A Piecewise Linear Discontinuous Finite Element Spatial Discretization of the $S_N$ Transport Equation for Polyhedral Grids in 3D Cartesian Geometry

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We are interested in developing spatial discretizations for arbitrary polyhedral grids

- Polyhedral grids can potentially reduce the number of spatial unknowns needed in a calculation
  - Potentially decrease run time
  - Potentially decrease memory requirements
  - Methods that work on polyhedral grids should be able to handle AMR grids

- 3D polyhedral discretizations are not automatically derived from 2D polygonal discretizations
  - Subcell divisions are easier in 2D
  - 3D faces much more complex than 2D edges

- We are interested in methods that preserve the diffusion limit
  - We will note that this method does preserve the diffusion limit, but do not present test problem results here
Possible discretizations for these problems have advantages and disadvantages

- **Piecewise Linear DFEMs**
  - Has been successful in 2D geometry
  - Must invert a dense matrix for every cell

- **Upstream Corner Balance Methods**
  - Can “sweep” a cell instead of invert a matrix
  - Requires ad-hoc closures, loses accuracy on distorted cells

- **Characteristic Methods**
  - Works well on concave cells in XY
  - Requires “piecewise” basis functions to expand the source on polygons, may be computationally expensive

- **CFEM-based DFEMs**
  - Works well in 2D
  - Not implemented in 3D yet, same or more computations as PWLD

- **Linear Discontinuous on tetrahedra and TriLD on hexahedra**
  - Efficient methods that have been tested on difficult problems
  - Not generalized for polyhedra, resulting in more unknowns
We develop machinery that can handle most generalized polyhedra

- We define an arbitrary polyhedron as a 3D volume with an arbitrary number of (faceted) faces
- In discretizations on these cell types we define a subcell volume called a side – tetrahedron
The PWLD discretization is a standard, Galerkin DFEM with special basis functions

- A standard DFEM solves an NxN matrix (N = number of unknowns in a cell) in each spatial cell for each quadrature point. We show the $i^{th}$ row of the matrix

$$
\sum_{f=\text{faces } \in \text{cell}} \int (\vec{\Omega}_m \cdot \vec{n}_f) v_i \left[ \left( \sum_{j=1}^{J} \psi_{m,j} u_j (x, y, z) \right) - \left( \sum_{j=1}^{J} \psi_{m,j} u_j (x, y, z) \right) \right] dA_f
$$

$$
+ \int_{V_{\text{cell}}} v_i \left[ \vec{\Omega}_m \cdot \vec{V} \left( \sum_{j=1}^{J} \psi_{m,j} u_j (x, y, z) \right) \right] dV
$$

$$
\sum_{V_{\text{cell}}} v_i \left[ \sigma (x, y, z) \sum_{j=1}^{J} \psi_{m,j} u_j (x, y, z) \right] dV = \int_{V_{\text{cell}}} v_i \sum_{j=1}^{J} Q_{m,j} u_j (x, y, z) dV
$$

- We have developed unlumped, lumped, and lumping parameter versions of the DFEM discretization
- If the weight/basis functions meet Adam’s surface matching and full-resolution diffusion limit requirements for polyhedral cells, then the discretization will work in the diffusion limit
We construct a 2D PWL basis function; 3D functions are extensions of 2D with extra face interpolation factors.

2D: \( u_j(r,z) = t_j(r,z) + \beta_j t_c(r,z) \)

3D: \( u_j(r,z) = t_j(r,z) + \sum_{\text{faces at } j} \alpha_{f,j} t_f(\vec{r}) + \beta_j t_c(r,z) \)

\[ t_j(r,z) + \beta_j t_c(r,z) = t_j(r,z) + \beta_j t_c(r,z) \]
We have implemented a PWLD XYZ method in the Texas A&M PDT code

- The PDT (“Parallel Deterministic Transport”) code is being developed at Texas A&M to provide accurate particle transport solutions on massively parallel computers
- PDT solves the time-dependent linear Boltzmann and thermal radiation equations
  - 3D (XYZ) or 2D (XY)
  - Multigroup in energy
  - Discrete ordinates (quadrature set can vary by energy group)
  - Various finite-volume and finite-element spatial discretizations
  - Multiple time discretization methods (fully-implicit, Crank-Nicolson, TBDF2)
  - Various partitioning algorithms (KBA, Volumetric, Hybrid, METIS)
  - Supports various iterative schemes (Sweeps, Block-Jacobi, Hybrid)
  - Supports various Krylov methods (GMRES, BiCGSTAB, CG)
  - Used as a methods test-bed, can also solve steady-state problems
We run test problems on orthogonal and random grids

- Orthogonal grids are well-behaved and we expect good results for most discretizations.
- Random grids have faces that will be faceted, and can create cyclical dependencies in the sweep order. We show a few cells on a random grid on the right.
Multiple test problems verify coding and explore properties of PWLD in XYZ

- We have developed a “one-cell” test problem to examine the robustness of the method as a cell becomes distorted.
  - One-cell test problems are particularly useful to examine the properties of DFEMs.

- We have developed a manufactured quadratic solution problem to test the truncation error of the method in an optically thin limit.

- We have run the Kobayashi benchmark test problems and show some selected results, noting run times.
The one-cell test problem demonstrates robustness

- We take a cell that is 4cm x 4cm x 4cm. The “origin” of this cell is at (0,0,0). We create five new cells, moving the “origin” of the cell incrementally towards the (4,4,4) vertex.
- As the origin moves towards the (4,4,4) vertex, three faces in the cell become extremely distorted potentially causing problems for our method.
- For PWLD, one potential problem is that the cell center point, about which we define our sides, moves outside of the cell, creating sides with negative volumes.
- Our test: Does PWLD retain its ability to exactly reproduce a spatially linear solution on these distorted one cell problems?
The one cell test problem shows that PWLD will not fail on highly distorted grids.

(0,0,0)  (1,1,1)  (2,2,2)  

(2.2857,2.2857,2.2857)  (3,3,3)  (4,4,4)
The quadratic manufactured solution problem in the optically thin limit

- We use a manufactured solution for our truncation error analysis. The exact analytic solution is known.
- The angular flux is

\[
\psi(x, y, z, \mu, \eta, \xi) = a + bx + c\mu + dx\mu + ex^2 + f\mu^2 + gy + h\eta + iy\eta + jy^2 + k\eta^2 \\
+ lz + m\xi + nz\xi + oz^2 + p\xi^2 + qxy + rxz + syz + t\mu\eta + u\mu\xi + v\eta\xi \\
+w\mu y + A\eta x + B\xi x + C\mu z + D\eta z + E\xi y
\]

- The scalar flux solution is only spatially dependent

\[
\phi(x, y, z) = 4\pi \left( a + bx + ex^2 + gy + jy^2 + lz + oz^2 + qxy + rxz + syz \right) + \frac{4\pi}{3} f + \frac{4\pi}{3} k + \frac{4\pi}{3} p
\]

- The TriLD basis functions better represent this solution space compared to the PWLD basis functions.
- We used an S_6 quadrature set, \( \sigma = 8, c = 0.5 \).
Our results indicate that PWLD is second-order accurate.
Even on extremely distorted grids, PWLD performs well.

Truncation Error Re-entrant Random Grid (0.33), Thin Limit

L2 Norm of the Error

Mesh Size

U PWLD  U TriLD  L PWLD  L TriLD  LP PWLD  LP TriLD  Reference
The Kobayashi benchmark problems provide more of a challenge for PWLD and PDT

- Analytic solutions exist for purely absorbing cases; highly resolved Monte Carlo calculations for problems with scattering.
- Problem domain is 120 cm x 200 cm x 120 cm

- We plot the scalar flux
  - Along the y axis at the x and z mid-planes (A)
  - Along the x axis at y=155, and the z mid-plane (B)
  - Along the x axis at y=195, z=90 (C)
PDT ran these benchmark problems efficiently

- Standard problem uses reflecting BC. PDT does not have reflecting BC, so we modeled the entire geometry
- Number of cells: 24 x 40 x 24, cell width = 5 cm
- Computational Performance
  - Single-core runs performed on a 2.3GHz Xeon E5345
  - Absorption problem
    - S8: 3 min. solution time
    - LDFE-2048*: 15 min. solution time.
  - Scattering problem:
    - S8: 10 min. solution time
    - LDFE-2048: 60 min. solution time.

* Quadrature set developed by Jarrell and Adams
Results for purely absorbing cases

- S8
- LDFE 2048
- Analytic

Graphs labeled A, B, C
Results for scattering cases

- S8
- LDFE 2048
- Benchmark

A

B

C
Conclusion

- We have provided a quick introduction to the PWLD method in XYZ geometry.
- Test problems indicate that the PWLD method is acceptably accurate, and surprisingly resilient on highly distorted grids.
- Diffusion limit analysis predicts good behavior in the thick diffusion limit because the 3D PWL basis functions conform to Adams’ surface matching and full resolution requirements.
- Diffusion limit test problems will be presented in the future.
Questions?