PhD Defense
Higher Order Grey Thermal Radiative Transfer

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Outline

1. New Results
2. Contributions
3. MIP for TRT
4. Su-Olson Problem
5. MMS
6. Marshak Wave
7. Conclusions

New for Today

Results

- Su-Olson Problem
- Manufactured Solutions
- High Resolution Marshak Wave Simulations

Coding

- Arbitrary DFEM trial space degree
- Arbitrary SDIRK schemes
- MIP diffusion operator for grey radiative transfer
- Done in C++ with lots of bells and whistles

Didn't Have All That Capability at Prelim?

- Was in MATLAB, now in C++
  - About 19,000 lines of C++ (PDT+TAXI-STAPL is about 106k lines)
  - Code leverages outside packages: CMAKE, PETSc, Eigen, TinyXml
  - DARK_ARTS can be read by / used by someone other than me
  - $> 20\times$ speed-up compared to MATLAB
- Used S2SA, now use MIP
- Incorporated extensive unit testing
- Framework for multi-frequency in place

Contributions to Discrete Ordinates Transport

1. Lumping framework (prelim)
2. Spatially varying cross section treatment (prelim)
3. Application of higher order DFEM to grey TRT (new)

Lumping Framework

- Introduced quadrature based self-lumping (SL) schemes for discrete ordinates
- Improved robustness versus traditional lumping (TL)
- Considered non-equally spaced DFEM interpolation points
- Demonstrated that SL schemes increased in accuracy with increased P
- Demonstrated that *TL* were at most third order convergent in space, for all P

Spatially Varying Cross Section

- Demonstrated poor accuracy of cell-wise constant approximation
- Demonstrated non-physical interaction rate of cell-wise constant schemes
- Modified SL schemes to account for within cell cross section variation (SLXS)
- SLXS schemes retained $P+1$ L^2 convergence for pure absorber and fuel depletion problem

Grey TRT

1. Adapting MIP diffusion operator to TRT linearization
2. Numerical Results
   - Validation (Su-Olson problem)
   - Order of convergence (Method of Manufactured Solutions)
   - High resolution capability (Marshak wave problem)

Grey TRT Equations

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu_d \frac{\partial I}{\partial x} + \sigma_t I = 2\pi \int_{-1}^{1} \sigma_s(\mu' \to \mu_d) I d\mu + \sigma_a B + S_I$$

$$C_v \frac{\partial T}{\partial t} = \sigma_a \left(\phi - 4\pi B\right) + S_T$$

- $I(x, \mu_d, t)$ - intensity $\left[\frac{energy}{area - time - ster}\right]$
- $\phi(x, t)$ - angle integrated intensity $\left[\frac{energy}{area - time}\right]$
- $T(x, t)$ - temperature
- σ_a - absorption opacity $\left[length^{-1}\right]$
- σ_s - scattering opacity $\left[length^{-1}\right]$
- C_v - heat capacity $\left[\frac{energy}{volume - temperature}\right]$
- B - Planck function $\left[\frac{energy}{area - time - ster}\right]$

Solution Methodology

1. Linearize Planckian in temperature
2. Expand Planckian in P degree trial space
3. Use temperature equation to make radiation equation linear (for a given temperature iterate)
4. Ignore non-linearity of material properties
5. Assume SDIRK time integration
6. Iterate for temperature using damped Newton iteration, with time step control

Spatially Analytic Linearized TRT Radiation Equation

$$\mu_d \frac{\partial I_i}{\partial x} + \sigma_{\tau,i} = \frac{1}{4\pi}\sigma_s \phi_i + \frac{1}{4\pi}\nu_i \sigma_a \phi_i + \xi_i \tag{1}$$

$$\nu_i = \frac{4\pi a_{ii} \Delta t \sigma_a D_*}{C_v + 4\pi a_{ii} \Delta t \sigma_a D_*} \tag{2a}$$

$$\sigma_{\tau,i} = \frac{1}{a_{ii} \Delta t c} + \sigma_t \tag{2b}$$

- a_{ii} is an SDIRK constant
- D_* is Planck derivative:

$$D_* = \left.\frac{\partial B}{\partial T}\right|_{T=T_*}$$

Spatially Discretized Equations

$$\mu_d \mathbf{G} \vec{I}_i + \overline{\overline{\mathbf{R}}}_{\sigma_\tau,i} \vec{I}_i = \frac{1}{4\pi} \mathbf{R}_{\sigma_s} \vec{\phi}_i + \frac{1}{4\pi} \overline{\overline{\nu}}_i \mathbf{R}_{\sigma_a} \vec{\phi}_i + \overline{\overline{\xi}}_{d,i} + \mu_d \vec{f} I_{in,i}$$

- $\mathbf{G}$ - local gradient operator (for $\mu_d > 0$)

$$b_i(1) b_j(1) - \int_{-1}^{1} \frac{\partial b_i}{\partial s} b_j(s)\ ds\,.$$

- $\vec{f}$ - upwinding term

$$\vec{f}_i = \begin{cases} b_i(-1) & \text{for } \mu_d > 0 \\ -b_i(1) & \text{for } \mu_d < 0 \end{cases}$$

- $\mathbf{R}_{\sigma_t}$ - reaction matrix for material property f

$$\frac{\Delta x}{2} \int_{-1}^{1} \sigma_t(s) b_i(s) b_j(s)\ ds\,.$$

More Terms

$$\begin{aligned}
\overline{\overline{\nu}}_i &= 4\pi\Delta t a_{ii}\mathbf{R}_{\sigma_a}\mathbf{D}_* \left[\mathbf{I} + 4\pi\Delta t a_{ii}\mathbf{R}_{C_v}^{-1}\mathbf{R}_{\sigma_a}\mathbf{D}_*\right]^{-1}\mathbf{R}_{C_v}^{-1} \\
\overline{\overline{\mathbf{R}}}_{\sigma_\tau,i} &= \mathbf{R}_{\sigma_t} + \frac{1}{c\Delta t a_{ii}}\mathbf{M}\,,
\end{aligned}$$

- $\mathbf{I}$ - $N_P \times N_P$ identity matrix, $N_P = P + 1$
- $\mathbf{M}$ - mass matrix
- $\mathbf{D}_*$ - diagonal matrix of Planck derivatives

$$\mathbf{D}_{*,ii} = \left.\frac{dB}{dT}\right|_{T=T_{i,*}}\,.$$

MIP Diffusion Coefficient

MIP diffusion operator defined for a problem of the form:

$$\nabla \widetilde{D} \nabla \phi + \widetilde{\Sigma_a} \phi = S$$

- Need $\widetilde{D}$ point evaluations (cell edges)
- Need $\mathbf{R}_{\widetilde{\Sigma}_a}$
- Spatially discretized TRT equations only give

$$\begin{aligned} \mathbf{R}_{\widetilde{\Sigma}_t} &= \overline{\overline{\mathbf{R}}}_{\sigma_\tau,i} = \mathbf{R}_{\sigma_t} + \frac{1}{c\Delta t a_{ii}} \mathbf{M} \\ \mathbf{R}_{\widetilde{\Sigma}_s} &= \overline{\overline{\nu}}_i \mathbf{R}_{\sigma_a} + \mathbf{R}_{\sigma_s} \end{aligned}$$

If the spatially analytic linearization and spatially discretized linearization yield the same $\mathbf{R}_{\widetilde{\Sigma}_t}$ in theory we can use MIP accelerator

Equivalence for $\widetilde{\Sigma}_t$

If we establish

$$\overline{\overline{\mathbf{R}}}_{\sigma_\tau,i} = \mathbf{R}_{\sigma_\tau,i} \,,$$

we may then evaluate

$$\widetilde{D} = \frac{1}{3\widetilde{\Sigma}_t} \,.$$

at all necessary points.

By definition:

$$\mathbf{R}_{\sigma_\tau,i,jk} = \frac{\Delta x}{2} \int_{-1}^{1} b_j(s) b_k(s) \left(\sigma_t(s) + \frac{1}{c a_{ii} \Delta t} \right) \, ds$$

Equivalence for $\widetilde{\Sigma}_t$

Likewise

$$\overline{\overline{\mathbf{R}}}_{\sigma_{\tau,i}} = \frac{1}{a_{ii}c\Delta t}\mathbf{M} + \mathbf{R}_{\sigma_t}$$

$$\overline{\overline{\mathbf{R}}}_{\sigma_{\tau,i}} = \frac{1}{a_{ii}c\Delta t}\frac{\Delta x}{2}\int_{-1}^{1} b_j(s)b_k(s)\ ds + \frac{\Delta x}{2}\int_{-1}^{1}\sigma_t(s)b_j(s)b_k(s)\ ds$$

$$\overline{\overline{\mathbf{R}}}_{\sigma_{\tau,i},jk} = \frac{\Delta x}{2}\int_{-1}^{1}\left(\frac{1}{a_{ii}c\Delta t} + \sigma_t(s)\right) b_j(s)b_k(s)\ ds$$

$$\therefore \overline{\overline{\mathbf{R}}}_{\sigma_{\tau,i},jk} = \mathbf{R}_{\sigma_{\tau,i},jk}$$

This does not hold for $\widetilde{\Sigma}_a$, unless using SLXS or cell-wise constant schemes. For generality, we define:

$$\mathbf{R}_{\widetilde{\Sigma}_a} = \overline{\overline{\mathbf{R}}}_{\sigma_{\tau,i}} - \left(\mathbf{R}_{\sigma_s} + \overline{\overline{\nu}}_i\mathbf{R}_{\sigma_a}\right)$$

MIP Iterative Effectiveness

Iteration Count for Upcoming Results

Problem Description	Scheme	Average DSA+SI Iterations	Average SI Iterations
MMS Constant Time 8 cells	Cubic SLXS Lobatto	1.6	2.3
MMS1 2 cells	Quadratic SLXS Gauss	2.0	13.5
MMS2 2 cells	Linear SLXS Gauss	1.0	2.7
MMS Constant Space Alexander 3-3, $\Delta t = 1$	Quartic SLXS Lobatto	17.0	39.0
MMS Constant Space Alexander 3-3, $\Delta t = \frac{1}{128}$	Quartic SLXS Lobatto	2.3	4.9
Marshak Wave 20 cells, largest Δt	Linear SLXS Lobatto	2.1	2.9

Designed Optically Thick Problem

S_8, 50 cells, P1 SLXS Lobatto, IE SDIRK, initially cold slab with $T = 0.5$. Incident current of 100 on LHS, vacuum RHS.

$$\begin{aligned} a = \quad c &= 1 \\ C_v &= 0.05 \\ \sigma_a &= \frac{5000}{T^2} \\ \sigma_s &= 0 \\ x &\in [0, 100] \\ t &\in [0, 5] \\ \Delta t_{max} &= 0.1 \end{aligned}$$

Iterative Strategy	Average Iterations
SI+MIP	2.5
SI	4460.7

Solution Algorithm

```
while !end_of_time
{
  for stage = 1:1:n_stage
  {
    while !thermal_converged
    {
      while !intensity_converged
      {
        phi_new = calculate_new_intensity_iterate(t_star)
        change_phi = normalized_diff(phi_new, phi_old)
        intensity_converged = change_phi < epsilon_phi
      }
      [t_star, change_t] = update_temperature(t_star, phi_new)
      thermal_converged = change_t < epsilon_temperature
    }
    k_I[stage] = calculate_k_I(t_star, phi_new)
    k_T[stage] = calculate_k_T(t_star, phi_new)
  }
  advance_intensity(i_old, k_I)
  advance_temperature(t_old, k_T)
}
```

Numerical Methods

1. **TL**- traditional lumping, equally spaced DFEM interpolation points, volume average C_v and σ, for historical comparison
2. **SL Lobatto**- self-lumping, Lobatto DFEM interpolation points, volume average C_v and σ
3. **SL Gauss**- self-lumping, Gauss DFEM interpolation points, volume average C_v and σ
4. **SLXS Lobatto**- self-lumping incorporating spatial variation of material properties, Lobatto DFEM interpolation points
5. **SLXS Gauss**- self-lumping incorporating spatial variation of material properties, Gauss DFEM interpolation points

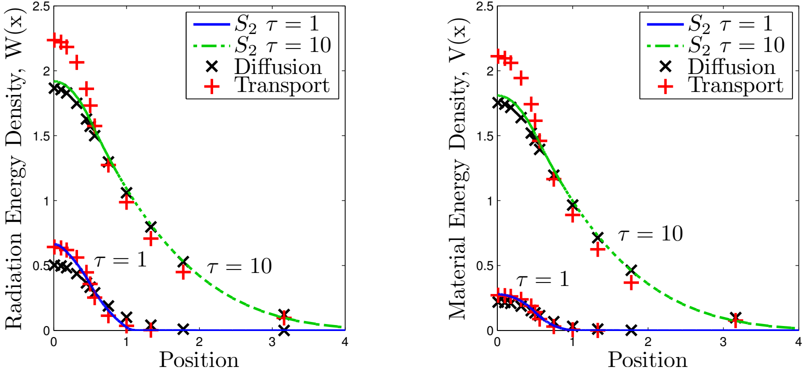
Su-Olson Description

- Initially cold (absolute zero) half space
- Volumetric source near origin for a finite period of time
- Constant opacity
- $C_v = \alpha T^3$
  - C_v assumption causes TRT equations to be linear in I and T^4/material energy density
  - Computationally challenging if not tracking material energy density(IMC)
  - We impose

$$C_v = \epsilon + \alpha T^3$$

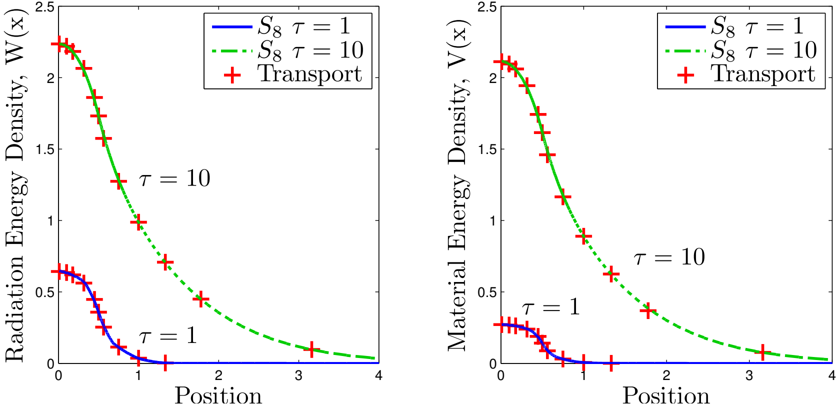
We choose $\sigma_a = 1,\ \sigma_s = 0,\ a = c = 1,\ \&\alpha = 4.$ We truncate the half-space to be $x \in [0, 10]$ and the source is located in $x \in [0, 0.5]$.

Su-Olson Results with S_2



Calculated using 200 cells, linear SLXS Lobatto, $\Delta t = 10^{-3}$

Su-Olson Results with S_8



Calculated using 200 cells, linear SLXS Lobatto, $\Delta t = 10^{-3}$

Error Measures

$$E_\phi = \sqrt{\sum_{c=1}^{N_{cell}} \frac{\Delta x}{2} \sum_{q=1}^{N_{qf}} w_q \left(\widetilde{\phi}(s_q, t_{end}) - \phi(s_q, t_{end}) \right)^2}$$

$$E_{\phi_A} = \sqrt{\sum_{c=1}^{N_{cell}} \frac{\Delta x}{2} \left(\frac{1}{2} \sum_{q=1}^{N_{qf}} w_q \widetilde{\phi}(s_q, t_{end}) - \frac{1}{2} \sum_{q=1}^{N_{qf}} w_q \phi(s_q, t_{end}) \right)^2}$$

E_T and E_{T_A} are defined analogously. $N_{qf} = 2P + 7$, Gauss quadrature

Choice of MMS

Elect to use separable solution of the form

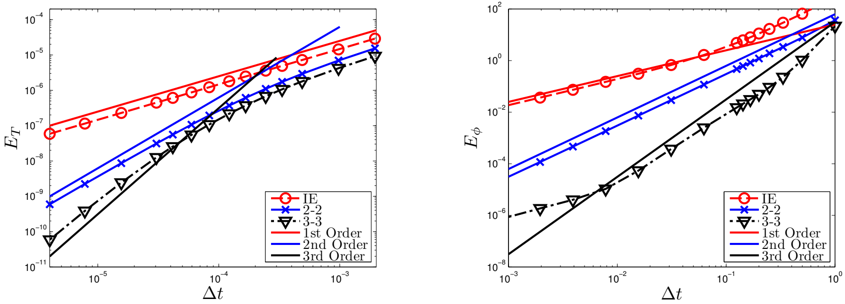
$$
\begin{aligned}
I_d(x,\mu_d,t) &= M(\mu_d)F(t)W_I(x) && (3)\\
T(x) &= F(t)W_T(x) && (4)\\
\phi(x) &= C_M F(t)W_I(x) && (5)\\
C_M &= \sum_{d=1}^{N_{dir}} w_d M(\mu_d) && (6)
\end{aligned}
$$

SDIRK Order of Convergence

$$
\begin{aligned}
M(\mu_d) &= \frac{1}{4\pi} \\
W_I(x) &= \frac{10}{4\pi} \\
W_T(x) &= 10 \\
F(t) &= 45\cos\left(\pi t\right) + 46 \\
t &\in [0, 1] \\
\sigma_s &= 0.1 \\
\sigma_a &= 2.5 \\
C_v &= 0.2 \\
x &\in [0, 10]
\end{aligned}
$$

10 equally-spaced cells, quartic SLXS Gauss

SDIRK Order of Convergence



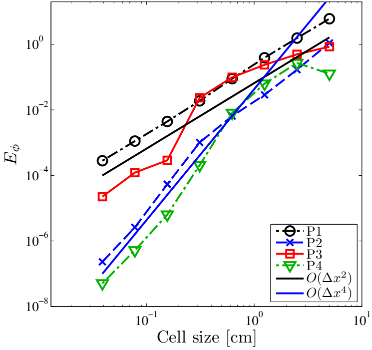
Constant Material Properties- MMS1

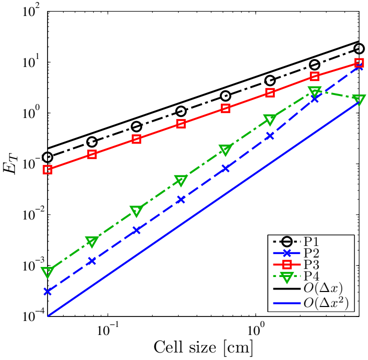
$$
\begin{aligned}
M(\mu_d) &= \frac{1}{4\pi} \\
F(t) &= 1 + .02t \\
W_I(x) &= 10\cos\left(\frac{\pi x}{10} - \frac{\pi}{2}\right) + 15 \\
W_T(x) &= 25\cos\left(\frac{\pi x}{10} - \frac{\pi}{2}\right) + 30 \\
C_v &= 0.1 \\
\sigma_a &= 100 \\
\sigma_s &= 0.5 \\
t &\in [0, 1] \\
\Delta t &= 0.01
\end{aligned}
$$

Used S_8 quadrature, 2-2 SDIRK scheme

TL- MMS1 Results

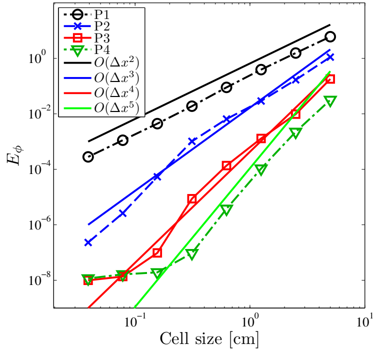
TL does not get better applied to a harder problem

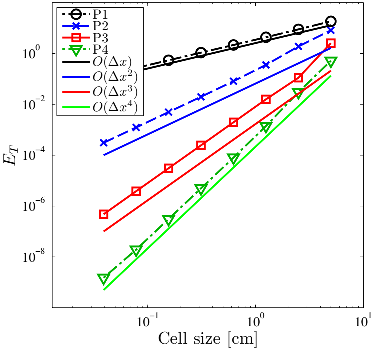




SL Lobatto- MMS1 Results

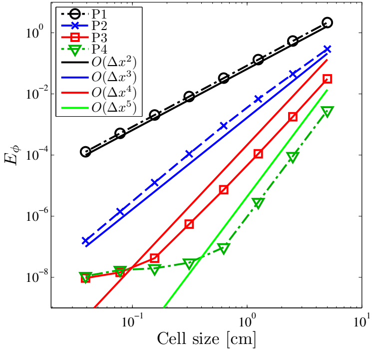
SL Lobatto loses an order in T

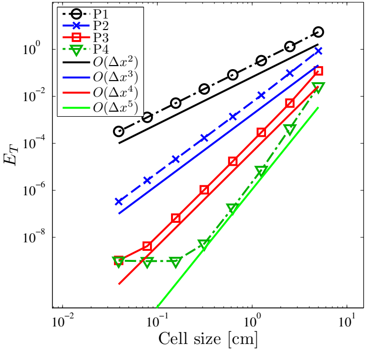




SL Gauss- MMS1 Results

SL Gauss picks up an order for T?





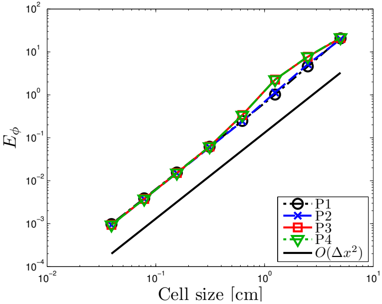
Variable Material Properties- MMS2

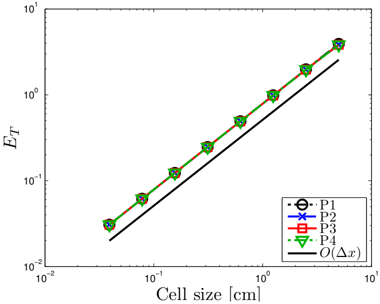
$$
\begin{aligned}
M(\mu_d) &= \frac{1}{4\pi} \\
W_I(x) &= 9\cos\left(\frac{\pi x}{10} - \frac{\pi}{2}\right) + 3 \\
W_T(x) &= 5\cos\left(\frac{\pi x}{10} - \frac{\pi}{2}\right) + 5 \\
F(t) &= 1 + .02t \\
C_v &= 0.2 + 0.01\,T^3 \\
\sigma_a &= \frac{10^4}{T^3} \\
\sigma_s &= 0.5
\end{aligned}
$$

3-3 Alexander, $\Delta t = 10^{-3}$

Must Account for Spatially Varying Material Properties

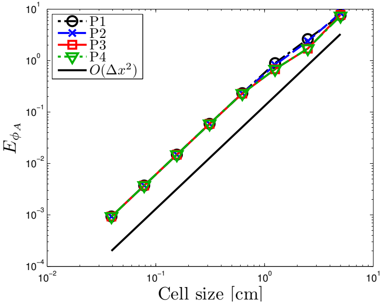
SL Gauss, $P \in [1, 4]$. Limited L^2 convergence.

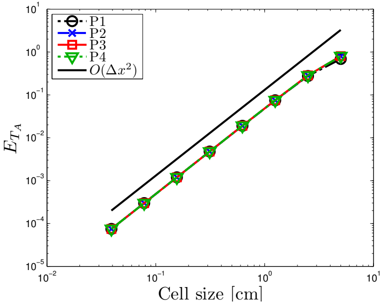




Not Lucky This Time

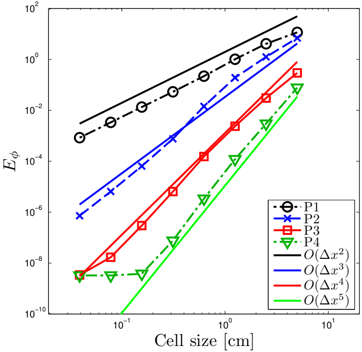
SL Gauss, $P \in [1, 4]$. High convergence of CXS DFEM for neutronics was problem specific luck/fluke





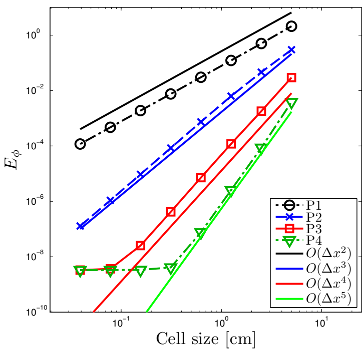
SLXS E_ϕ Convergence

SLXS Lobatto



$\propto P+1$

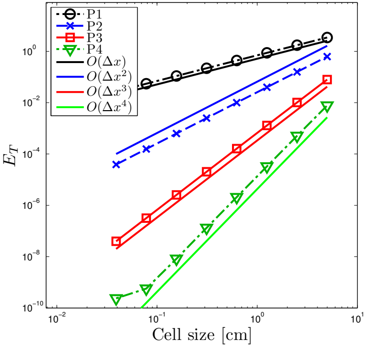
SLXS Gauss



$\propto P+1$

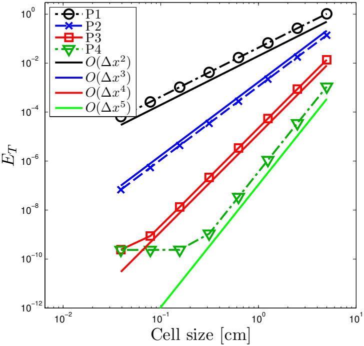
SLXS E_T Convergence

SLXS Lobatto



$\propto P$

SLXS Gauss



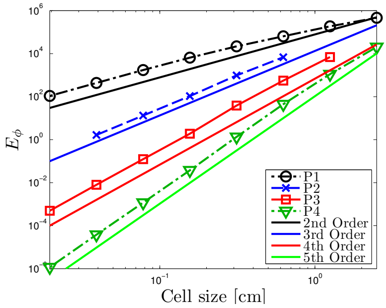
$\propto P+1$

Steady-state problem

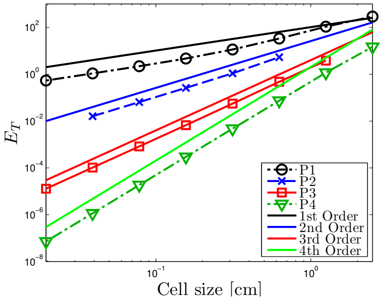
$$
\begin{aligned}
M(\mu_d) &= \frac{1}{4\pi} \\
W_I(x) &= 19\cos\left(\frac{\pi x}{2}\right) + 20\,, \\
W_T(x) &= 15\cos\left(\frac{\pi x}{2}\right) + 20\,, \\
F(t) &= 10 \\
C_v &= 0.1 + 0.2\,T^2 \\
\sigma_a &= \frac{5}{T^2} \\
\sigma_s &= 0.01
\end{aligned}
$$

SLXS Lobatto L^2 Convergence

E_ϕ



E_T



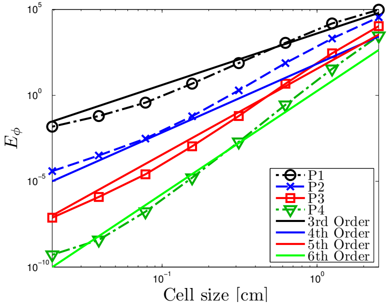
$\propto P+1$

$\propto P$

No surprises

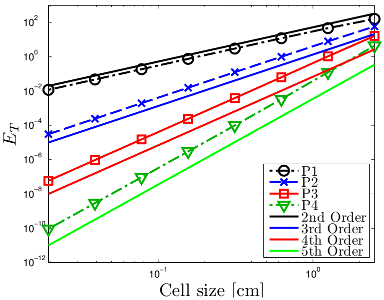
SLXS Gauss L^2 Convergence

E_ϕ



$\propto P+2$

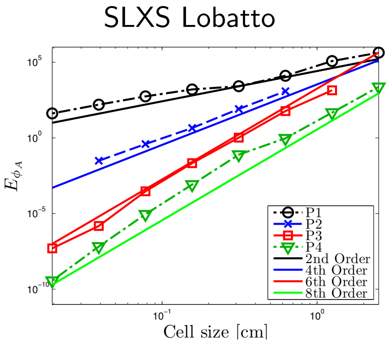
E_T

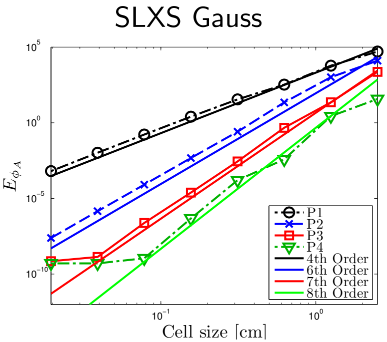


$\propto P+1$

Where did the extra order in E_ϕ come from?

E_{ϕ_A} Convergence



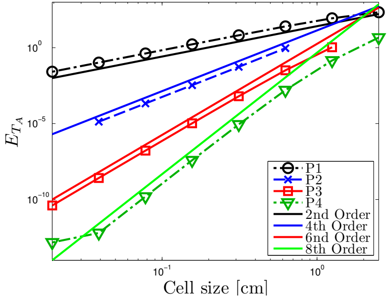


TRT $E_{\phi_A} \propto 2P$
Neutronics $E_{\psi_A} \propto 2P$

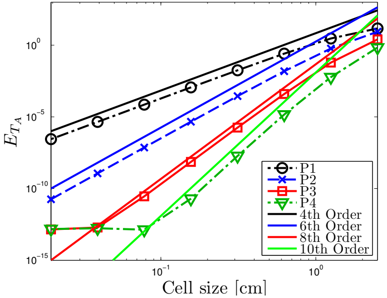
TRT $E_{\phi_A} < 2P + 2$
Neutronics $E_{\psi_A} \propto 2P + 1$

E_{T_A} Convergence

SLXS Lobatto



SLXS Gauss



TRT $E_{T_A} \propto 2P$
Neutronics $E_{\psi_A} \propto 2P$

TRT $E_{T_A} \propto 2P + 2$
Neutronics $E_{\psi_A} \propto 2P + 1$

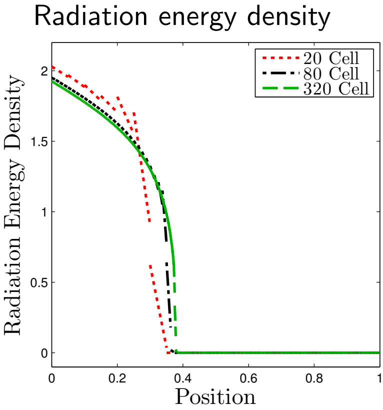
Marshak Wave Problem

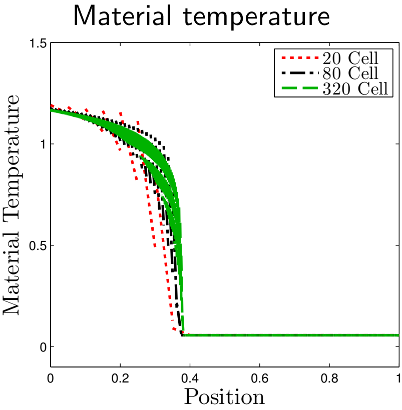
Unit current incident intensity on left face. Vacuum right boundary condition. Initially cold slab. No analytic solution.

$$
\begin{aligned}
a &= c = C_v = 1 \\
x &\in [0,1] \\
t &\in [0,1] \\
T_0^4 &= 1E-5 \\
\sigma_s &= 0 \\
\sigma_a &= \frac{1}{T^3}
\end{aligned}
$$

Blading with Cell-Wise Constant Assumption

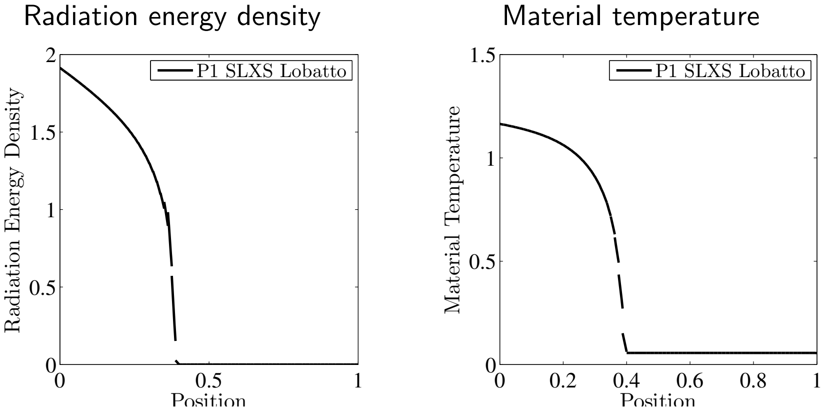
Linear TL, volumetric average opacity





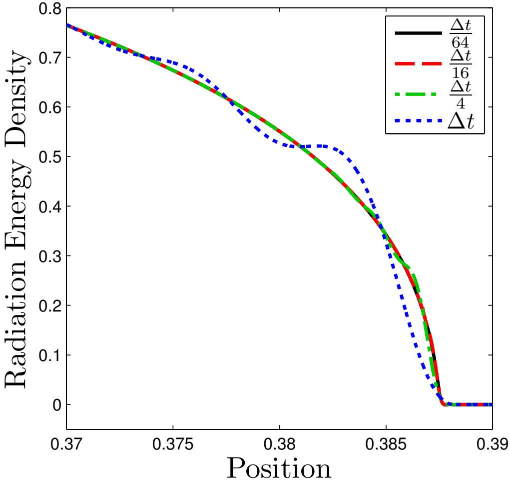
SLXS Treatment

Linear SLXS Lobatto

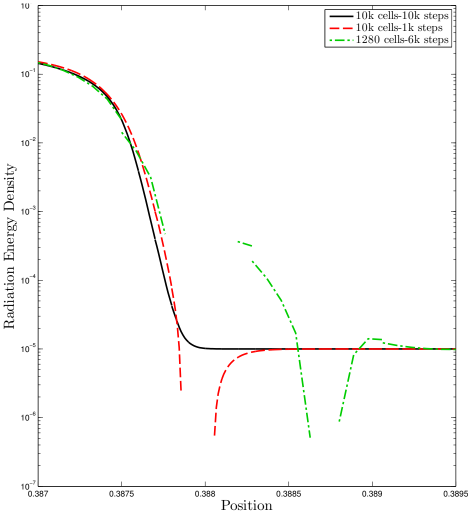


Time Resolution Cannot Be Neglected

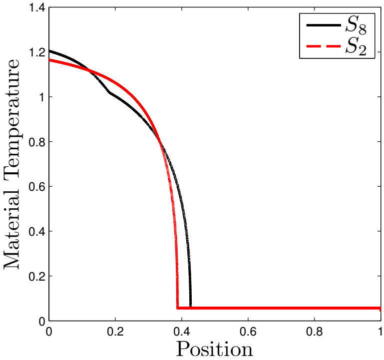
Quartic SLXS Lobatto, 1280 mesh cells, 2-2 SDIRK, $\Delta t = 0.01$

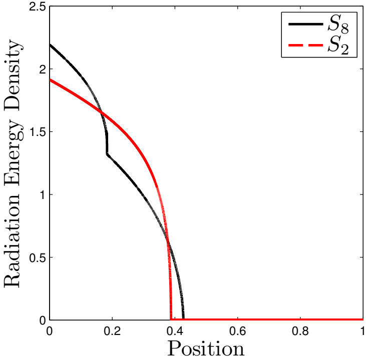


Extreme Zoom of S_2 Radiation Energy Density



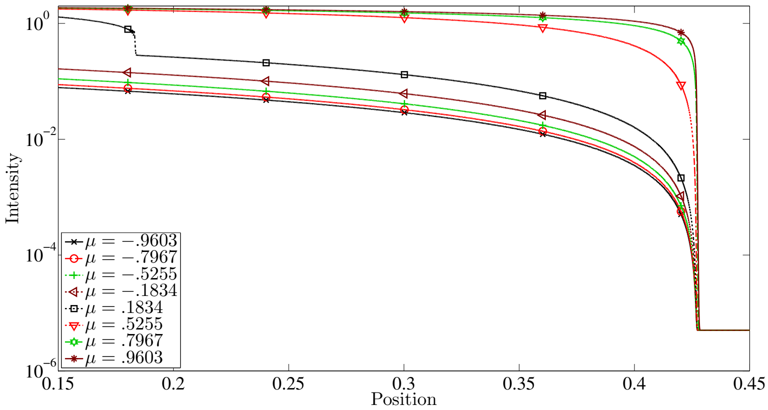
S_2 vs S_8



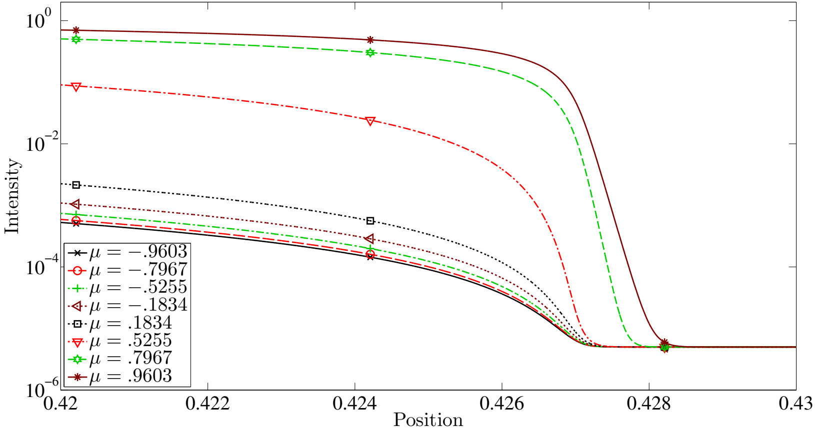


5000 mesh cells, P4 SLXS Gauss, 5k time steps, 2-2 scheme

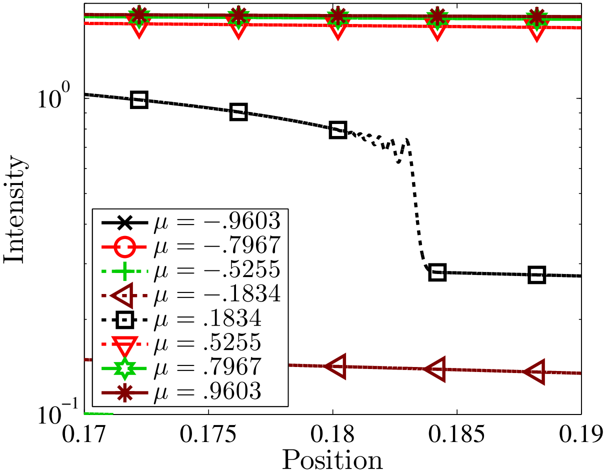
S_8 Angular Intensity



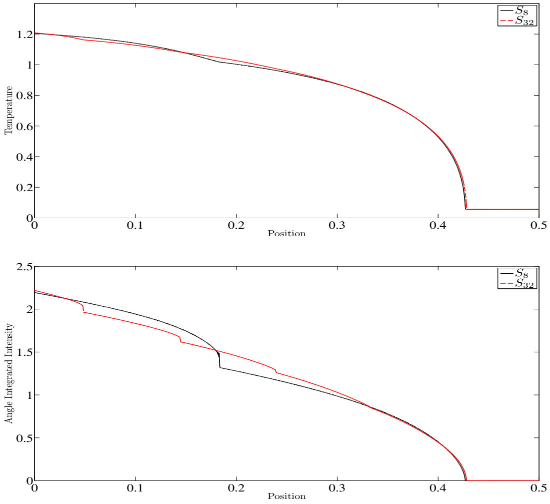
Wavefront Boundary Layers



Need More Resolution for Interior Boundary Layer

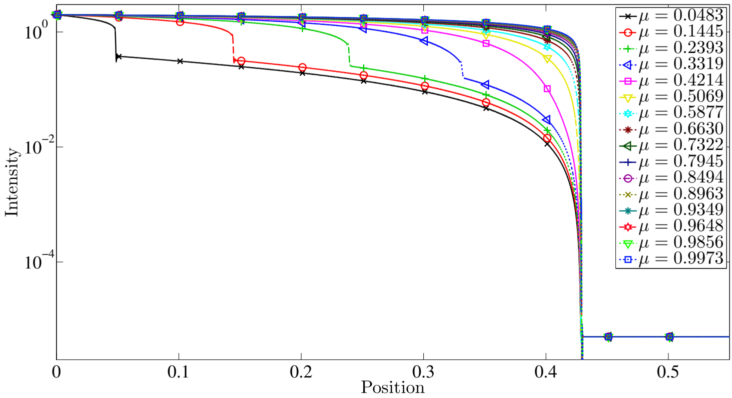


S_8 vs S_{32} Solutions



S_{32} solution- 1000 mesh cells, quartic SLXS Gauss, 5000 time steps

S_{32}, $\mu_d > 0$ intensities



Conclusions

In PhD we have

1. Developed a matrix lumping framework that is effective for arbitrary P
2. Demonstrated the need to consider spatial variation of material properties
3. Applied MIP diffusion operator to TRT acceleration

Today we have

- Applied higher order DFEM to grey TRT
- Examined the asymptotic accuracy of higher order DFEM for coupled grey TRT problems
- Generated high resolution discrete ordinates results for grey TRT problems

Potential Future Work

- Complete multi-frequency capabilities
- Diffusion limit analysis of higher order DFEM
- Extend lumping framework to multiple spatial dimensions

Acknowledgments

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