Finite Element Particle Transport using Wachspress Rational Basis Functions

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CSGF Annual Conference
June 20
Outline

1. Introduction
   - Introduction to Particle Transport
   - Introduction to the Finite Element Method
   - Motivation of Research

2. Properties of Wachspress rational functions
   - Proper basis functions
   - Comparison between PWL and WRF

3. Construction of Wachspress Rational Functions

4. Integration of Wachspress Rational Functions

5. Numerical Results
Particle transport is concerned with describing how radiation flows through materials. We are only concerned with time-independent and energy-independent two-dimensional particle transport.
Introduction to Particle Transport

- Particle transport is concerned with describing how radiation flows through materials.
- We are only concerned with time-independent and energy-independent two-dimensional particle transport.
Particle transport is described by the linear Boltzmann transport equation:

$$\Omega \cdot \nabla \psi(x, \Omega) + \Sigma_t \psi(x, \Omega) = \frac{\Sigma_s}{2\pi} \int_{2\pi} \psi(x, \Omega') d\Omega' + \frac{Q}{2\pi}$$  \hspace{1cm} (1)
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\] (1)

Streaming Term: Rate that particles at position \(x\) and angle \(\Omega\) stream through the background media.
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$$

Collision Term: Rate that particles in \((x, \Omega)\) collide with nuclei
Introduction to Particle Transport

Particle transport is described by the linear Boltzmann transport equation:

$$\Omega \cdot \nabla \psi(x, \Omega) + \sum_i \psi(x, \Omega) = \frac{\Sigma_s}{2\pi} \int_{2\pi} \psi(x, \Omega') d\Omega' + \frac{Q}{2\pi}$$  \hspace{1cm} (1)$$

Scattering Term: Rate that particles at $x$ scatter into angle $\Omega$.
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Source Term: Rate that particles are created at position \( x \) and angle \( \Omega \)
Break the spatial domain into zones:

Main idea: Represent $\psi(x, \Omega)$ as an expansion in basis functions:

$$\psi(x, \Omega) = \sum_{i=1}^{4} \psi_i(\Omega) b_i(x)$$  \hspace{1cm} (2)
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Introduction to the Finite Element Method

- Multiply by a weight function and integrate over the zones
- Apply the divergence theorem to the streaming term
- Substitute the expansion into the transport equation
- When we’re all done we end up with, in each zone:

\[
A \psi(\Omega) = B \int_{2\pi} \psi(\Omega) \, d\Omega + \frac{1}{2\pi} Q \quad (3)
\]

- The matrices $A$ and $B$ involve integrals of the (known) basis and weight functions
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Motivation of Research

- Traditionally, finite element methods are restricted to the finite element zoo:

- Wachspress rational functions are shape functions (or interpolation functions, or basis functions) that can be built on a variety of zone shapes.

- Some discretizations give unphysical solutions in the thick diffusive limit, but Adams (2001) predicted that Wachspress rational functions will have full resolution in the thick diffusive limit.
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Wachspress asserted four requirements for a “proper” basis function:

- Continuous over the zone
- Normalized to unity at its anchor vertex
- Linear on the two sides adjacent to the anchor
- Equal to zero on the sides opposite the anchor

Two new bases are being investigated for extending the finite element method: Wachspress rational functions and piecewise-linear functions.
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Adams (2001) found that for full-resolution, weight functions must have locality and surface-matching. 

- **Locality**: The function is non-zero only within a certain region, known as the anchor. 
- **Surface-Matching**: The function matches the surface of the cell, ensuring accuracy.
## Comparison between PWL and WRF

<table>
<thead>
<tr>
<th>Property</th>
<th>PWL</th>
<th>WRF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polygons and Polyhedra</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Polycons and Polypols</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Full-resolution</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Continuous in zone</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Smooth in zone</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Easily integrated</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>
A Wachspress Rational Function
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Construction of Wachspress Rational Functions

\[ b_i(x, y) = k_i \frac{l_{opp1}(x, y)l_{opp2}(x, y)}{l_{ext}(x, y)} \] (4)
Normalize $k_i$ such that $b_i(x, y) = 1$ at the anchor node.
More complex polygons can be constructed using Dasgupta’s (2003) method
This works:  

This doesn’t:
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Integration of Wachspress Rational Functions

- **Isoparametric Mapping**
  - Maps the quadrilateral onto an isoparametric square
  - Integral done numerically in isoparametric space
  - **Only for quadrilaterals!**

- **Dasgupta Integration (2003)**
  - Repeatedly apply Divergence Theorem
  - End up with integrals around zone edges
  - Integrand becomes very complex
  - Requires a computer algebra system!
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Strongly Heterogeneous Problem, Adams, (1991)

Problem was accelerated using Asymptotic-P1 DSA
Strongly Heterogeneous Problem, Adams, (1991)

FL Orthogonal Mesh Results

FL Skewed Mesh Results
Wachspress Rational Functions in Computer Graphics
(Dasgupta, Malsch, 2001)

Particle Transport using Wachspress Functions
Wachspress Rational Functions in Computer Graphics
(Dasgupta, Malsch, 2001)

Using triangular interpolation:
Using Wachspress interpolation:
Conclusions

- Wachspress rational functions provide smooth interpolation over polygonal domains.
- Wachspress rational functions can be integrated over quadrilateral domains numerically.
- Wachspress rational functions provide a full-resolution discretization to the particle transport equation.
- Wachspress rational functions can provide numerically robust solutions to the particle transport equation in the diffusive limit.
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Future Work

- Investigate construction of Wachspress rational functions in 3-D
- Investigate behavior on concave zones
- Faster integration!
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Acknowledgements

This research was funded by the DOE Computational Science Graduate Fellowship