School of Nuclear Science and Engineering

COLLEGE OF ENGINEERING

High Order Finite Element S_N Transport in X-Y Geometry on Meshes with Curved Edges

M.S. Thesis Defense

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Introduction

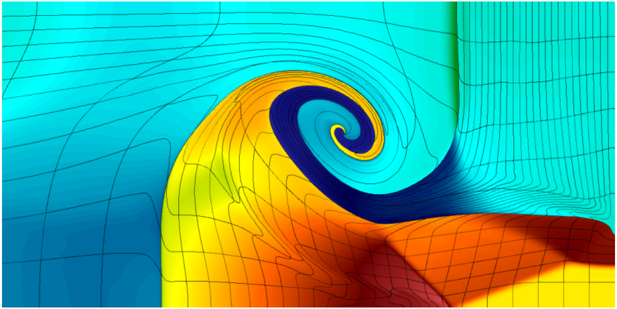
- Radiation hydrodynamics
- Past research in finite element radiation transport
- Current research objectives
- Methodology
- Test problems and results
- Conclusion
- Future work

Introduction

- Radiation hydrodynamics
  - High energy density problems - astrophysics, inertial confinement fusion
  - Fluid emits, absorbs, and scatters photons
  - Radiation field within a fluid influences the energy and momentum of the fluid
- Can be impractical to performed experimentally but experiments are performed

  `https://lasers.llnl.gov/media/video-gallery/ride-the-beamline`
- High energy density physics simulation tools
  - Behavior of fluid (kinematics and thermodynamics)
  - Generation, transport, absorption of radiation

Introduction



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

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

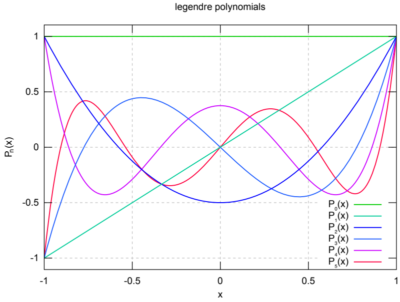
- BLAST: shock hydrodynamics code developed at LLNL
  - In particular, model National Ignition Facility (NIF) shots
- High order finite elements
- Unstructured meshes with curved edges/surfaces
- No radiation transport implementation

Introduction

- Transport community studying/using finite element method for radiation transport for several decades
  - Previously, other spatial discretization methods were employed (e.g. finite difference)
- Three applicable areas of development: finite element order, diffusion limit, and meshes

Introduction

- High-order finite elements
  - Early (and continual) development in low order methods (LD, BLD, PWLD)
  - Obtain accuracy by increasing order instead of refining the mesh
  - Higher order is more computationally expensive; it has begun to be researched with the development of advanced computers



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Introduction

- Research in the thick diffusion limit in the last several decades
  - Asymptotic analysis
  - Developed criteria to evaluate performance of a method[1]
- Research of various spatial grids in Cartesian geometry
  - Quadrilateral and triangular in 2-D, Tetrahedral in 3-D
  - Structured/unstructured meshes
  - Several papers acknowledge meshes with curved edges/surfaces but do not perform studies
  - It is common to study straight mesh edges, or approximate edges with an average outward normal direction

[1] Marvin L. Adams. Discontinuous finite element transport solutions in thick diffusive problems. *Nuclear Science and Engineering*, (137):298-333, 2001.

Research Objectives

- Develop radiation transport solver to eventually integrate with BLAST
  - High order finite elements
  - Meshes with curved edges
  - Use Modular Finite Element Methods (MFEM) to set up system of equations
    - General finite element library developed at LLNL
- Characterize the spatial discretization of the solver with a suite of test problems
  - Analytic uniform infinite medium problem
  - Multi-material problem
  - Convergence study on mesh refinement and finite element order
  - Homogeneous diffusion limit problems
  - Diffusion limit boundary layer problem
  - Multi-region problem with varying optical thicknesses

Transport Discretization

- Transport equation has seven variables
  - Cannot solve analytically
  - Make assumptions - discretize
- Assume steady-state and mono-energetic
- Currently not investigating the effects of quadrature discretization
- Using level-symmetric angular quadrature
- Load pre-generated quadrature set at run time

Finite Element Discretization

- Multiply transport equation by weight function and integrate over cell k

$$\int_{\mathbb{V}} w_{ki} \boldsymbol{\Omega} \cdot \nabla \psi\left(\boldsymbol{x}, \boldsymbol{\Omega}\right) + \int_{\mathbb{V}} w_{ki} \sigma \psi\left(\boldsymbol{x}, \boldsymbol{\Omega}\right) = \frac{1}{4\pi} \int_{\mathbb{V}} w_{ki} \sigma_s \phi\left(\boldsymbol{x}\right) + \frac{1}{4\pi} \int_{\mathbb{V}} w_{ki} S_0$$

- Approximate flux in terms of high-order polynomial basis functions for all J_k basis and weight functions

$$\psi\left(\boldsymbol{x}, \boldsymbol{\Omega}\right) \approx \sum_{j=1}^{J_k} \psi_{kj}\left(\boldsymbol{\Omega}\right) b_{kj}\left(\boldsymbol{x}\right)$$

- This results in a system of equations to solve for the angular flux at every support point in the mesh
- System of equations solved using UMFPack (i.e. LU decomposition)

Solution Methods

- Two methods to solve for scalar flux:

1. Source iteration
   - Can solve for each angular flux for each angle in parallel
   - Sum weighted angular fluxes
   - Converge on scalar flux

$$\boldsymbol{\Omega} \cdot \nabla \psi_m^{(l+1)} + \sigma \psi_m^{(l+1)} = \frac{1}{4\pi} \sigma_s \phi^{(l)} + \frac{1}{4\pi} S_0$$

$$\phi^{(l+1)} = \sum_{m=1}^{M} \Delta_m \psi_m^{(l+1)}$$

$$||\phi^{(l+1)} - \phi^{(l)}||_\infty < \epsilon_{\text{conv}}$$

2. Directly solving for angular flux in all directions
   - Discussed later

Test Problem 1: Uniform Infinite Medium with Scattering

- Steady-state, mono-energetic transport equation

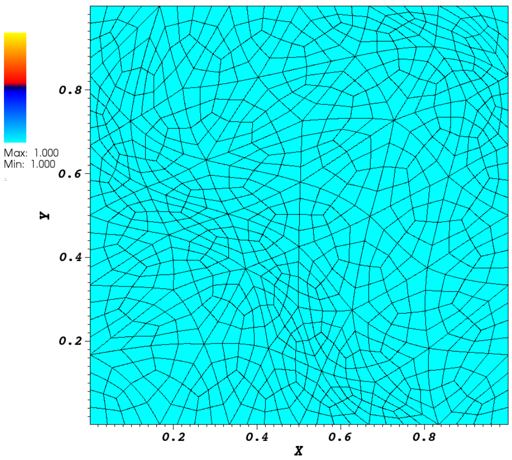
$$\boldsymbol{\Omega} \cdot \nabla\psi\left(\boldsymbol{x}, \boldsymbol{\Omega}\right) + \sigma\psi\left(\boldsymbol{x}, \boldsymbol{\Omega}\right) = \frac{1}{4\pi}\int_{4\pi}\sigma_s\psi\left(\boldsymbol{x}, \boldsymbol{\Omega'}\right)d\Omega' + \frac{1}{4\pi}S_0$$

- Analytical solution is not spatially dependent

$$\begin{aligned} \sigma\psi &= \frac{1}{4\pi}\sigma_s\phi + \frac{1}{4\pi}S_0 \\ \sigma\phi &= \sigma_s\phi + S_0 \\ \phi &= \frac{S_0}{\sigma_a} \end{aligned}$$

- Tests spatial discretization, quadrature, boundary conditions, and source iteration implementation

Test Problem 1: Uniform Infinite Medium with Scattering

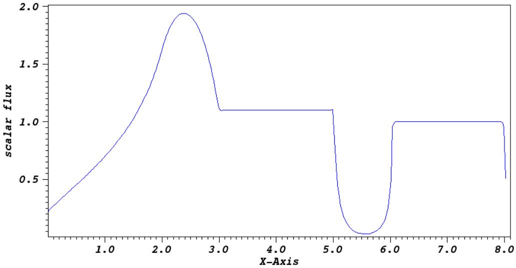


- $\sigma = 1\ \text{cm}^{-1}$
- $\sigma_s = 0.3\ \text{cm}^{-1}$
- $S_0 = 0.7\ \text{cm}^{-2}\ \text{s}^{-1}$
- $\psi_{inc} = \frac{S_0}{4\pi\sigma_a}$
- S_8 level-symmetric quadrature
- 8th order finite elements
- 8th order mesh edges
- 71,928 unknowns
- 888 zones

Test Problem 2: Reed-Hill Problem

Reed-Hill problem description

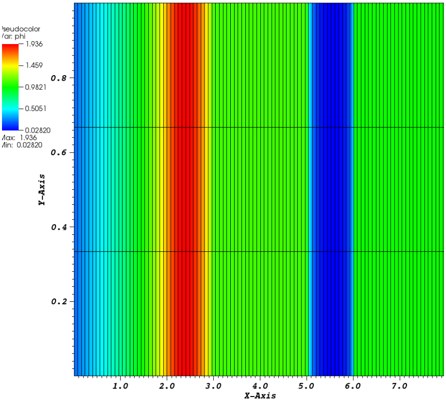
	$x \in (0, 2)$	$x \in (2, 3)$	$x \in (3, 5)$	$x \in (5, 6)$	$x \in (6, 8)$
S_0	0	1.0	0	0	50
σ	1.0	1.0	0	5.0	50
σ_s	0	0.9	0	0	0
σ_a	1.0	0.1	0	5.0	50



Reed-Hill DGFEM solution

- Multiregion 1-D problem
  - Scattering ratio of 0.9 region
  - Void region
  - Strong absorption region
  - Strong absorption and source region
- Sharp flux changes between regions
- Vacuum boundary on left
- Reflecting boundary on right

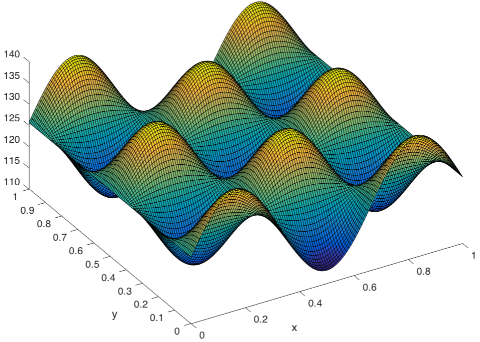
Test Problem 2: Reed-Hill Problem



Reed-Hill DGFEM solution on 2-D mesh

- Periodic boundaries on top and bottom
- S_8 level-symmetric quadrature
- 8th order finite elements
- 100 spatial cells across
- Reference solution: 1-D step differencing on 16,000 spatial cells
- Relative L_2 error is 0.04167
- Error may be reduced by ignoring the “tail”

Test Problem 3: Convergence Study

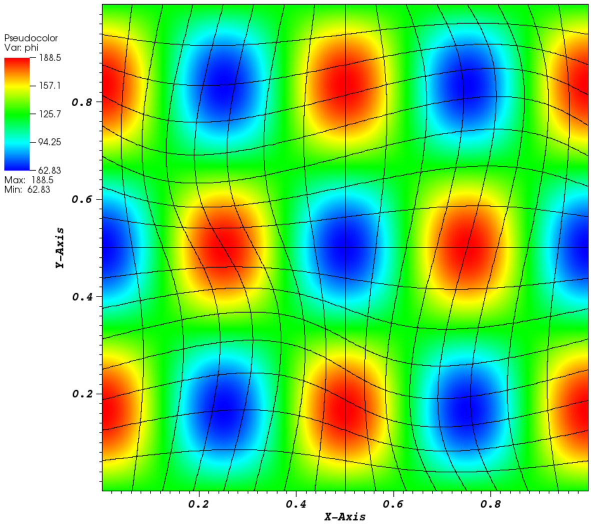


- Converge to reference solution by refining mesh and/or increasing finite element order
- Method of manufactured solutions
- Cannot be modeled exactly with polynomials

$$\psi\left(x, y, \mu, \eta\right) = a + b\mu + c\eta + d\cos\left(4\pi x\right)\sin\left(3\pi y\right)$$

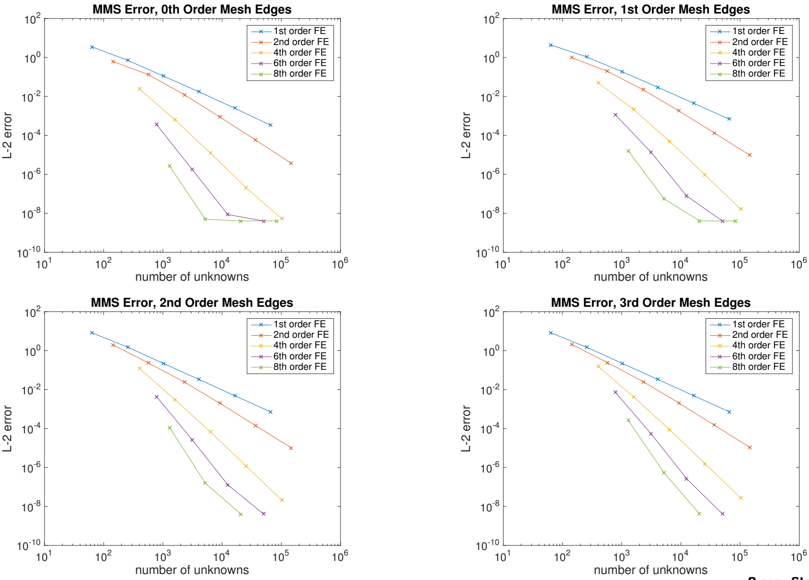
$$a = 10, \quad b = 1, \quad c = 5, \quad d = 1$$

Test Problem 3: Convergence Study



- 3rd order mesh DGFEM solution (typical)
- 0th-, 1st-, 2nd-, and 3rd-order mesh edges
- Varying number of mesh cells and finite element order

Test Problem 3: Convergence Study



Test Problem 3: Convergence Study

- Minimum achievable error on the order of 10^{-9} due to a precision limitation currently under investigation
- Convergence rates determined from the slopes of the error plots
  - Data points judged to be smaller than this maximum achievable accuracy were omitted from this calculation

		mesh edge order			
		0	1	2	3
element order	1	1.340	1.279	1.355	1.353
	2	1.770	1.692	1.763	1.765
	4	2.818	2.709	2.817	2.812
	6	3.836	3.462	3.759	3.688
	8	-	4.067	4.745	4.465

Table of convergence rates

Diffusion Limit

- Arises in radiation transport problems
- Transport equation is useful for cells of few mean free paths thick
- Diffusion limit problems are highly scattering
  - Mesh cells are many mean free paths thick
- Diffusion equation cannot model large changes in materials, strong absorbers, or voids
- Computational limitation on refining mesh
- Transport equation is accurate but converges slowly

Scaled Transport Equation

- Steady-state diffusion equation with scaling factor

$$-\nabla \frac{\epsilon}{3\sigma} \cdot \nabla \phi + \epsilon \sigma_a \phi = \epsilon S_0$$

- Scaled physics parameters

$$\sigma \rightarrow \frac{1}{\epsilon}\sigma \qquad \sigma_a \rightarrow \epsilon \sigma_a \qquad S_0 \rightarrow \epsilon S_0$$

- The equivalently scaled transport equation becomes

$$\boldsymbol{\Omega} \cdot \nabla \psi + \frac{\sigma}{\epsilon}\psi = \frac{1}{4\pi}\left(\frac{\sigma}{\epsilon} - \epsilon \sigma_a\right)\phi + \frac{1}{4\pi}\epsilon S_0$$

- As $\epsilon \rightarrow 0$, the transport equation solution converges to the diffusion equation solution

Scaled Transport Equation

- Highly scattering problems converge slowly
- Modified convergence criteria protects against false convergence

$$||\phi^{(l+1)} - \phi^{(l)}||_\infty < \epsilon_{\text{conv}} \left(1 - \rho\right) ||\phi^{l+1}||_\infty$$

- Spectral radius is a measure of the convergence rate

$$\rho \approx \frac{||\phi^{(l+1)} - \phi^{(l)}||_\infty}{||\phi^{(l)} - \phi^{(l-1)}||_\infty}$$

Test Problem 4: 1-D Diffusion Problem

- This problem is defined by

$$\sigma = \frac{1}{\epsilon}, \qquad \sigma_a = \epsilon, \qquad S_0 = \epsilon, \qquad \phi(0) = \phi(1) = 0$$

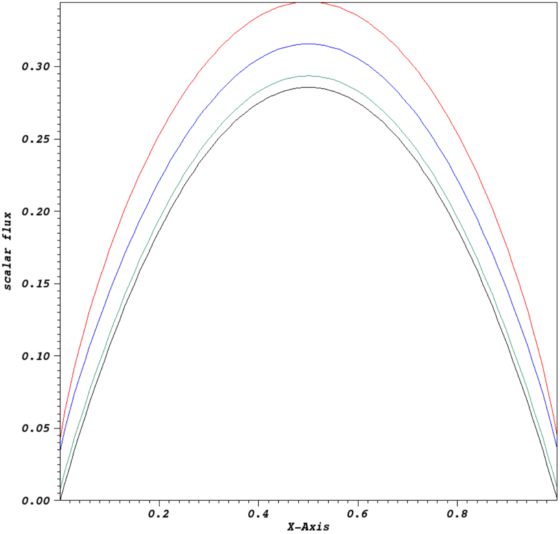
- Analytical diffusion equation solution where $L^2 = D/\sigma_a$,

$$\phi(x) = \frac{S_0}{\sigma_a}\left[\left(\frac{e^{-1/L}-1}{e^{1/L}-e^{-1/L}}\right)e^{x/L} - \left(\frac{e^{-1/L}-1}{e^{1/L}-e^{-1/L}}+1\right)e^{-x/L}+1\right]$$

- The steady-state transport equation for this problem becomes

$$\mathbf{\Omega}\cdot\nabla\psi + \frac{1}{\epsilon}\psi = \frac{1}{4\pi}\left(\frac{1}{\epsilon}-\epsilon\right)\phi + \frac{1}{4\pi}\epsilon$$

Test Problem 4: 1-D Diffusion Problem



- DGFEM solutions; $\epsilon = 0.1$ (red), $\epsilon = 0.05$ (blue), $\epsilon = 0.01$ (green), and analytical diffusion equation solution (black).

Test Problem 4: 1-D Diffusion Problem

ϵ	scattering ratio $c = 1 - \epsilon^2$	spectral radius	L_2 error
0.1	0.9900	0.96	0.066
0.05	0.9975	0.99	0.034
0.01	0.9999	0.9996	0.0069

- 1-D problem modeled on 2-D periodic mesh
- S_8 level-symmetric quadrature, 8th order finite elements, 0th order orthogonal mesh edges
- As $\epsilon \rightarrow 0$, the transport solution trends toward the exact diffusion solution
- This does not confirm achievement of the diffusion limit
  - Need to solve for $\epsilon \rightarrow 10^{-6}$
  - Requires source iteration acceleration

Test Problem 5: 2-D Diffusion Problem

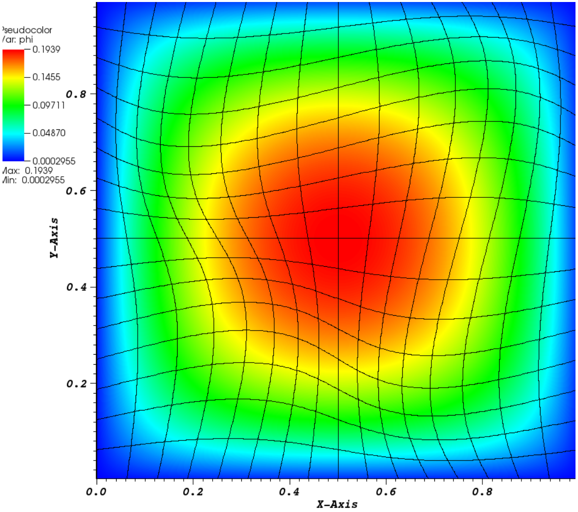
- This problem is defined on $x, y \in (0, 1)$

$$\sigma = \frac{1}{\epsilon}, \qquad \sigma_a = \epsilon, \qquad S_0 = \epsilon, \qquad \phi(0) = \phi(1) = 0$$

- Reference solution from FEM diffusion equation solve on the same mesh with the same order of finite elements
- The steady-state transport equation for this problem becomes

$$\mathbf{\Omega} \cdot \nabla \psi + \frac{1}{\epsilon}\psi = \frac{1}{4\pi}\left(\frac{1}{\epsilon} - \epsilon\right)\phi + \frac{1}{4\pi}\epsilon$$

Test Problem 5: 2-D Diffusion Problem



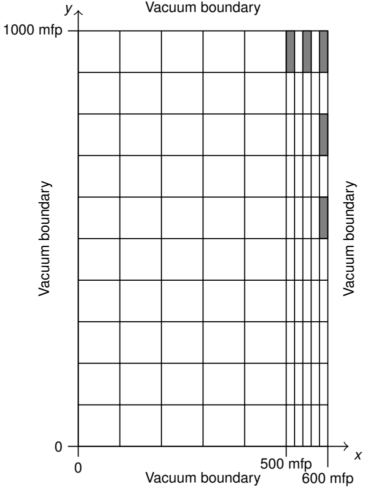
- DGFEM solution to 2-D diffusion problem for $\epsilon = 0.01$.
- S_8 level-symmetric quadrature
- 8th order finite elements
- 8th order curved mesh edges

Test Problem 5: 2-D Diffusion Problem

ϵ	scattering ratio $c = 1 - \epsilon^2$	spectral radius	L_2 norm
0.1	0.99	0.94	0.684
0.05	0.9975	0.98	0.346
0.01	0.9999	0.999	0.0663

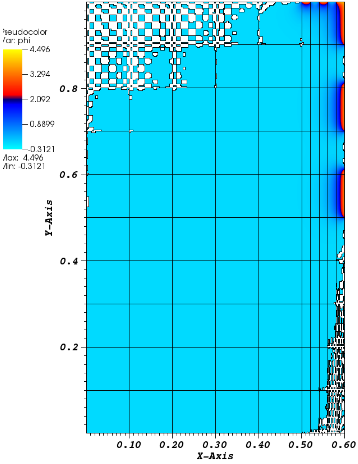
- 20,736 unknowns, 256 zones
- As $\epsilon \to 0$, the transport solution trends toward the diffusion solution
- This does not confirm achievement of the diffusion limit
  - Need to solve for $\epsilon \to 10^{-6}$
  - Requires source iteration acceleration

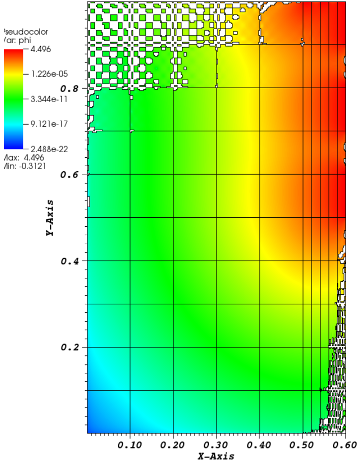
Test Problem 6: Optically Thick Boundary Layer



- Homogeneous, optically thick ($c = 0.999$)
- Gray cells indicate boundaries with incident flux, rest are vacuum
- Designed to illuminate boundary layers on the interior solution and exercise the code
- No matrix lumping implemented

Test Problem 6: Optically Thick Boundary Layer





- scalar flux; white space indicates negative flux
- log of scalar flux; white space indicates negative flux

Test Problem 6: Optically Thick Boundary Layer

- Oscillations near zero result in negative fluxes
- Negative fluxes between incident flux locations
- Oscillations expected to be damped using lumped methods[2] [3]
- Polynomials smoothly model exponential function over 22 orders of magnitude
- S_4 level-symmetric quadrature
- 8th order finite elements

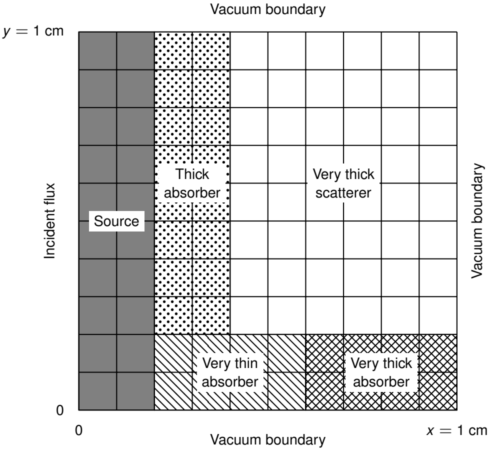
[2]Marvin L. Adams. Discontinuous finite-element transport solutions in the thick diffusion limit in Cartesian geometry. The American Nuclear Society International Topical Meeting, 1991

[3]Todd S. Palmer. Curvilinear Geometry Transport Discretization in Thick Diffusive Regions. PhD thesis, University of Michigan, 1993

Test Problem 7: Optically Thick Multi-region

Material Region	σ cm^{-1}	σ_s cm^{-1}
Source	1.0	1.0
Very thin absorber	0.0001	0.0
Thick absorber	10.0	0.0
Very thick absorber	100.0	0.0
Very thick scatterer	1000.0	1000.0

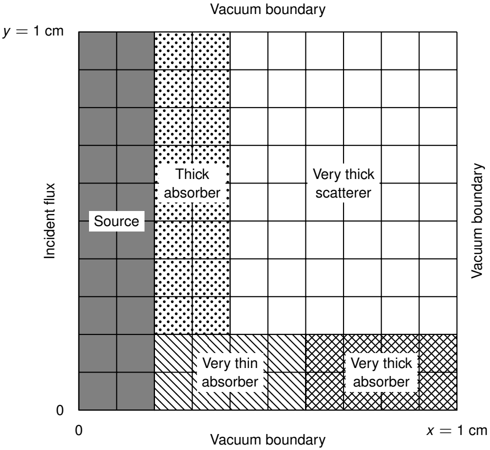
- Incident flux and source on the left drive the problem
- Vacuum on remaining sides
- Designed to test optical thicknesses ranging several orders of magnitude simultaneously



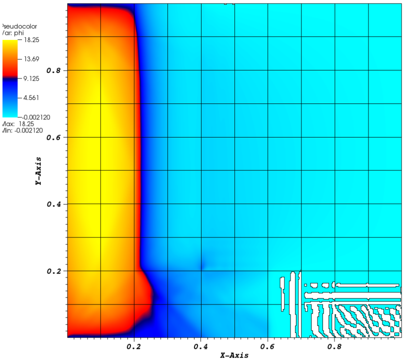
Test Problem 7: Optically Thick Multi-region

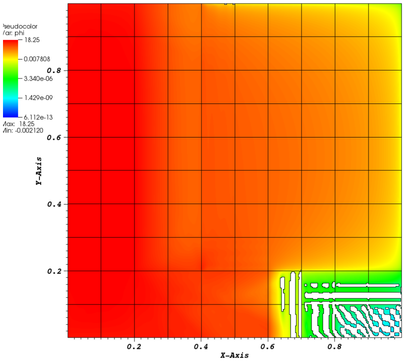
Material Region	σ cm^{-1}	σ_s cm^{-1}
Source	1.0	1.0
Very thin absorber	0.0001	0.0
Thick absorber	10.0	0.0
Very thick absorber	100.0	0.0
Very thick scatterer	1000.0	1000.0

- Also designed to force anisotropic fluxes incident into the scattering region
- Test the boundary condition of the interior solution



Test Problem 7: Optically Thick Multi-region





- scalar flux; white space indicates negative flux
- log of scalar flux; white space indicates negative flux

Test Problem 7: Optically Thick Multi-region

- Oscillations near zero result in negative fluxes
- Oscillations expected to be damped using lumped methods[4]
- Polynomials smoothly model exponential function over 14 orders of magnitude
- No issues with the negative flux due to anisotropic incident flux
  - Perhaps the source is too strong
- S_4 level-symmetric quadrature
- 8th order finite elements
- No lumping technique implemented

[4] Todd S. Palmer. Curvilinear Geometry Transport Discretization in Thick Diffusive Regions. PhD thesis, University of Michigan, 1993

Solution Methods

- Two methods to solve for scalar flux:
  1. Source iteration
  2. Directly solving for angular flux in all directions
     - Expand scalar flux in terms of weights and angular fluxes

$$\mathbf{\Omega} \cdot \mathbf{\nabla} \psi_m + \sigma \psi_m = \frac{1}{4\pi} \sigma_s \left(\Delta_1 \psi_1 + \cdots + \Delta_m \psi_m + \cdots + \Delta_M \psi_M \right) + \frac{1}{4\pi} S_0$$

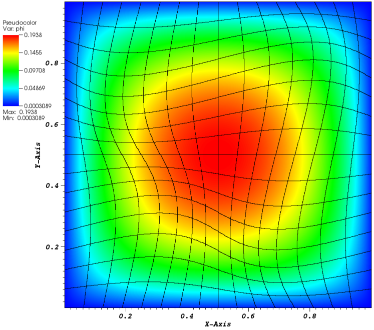
     - Large matrix to solve for all angular fluxes simultaneously

$$\left[\left(feOrder + 1 \right)^2 \times numCells \times \left(numAngles \right)^2 \right]$$

     - Sum weighted angular fluxes

$$\phi = \sum_{m=1}^{M} \Delta_m \psi_m$$

Test Problem 8: Direct Solve



2-D diffusion problem solved with direct solve method.

- $\epsilon = 0.01$; $c = 0.9999$
- S_4 angular quadrature
- 4th order finite elements, 2nd order mesh
- 1600 unknowns in 64 zones
- 1920 by 1920 matrix
- This may be the practical limit of unknowns
- Begins to fail for $\epsilon < 0.001$; matrix is ill-conditioned

Conclusions

- Developed a transport solver
  - Using MFEM
  - High order finite elements
  - Meshes with curved edges
  - X-Y geometry
- Characterized on various test problems
  - Uniform infinite medium problem with analytical solution was modeled well, indicating preliminary success in the implementation of the finite element method, angular quadrature, incident boundary conditions, and source iteration method
  - Reed-Hill problem exposed the need for reflecting boundary conditions
  - Convergence study smoothly modeled a sine/cosine function; revealed error reduction by increasing the number of unknowns; illuminated a precision limitation within MFEM

Conclusions

- Characterized on various test problems (continued)
  - 1- and 2-D diffusion limit problems were modeled smoothly trending toward the diffusion solution; demonstrates the need for source iteration acceleration
  - Boundary layer problem exponential solution was smoothly modeled with polynomials; transport solution has nonphysical negative fluxes; lumping may help at the cost of accuracy
  - Multi-region problem was smoothly modeled; negative fluxes in optically thick regions; lumping may fix negative fluxes at the cost of accuracy and potentially introducing errors in optically thin regions
  - Direct solve method solves the 2-D diffusion limit problem much faster than the source iteration; size of the problem is very limited; large operator matrix is ill-conditioned

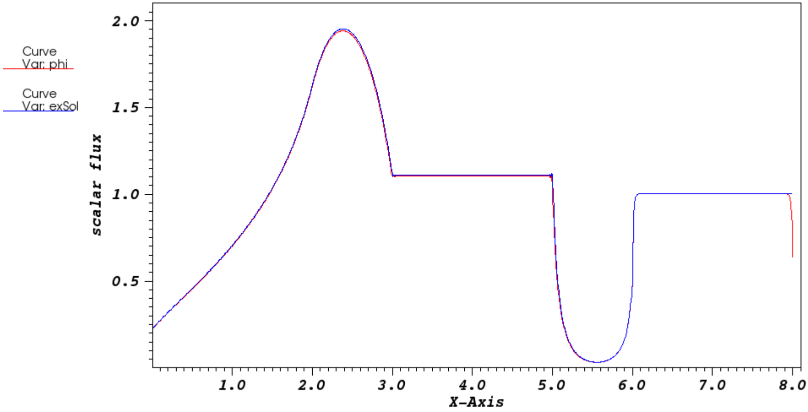
Future Work

- Implement synthetic acceleration
- Reflecting mesh boundaries
- More rigorous MMS convergence study
- Investigate MFEM precision limitation
- Perform asymptotic analysis
- Investigate usage of various lumping techniques
- Correct the direct solve method

Questions?

Thank you...
Dr. Todd Palmer, OSU
Dr. Tom Brunner, LLNL
Dr. Teresa Bailey, LLNL
BLAST Team, LLNL
MFEM Team, LLNL

1-D Adams Problem Solution



Convergence Study - 0th order mesh

		finite element order				
		1	2	4	6	8
number of mesh cells	16	3.4800	0.61775	0.024481	3.5636E-4	2.6695E-6
	64	0.70630	0.13003	6.3048E-4	1.7471E-6	5.0385E-9
	256	0.11068	0.012167	1.2076E-5	8.6389E-9	4.0750E-9
	1024	0.017186	8.6984E-4	2.0242E-7	4.0752E-9	4.0750E-9
	4096	2.4856E-3	5.7499E-5	5.2170E-9	-	-
	16,384	3.3718E-4	3.7238E-6	-	-	-

Table: L^2 norm for given order of finite elements and mesh cells for 0^{th}-order orthogonal edges.

Convergence Study - 1st order mesh

		finite element order				
		1	2	4	6	8
number of mesh cells	16	4.3779	0.97822	0.049514	1.1404E-3	1.5779E-5
	64	1.0636	0.19437	2.1084E-3	1.3649E-5	5.6172E-8
	256	0.18427	0.021919	5.0502E-5	7.7349E-8	4.0757E-9
	1024	0.02944	1.8227E-3	9.3964E-7	4.0887E-9	4.0750E-9
	4096	4.4956E-3	1.3200E-4	1.6471E-8	-	-
	16,384	6.8033E-4	9.4817E-6	-	-	-

Table: L^2 norm for given order of finite elements and mesh cells with 1^{st} order curvilinear edges.

Convergence Study - 2nd order mesh

		finite element order				
		1	2	4	6	8
number of mesh cells	16	8.1134	1.9689	0.12230	4.2791E-3	1.1468E-4
	64	1.4893	0.22841	3.0402E-3	2.6284E-5	1.5944E-7
	256	0.21937	0.024236	6.5709E-5	1.2746E-7	4.0793E-9
	1024	0.032682	1.9632E-3	1.1772E-6	4.1112E-9	-
	4096	4.8375E-3	1.4116E-4	2.0566E-8	-	-
	16,384	7.2294E-4	1.0184E-5	-	-	-

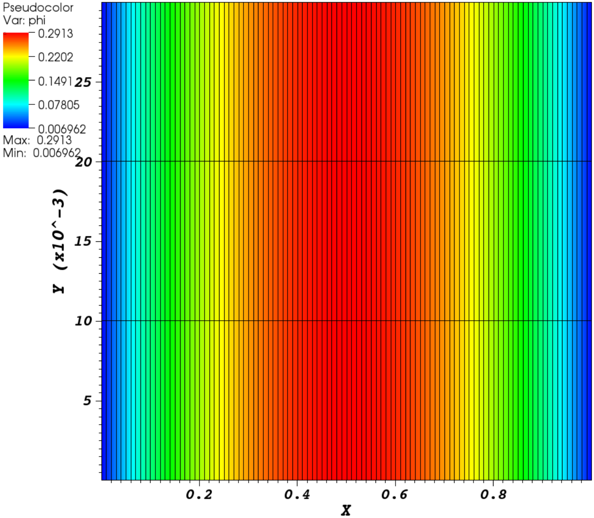
Table: L^2 norm for given order of finite elements and mesh cells with 2^{nd}-order curvilinear edges.

Convergence Study - 3rd order mesh

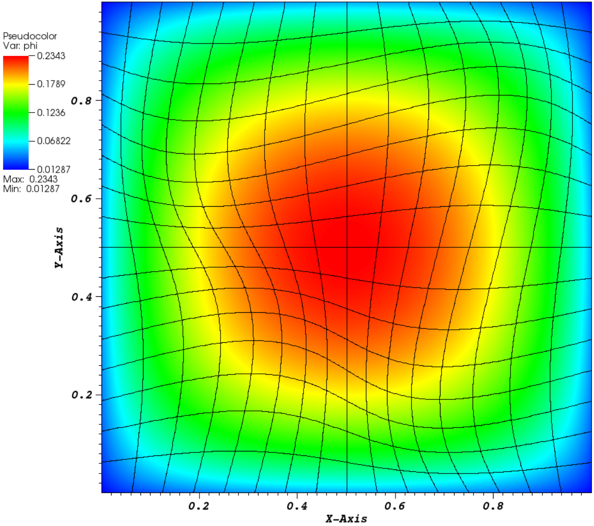
		finite element order				
		1	2	4	6	8
number of mesh cells	16	8.1099	2.0451	0.15364	7.2457E-3	2.6153E-4
	64	1.4891	0.24304	4.1710E-3	5.3909E-5	5.3647E-7
	256	0.22057	0.025530	8.9648E-5	2.6227E-7	4.1221E-9
	1024	0.033012	2.0550E-3	1.5906E-6	4.2185E-9	-
	4096	4.8894E-3	1.4711E-4	2.6972E-8	-	-
	16,384	7.2936E-4	1.0551E-5	-	-	-

Table: L^2 norm for given order of finite elements and mesh cells with 3^{rd}-order curvlinear edges.

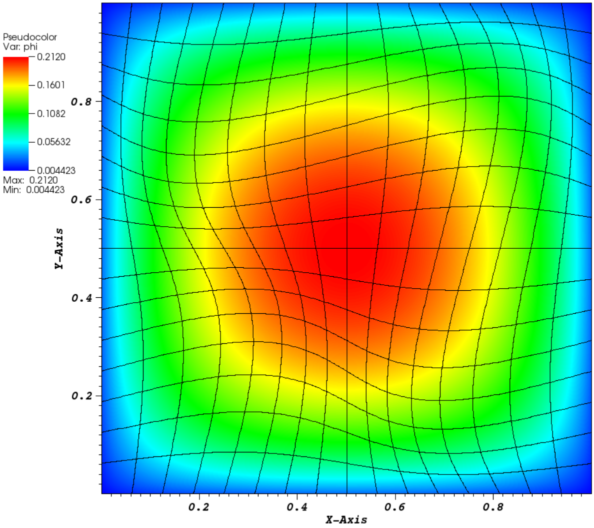
1-D Adams Problem Solution



2-D Adams Problem Solution $\epsilon = 0.1$



2-D Adams Problem Solution $\epsilon = 0.05$



Test Problem 8: Direct Solve

ϵ	scattering ratio	L^2 norm
0.1	0.99	0.04654713
0.05	0.9975	0.023714251
0.01	0.9999	0.0048038978
0.005	0.999975	0.0024034884
0.001	0.999999	0.00048896782
0.0005	0.99999975	0.00027587357
0.0001	0.99999999	0.040468175