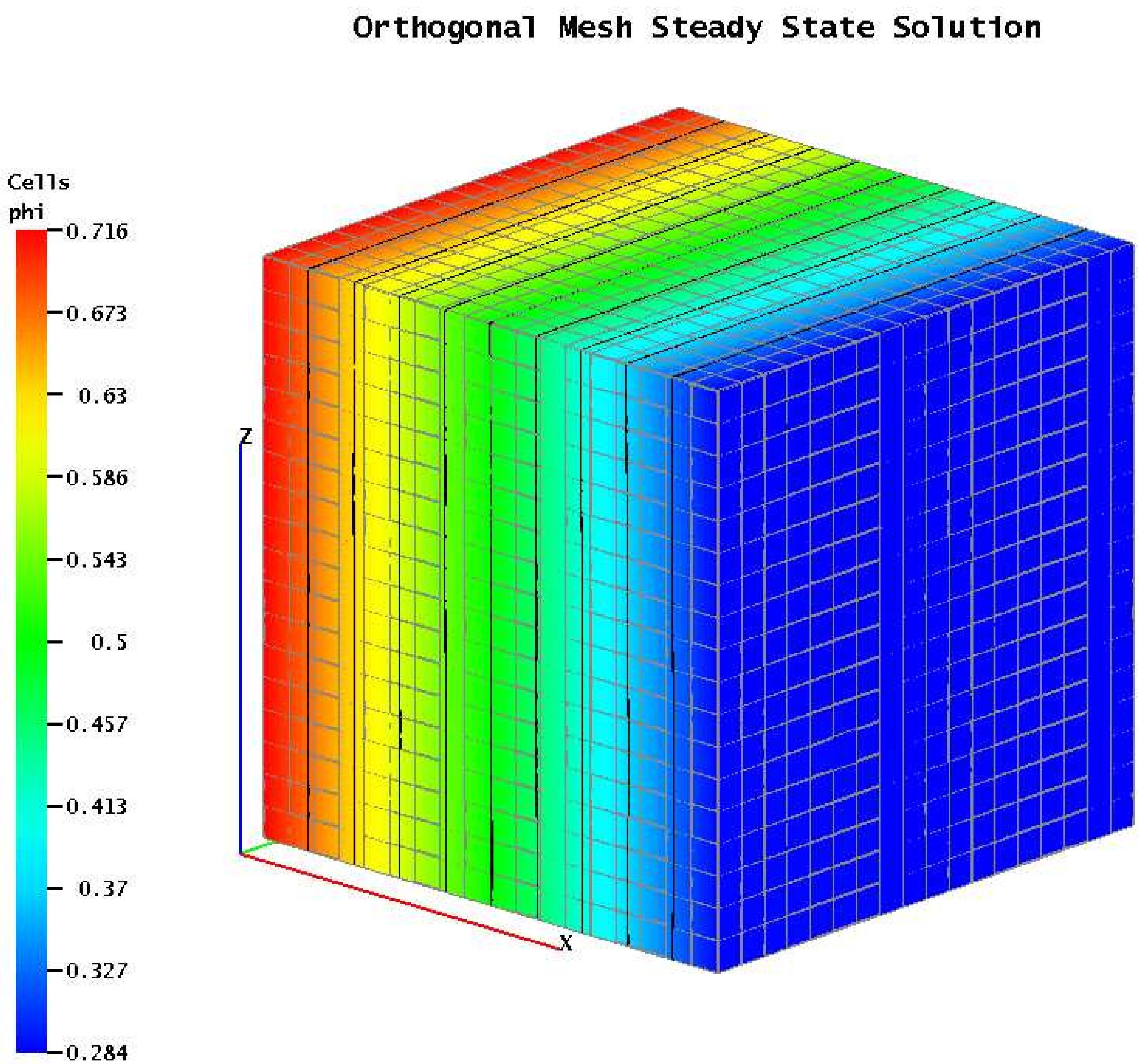
Actual Mesh (Cell Nodes)



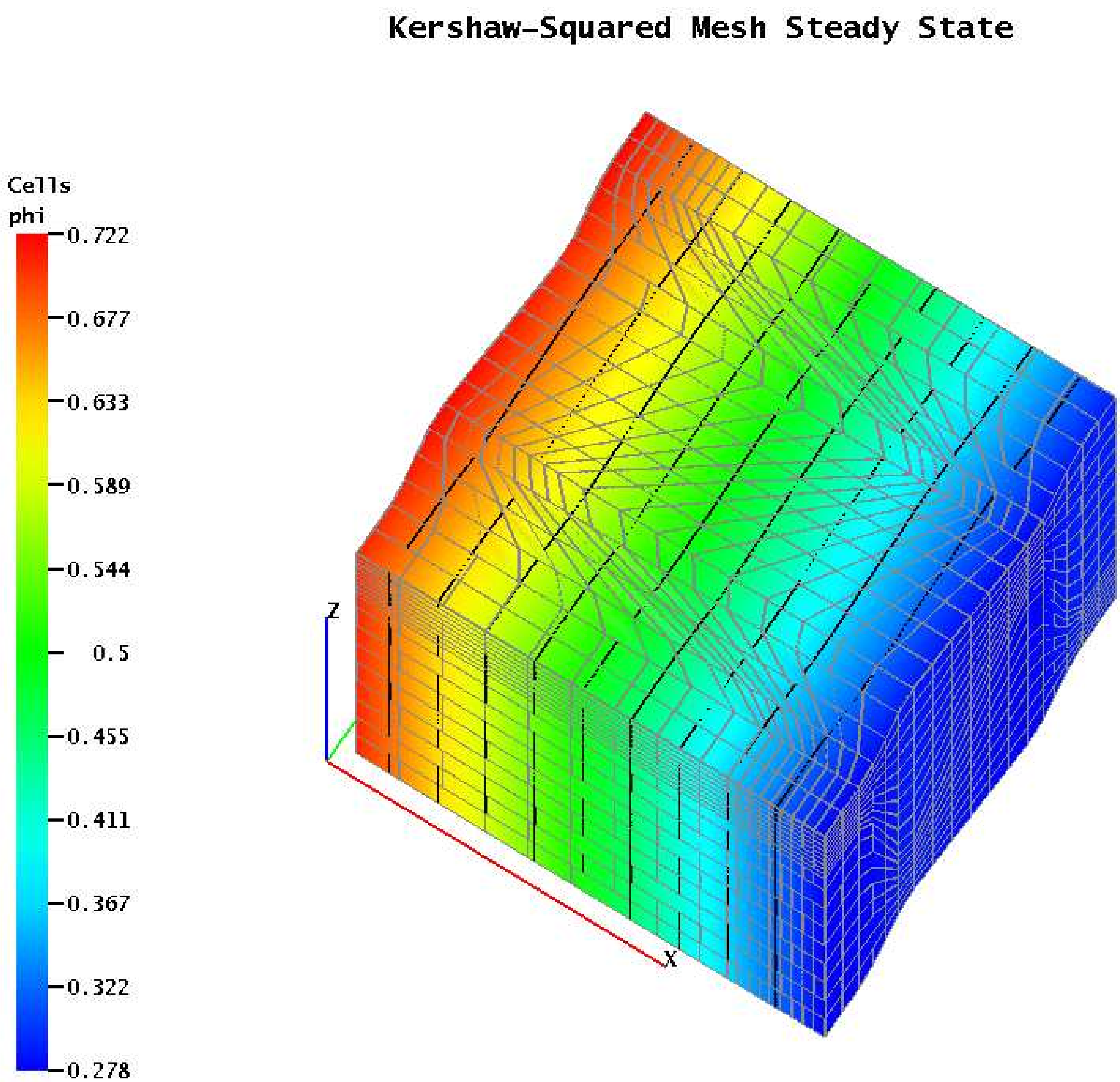
Dual Mesh (Cell Centers)



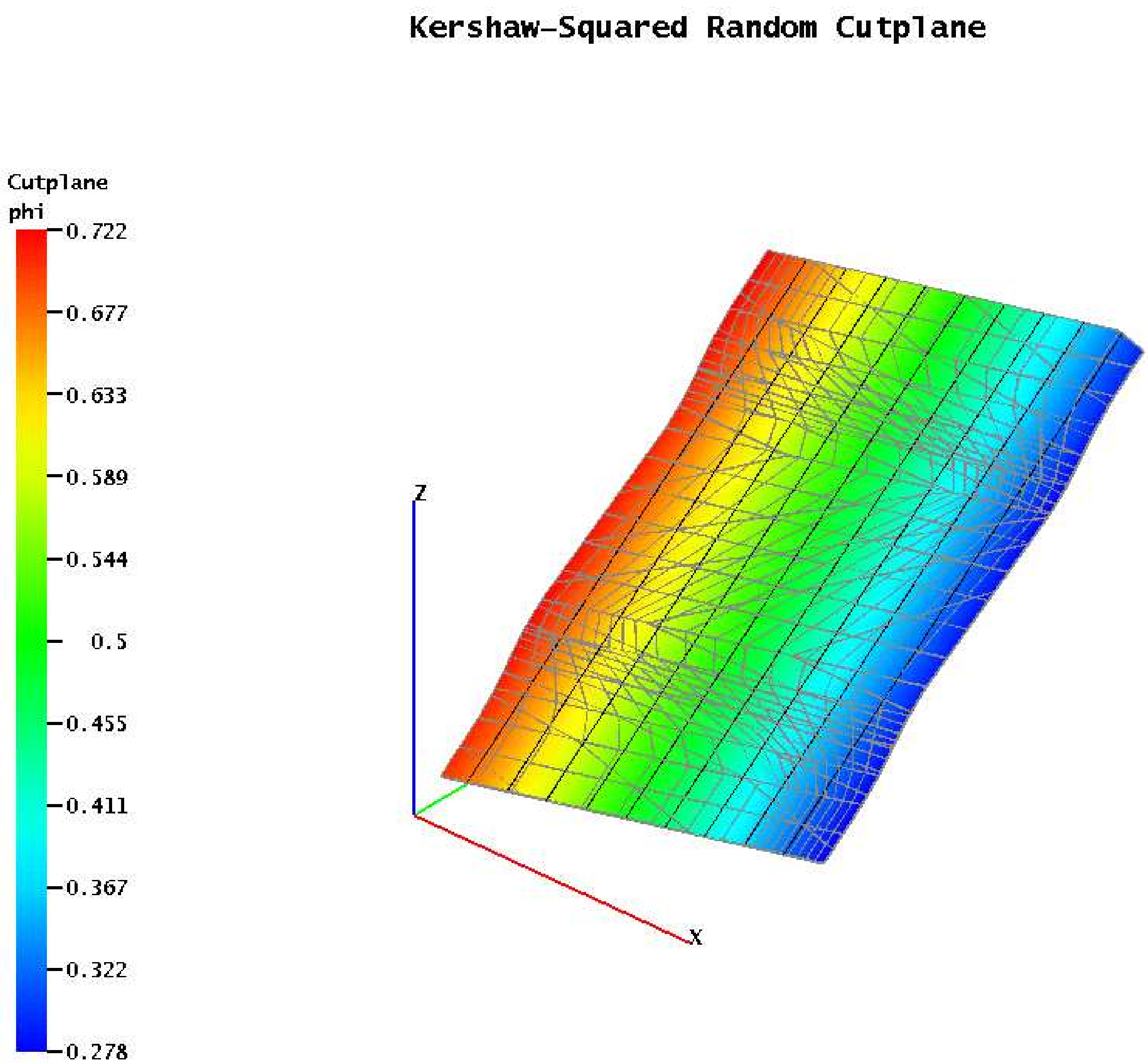
Results: Sample Problem



Results: Sample Problem



Results: Sample Problem



Future Work

- Parallel (JTpack90, PGSlib, SPAM)

- Object-based, design-by-contract F90

- Generic programming?

- Integrated documentation (HTML, PS)

- Newton-Krylov solution method?

- Alternate angular discretization?

- Self-adjoint equation set?