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

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4 / 22 / 98

Outline

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  – Properties
  
  – Solution Strategy

• Diffusion ($P_1$)
  
  – 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

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Method Overview: Spartan

- Energy/Temperature Discretization
  - Solves $2T + \text{Multi-Group Even-Parity Equations}$
  - Can yoke $T_e$ and $T_i$ together to make $1T$
  - Can use a single-group radiation treatment to make $3T$

- 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:

<table>
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<tr>
<th>Dimension</th>
<th>Geometries</th>
<th>Type of Elements</th>
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<tr>
<td>1-D</td>
<td>spherical, cylindrical or cartesian</td>
<td>line segments</td>
</tr>
<tr>
<td>2-D</td>
<td>cylindrical or cartesian</td>
<td>quadrilaterals or triangles</td>
</tr>
<tr>
<td>3-D</td>
<td>cartesian</td>
<td>hexahedra or degenerate hexahedra (tetrahedra, prisms, pyramids)</td>
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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:

$$\frac{1}{c} \frac{\partial}{\partial t} \xi_{m,g} + \nabla \cdot \Gamma_{m,g} + \sigma_t \xi_{m,g} = \sigma_s \phi_g + \sigma_e B_g + C_g,$$

$$\frac{1}{c} \frac{\partial}{\partial t} \Gamma_{m,g} + \mu_m^2 \nabla \xi_{m,g} + \sigma_t \Gamma_{m,g} = \mathcal{C}_m g$$

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

Temperature equations:

$$C_{vi} \frac{\partial T_i}{\partial t} = \alpha (T_e - T_i) + Q_i,$$

$$C_{ve} \frac{\partial T_e}{\partial t} = \alpha (T_i - T_e) + Q_e + \sum_{g=1}^{G} \left( \sigma_a \phi_g^{(0)} - \sigma_e B_g \right),$$

where

$$\xi_{m,g} = \text{Even-parity pseudo-angular energy intensity},$$

$$\Gamma_{m,g} = \text{Even-parity pseudo-angular energy current},$$
Simplified Spherical Harmonics \((SP_N)\) 
Even-Parity Equation Set (cont)

\[
\mathcal{C}^s_g = \left(\sigma^a_g - \sigma^s_g\right) \vec{F}^{(0)}_g \cdot \frac{\vec{v}}{c},
\]

\[
\mathcal{C}^v_{m,g} = 3\mu^2_m \sigma^t_g (P_g + \phi_g) \frac{\vec{v}}{c},
\]

\[
\phi_g = \sum_{m=1}^{M} \xi_{m,g} w_m,
\]

\[
P_g = \sum_{m=1}^{M} \xi_{m,g} \mu^2_m w_m,
\]

\[
\vec{F}^v_g = \sum_{m=1}^{M} \vec{\Gamma}_{m,g} w_m,
\]

\[
\phi_g^{(0)} = \phi_g - 2 \vec{F}^{(0)}_g \cdot \frac{\vec{v}}{c},
\]

\[
\vec{F}^{(0)}_g = \vec{F}_g - (P_g + \phi_g) \frac{\vec{v}}{c},
\]

\[
M = (N + 1) / 2.
\]
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 $\rightarrow$ no ray effects.

- $SP_N$ is a non-convergent method. It is an asymptotic approximation associated with the diffusion limit. As $N \rightarrow \infty$, 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 $c$ 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:

$$
\frac{1}{c} \frac{\partial}{\partial t} \xi_{m,g} + \nabla \cdot \Gamma_{m,g} + \sigma_g^t \xi_{m,g} = \sigma_g^s \phi_g + \sigma_g^e B_g + C_g^s ,
$$

$$
\frac{1}{c} \frac{\partial}{\partial t} \Gamma_{m,g} + \mu_m^2 \nabla \xi_{m,g} + \sigma_g^t \Gamma_{m,g} = \Gamma_v \Gamma_{m,g}
$$

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

Temperature equations:

$$
C_{vi} \frac{\partial T_i}{\partial t} = \alpha (T_e - T_i) + Q_i ,
$$

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

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:

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

Which can be written

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

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

Where

$$\Phi = \text{Intensity}$$
$$\vec{F} = \text{Flux}$$
$$D = \text{Diffusion Coefficient}$$
$$\alpha = \text{Time Derivative Coefficient}$$
$$\sigma = \text{Removal Coefficient}$$
$$S = \text{Intensity Source Term}$$
$$\vec{J} = \text{Flux Source Term}$$
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


  which is an extension of


  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


  to 3-D unstructured meshes, with an alternate derivation.
**Diffusion Discretization Stencil**

The flux at a given face, for example the $+k$-face,

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

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 \((4n_c + n_b/2)^2\) squared
  - Maximum of 11 non-zero elements per row

- Main Matrix System (Support Operator Method):
  - Symmetric – can use CG to solve
  - Size is \((4n_c + n_b/2)^2\) 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

Orthogonal Mesh Steady State Solution
Results: Sample Problem

Kershaw-Squared Mesh Steady State
Results: Sample Problem

Kershaw-Squared Random Cutplane
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?