High Order $S_N$ Transport in $R-Z$ Geometry on Meshes with Curved Surfaces

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October 18, 2017

ICTT-25
Monterey, CA
Introduction - BLAST hydrodynamics code

multi-material shock hydrodynamics problem solved with BLAST: 8th order kinematics, 7th order thermodynamics

https://computation.llnl.gov/project/blast/

- High-order finite element method
- Meshes with curved surfaces
  - Straight-edged meshes restrict the accuracy of the compressible Euler equations
  - “essential for higher-order accuracy”
- More accurately model:
  - fluid flow geometry in Lagrangian framework with curved meshes
  - shock front with increased resolution - can model a shock within a single zone
  - radial flow symmetry
Background

- High-order \((p \geq 2)\) \(S_N\) transport FEM research is relatively new
  - Cartesian coordinates
  - Spatial convergence of \(O(p + 1)\)
- \(R-Z\) geometry has only been developed using low-order \((p = 1)\) FEMs
  - LLD, FLBLD, PWLD are accurate in the diffusion limit
- Structured/unstructured quadrilateral and triangular meshes
  - Some research for meshes with curved surfaces
- Source iteration acceleration using MIP DSA
High-order mapping allows for meshes with curved surfaces.

(a) Reference element on the unit square

(b) Physical element has 2nd-order polynomial surfaces
Previous results in X-Y geometry

Orthogonal mesh

1st-order mesh

2nd-order mesh

3rd-order mesh

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X-Y MIP DSA source iteration acceleration

\[
b_{\text{MIP}}(\phi, w) = (\sigma_a \phi, w)_V + (D \nabla \phi, \nabla w)_V \\
+ (\kappa_e [\phi], [w])_{\partial V^i} + ([\phi], \{D \partial_n w\})_{\partial V^i} + (\{D \partial_n \phi\}, [w])_{\partial V^i} \\
+ (\kappa_e \phi, w)_{\partial V^d} - \frac{1}{2} (\phi, D \partial_n w)_{\partial V^d} - \frac{1}{2} (D \partial_n \phi, w)_{\partial V^d}
\]

\[
\ell_{\text{MIP}}(w) = \left(\sigma_s \left[\phi^{(l+1)} - \phi^{(l)}\right], w\right)_V
\]

\[
\kappa_{e_{IP}} = \begin{cases} 
\frac{c(p_+)}{2} \frac{D^+}{h^+} + \frac{c(p_-)}{2} \frac{D^-}{h^-}, & \text{on interior edges (i.e., } r \in E_h^i) \\
c(p) \frac{D}{h}, & \text{on boundary edges (i.e., } r \in \partial D_d^d) 
\end{cases}
\]

\[
\kappa_e = \max \left(\kappa_{e_{IP}}, \frac{1}{4}\right)
\]
X-Y MIP DSA source iteration acceleration unconditionally convergent

- MIP DSA equations are unconditionally convergent for all tested FEMs
- Peaks occur at switch from the interior penalty method to the DCF method
- Adding mesh curvature exhibits same basic behavior
Highly scattering problem

- Strong scatter with discontinuous BCs with MIP DSA problem geometry
  \[ \sigma_t = 1000, \sigma_s = 999, \quad S_0 = 0, \quad I_{inc} = 1 \]
- Plot log of scalar flux; white regions denote negative
- Gauss-Legendre basis functions - only mass lumped
- Fully lumping methods have demonstrated reduction in negativities
Objectives

• Numerically solve high-order $S_N$ transport equation in $R-Z$ geometry using MFEM, a general finite element library (mfem.org)
• Evaluate high-order solution with various test problems
• Investigate the impact of meshes with curved surfaces in $R-Z$ geometry
$R-Z$ streaming term introduces an angular derivative

\[
\frac{\mu}{r} \frac{\partial}{\partial r} r \psi (r, z, \Omega) + \xi \frac{\partial}{\partial z} \psi (r, z, \Omega) - \frac{1}{r} \frac{\partial}{\partial \omega} \eta \psi (r, z, \Omega)
\]

\[+ \sigma_t (r, z) \psi (r, z, \Omega) + \frac{1}{2\pi} \sigma_s (r, z) \phi (r, z, \Omega') + \frac{1}{2\pi} S_0 (r, z)
\]

\[
\mu = \sqrt{1 - \xi^2} \cos(\omega)
\]

\[
\eta = \sqrt{1 - \xi^2} \sin(\omega)
\]

\[
\xi = \cos(\theta)
\]
Level symmetric angular quadrature

- Angular discretization showing \((\xi_n, \mu_{n,m})\) pairs
R-Z angular derivative approximation - Morel Montry

\[-\frac{1}{r} \frac{\partial}{\partial \omega} \eta \psi (r, z, \Omega) = \frac{\alpha_{n}^{m+1/2} \psi_{n,m+1/2} - \alpha_{n}^{m-1/2} \psi_{n,m-1/2}}{r W_{n,m}}\]

- Define angular differencing coefficients to preserve uniform infinite medium solution
- Using level-symmetric angular quadrature to sweep through all \(\mu_{n,m}\) directions on level \(\xi_{n}\)

\[
\alpha_{n}^{m+1/2} = \alpha_{n}^{m-1/2} - \mu_{n,m} W_{n,m}
\]

\[
\alpha_{1/2} = \alpha_{Mn+1/2} = 0
\]
R-Z angular derivative approximation - Morel Montry

- Weighted diamond difference approximation for $\psi_{n,m}$ between $\psi_{n,m-1/2}$ and $\psi_{n,m+1/2}$, angular fluxes at the boundary of the discrete ordinate direction

\[
\psi_{n,m} = \tau_{n,m} \psi_{n,m+1/2} + (1 - \tau_{n,m}) \psi_{n,m-1/2}
\]

\[
\tau_{n,m} = \frac{\mu_{n,m} - \mu_{n,m+1/2}}{\mu_{n,m+1/2} - \mu_{n,m-1/2}}
\]

\[
\mu_{n,m+1/2} = \sqrt{1 - \xi_n^2} \cos(\gamma_{n,m+1/2})
\]

\[
\gamma_{n,m+1/2} = \gamma_{n,m-1/2} + \frac{\pi}{\sum_{M_n} W_{n,m}} W_{n,m}
\]

\[
\gamma_{n,1/2} = -\pi
\]
**R-Z angular derivative approximation - Morel Montry**

- Solve for starting directions $\psi_{n,1/2}$ using Cartesian geometry transport equation

\[ \Omega \cdot \nabla \psi_{n,1/2} + \sigma_t \psi_{n,1/2} = \frac{1}{2\pi} \sigma_s \phi + \frac{1}{2\pi} S_0 \]

- We relate the starting direction to the first $S_N$ direction

\[-\frac{1}{r} \frac{\partial}{\partial \omega} \eta \psi(r, z, \Omega) = \frac{\alpha_{m+1/2}^n \psi_{n,m+1/2} - \alpha_{m-1/2}^n \psi_{n,m-1/2}}{r \ w_{n,m}} \]

\[ \psi_{n,m} = \tau_{n,m} \psi_{n,m+1/2} + (1 - \tau_{n,m}) \psi_{n,m-1/2} \]
Create DFEM matrices using MFEM, solve using a direct solver

- MFEM generates local matrices and vectors for a variety of operators, assembles them into global $Ax = b$ system
  - Required modification to implement the radius factor
- Arbitrary finite element order
- Create and transform meshes with curved surfaces
- Solve linear system directly with UMFPack
  (http://faculty.cse.tamu.edu/davis/suitesparse.html)
$R-Z$ uniform infinite medium

- 1$^\text{st}$-order FEM
- 2$^\text{nd}$-order curved mesh
- $\sigma_t = 1.0$, $\sigma_s = 0.3$, $S_0 = 0.7$
- $S_4$ level-symmetric angular quadrature
$R-Z$ spatial and angular MMS (Lingus/Hendry?)

$$\psi = (1 - \mu^2)(1 - \xi^2) \sin \left(\frac{\pi}{2}r\right) \cos(\pi z)$$

- 2nd-order FEM
- Orthogonal quadrilateral mesh
- $\sigma_t = 1.0$, $\sigma_s = 0.3$, $S_0 = 0.7$
- $S_4$ level-symmetric angular quadrature
- $L_2$-error: 0.132
$R-Z$ MMS with only spatial dependence

\[ \psi = \sin \left( \frac{\pi}{2} r \right) \cos(\pi z) \]

- 2\textsuperscript{nd}-order FEM
- Orthogonal quadrilateral mesh
- $\sigma_t = 1.0$, $\sigma_s = 0.3$, $S_0 = 0.7$
- $S_4$ level-symmetric angular quadrature
- $L_2$-error: $4.59\times10^{-5}$
**Introduction**

**Methods**

**Numerical Results**

**Conclusions**

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**R-Z MMS convergence study**

\[ \psi = (\sin(\pi r) + 1 - r) \sin(\pi z) \]

- Bailey et al. demonstrated 2\textsuperscript{nd}-order convergence for PWL and BLD.
- We solve using \( p = \{1, 2, 4\} \) on an orthogonal and 2\textsuperscript{nd}-order curved mesh.
- \( S_4 \) level-symmetric angular quadrature.
$R-Z$ MMS convergence study shows $p + 1$ convergence

(a) Orthogonal quadrilateral mesh.
(b) 2$^{nd}$-order curved mesh.

\begin{align*}
p = 1 & : O(N^{-2}) \\
p = 2 & : O(N^{-3}) \\
p = 4 & : O(N^{-5})
\end{align*}
Conclusions and future work

• High-order convergence is preserved in $R$-$Z$ $S_N$ transport
• Weighted diamond differencing the angular derivative cannot resolve $\mu^2$ dependency
  • Increasing angular quadrature order may better resolve linear dependency
• Curvature of the mesh does not degrade spatial convergence
• Investigate optically thick problems
  • MIP DSA for $R$-$Z$ geometry
Thank you!

Questions?