Higher Order Grey Thermal Radiative Transfer

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DOE CSGF

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Outline

1. Theory
2. TRT Equations
3. TRT Results
4. Conclusions

Dissertation Goal

High-fidelity methods for discrete ordinates (S_N) radiative transfer

Requirements to Achieve Goal

1. Accurate Spatial Discretization
   - Higher degree trial space discontinuous finite element method (DFEM) trial spaces
   - Must address robustness
2. Accurate Spatial Treatment of Opacities
   - Cell-wise constant is a poor approximation for problems of interest
3. Efficient / Effective Acceleration
   - Computationally efficient
   - Compatible with spatial discretization

Matrix Lumping

1. One of three methods to improve the DFEM "robustness"
   - Other methods: ad-hoc fix-ups, strictly non-negative solution representations
   - Robustness (for S_N): solution positivity and resistance to oscillations
2. Lumping- makes diagonal mass matrices, does not guarantee increase in robustness
3. Two ways to lump mass matrices
   - Traditional lumping (TL): Collapse an exactly integrated mass matrix's entries to the main diagonal
   - Self-lumping (SL): Use quadrature restricted to the DFEM interpolation points
4. Both methods are equivalent for linear DFEM

Self-Lumping Concept

With interpolatory basis functions, restricting quadrature to the DFEM interpolation points (s_j) creates a diagonal mass matrix (**M**) *automatically*

Self-lumping (SL) M

$$\mathbf{M}_{ij} = \begin{cases} \frac{\Delta x}{2} w_i & i = j \\ 0 & \text{otherwise} \end{cases}$$

- Typically, s_j are chosen as equally-spaced points, and **M** is integrated analytically
- No requirement that s_j be equally-spaced, could use more accurate quadrature as the interpolation points
  - E.g. Gauss-Legendre (Gauss) or Lobatto-Gauss-Legendre (Lobatto)

Numerical Schemes

New to Dissertation

- Self-lumping with higher degree trial spaces
- Non equally-spaced interpolation points

- **SL Gauss**: Gauss quadrature as interpolation points, quadrature restricted to interpolation points
- **SL Lobatto**: Lobatto quadrature as interpolation points, quadrature restricted to interpolation points
- **SL Newton-Cotes**: Equally-spaced points, quadrature (closed Newton-Cotes) restricted to interpolation points
- **TL** (Traditional Lumping): Equally-spaced points, analytic integration, then collapse to main diagonal
- **Exact DFEM**: Equally-spaced points, analytic integration

Outflow Robustness

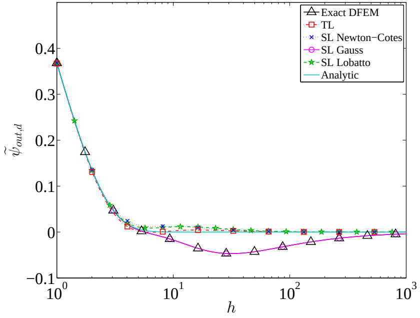


Figure: $P = 3$ Outflow as a function of h.

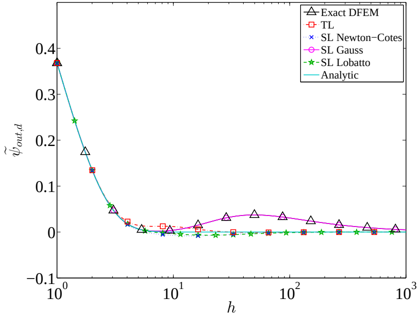


Figure: $P = 4$ Outflow as a function of h.

Motivation to Account for Cross Section Spatial Variation

- Many problems of interest to the NE community have within cell spatially varying cross section/opacity
  - Cross sections are functions of temperature, density, fuel burn-up, etc.
  - High fidelity simulations do not assume cell-wise constant values for these variables
- Neutronics examples: fuel depletion problems, coupled reactor physics...
- Radiative transfer: $\sigma = T^{-3}$

S_N Reaction Term

In DFEM spatial discretization of S_N transport and thermal radiative transfer equations, we have interactions terms like:

$$\frac{\Delta x}{2} \int_{-1}^{1} \sigma(s) b_i(s) \widetilde{\psi}(s)\ ds \tag{1}$$

Historically, for a P degree polynomial trial space representation with $N_P = P + 1$ degrees of freedom, this is approximated as

$$\bar{\sigma} \mathbf{M} \vec{\psi} \tag{2}$$

where

$$\vec{\psi} = \left[\psi_1 \dots \psi_{N_P+1}\right]^T , \quad \widetilde{\psi}(s) = \sum_{j=1}^{N_P} b_j(s) \psi_j$$

Eq. (2) exact iff $\sigma(s) = \bar{\sigma}$.

History

In neutronics:

- Some work has focused on assuming cross section is a linear function within cells
- Focus of this historical work has been on reproducing fine mesh results with coarser zoning

Radiative transfer/radiative diffusion calculations (sometimes) account for within cell variation by using vertex based quadrature integration

- Idea introduced by Adams and Nowak circa 1997
- Used by some (ex. Ober and Shadid 2004)
- Not by everyone

SL Schemes for Spatially Varying Cross Section Problems

Eq. (1) correctly represented as:

$$\mathbf{R}_\sigma \vec{\psi}$$

with

$$\mathbf{R}_{ij} = \frac{\Delta x}{2} \int_{-1}^{1} \sigma(s) b_i(s) b_j(s)\, ds$$

Self-Lumping Cross Section (SLXS) Schemes

Extension of self-lumping schemes to account for spatial variation of opacity/cross section

$$\mathbf{R}_{\sigma,ij} = \begin{cases} \frac{\Delta x}{2}\sigma(s_i) w_i & i = j \\ 0 & \text{otherwise} \end{cases}$$

- **SLXS Lobatto**- self-lumping incorporating spatial variation of material properties, Lobatto DFEM interpolation points
- **SLXS Gauss**- self-lumping incorporating spatial variation of material properties, Gauss DFEM interpolation points

Grey Thermal Radiative Transfer Equations

Grey (frequency integrated) thermal radiative transfer (TRT) equations:

$$\begin{aligned}
\frac{1}{c}\frac{\partial I}{\partial t} + \mu_d \frac{\partial I}{\partial x} + \sigma_t I &= 2\pi \int_{-1}^{1} \sigma_s(\mu' \rightarrow \mu_d) I d\mu + \sigma_a B + S_I \\
C_v \frac{\partial T}{\partial t} &= \sigma_a \left(\phi - 4\pi B\right) + S_T
\end{aligned}$$

$I(x, \mu_d, t)$- intensity $\left[\frac{energy}{area-time-ster}\right]$

$\phi(x, t)$- angle integrated intensity $\left[\frac{energy}{area-time}\right]$

$B(T) = \frac{acT^4}{4\pi}$- Planck function $\left[\frac{energy}{area-time-ster}\right]$

$C_v(x, T)$- heat capacity $\left[\frac{energy}{volume-temperature}\right]$

$T(x, t)$- temperature

$\sigma_a(x, T)$- absorption opacity $\left[length^{-1}\right]$

$\sigma_s(x, T)$- scattering opacity $\left[length^{-1}\right]$

Solution Methodology

1. Linearize Planckian in temperature

$$
\begin{aligned}
B(T) &\approx B(T_*) + \left.\frac{dB}{dT}\right|_{T=T_*} (T - T_*) \\
B_* &= B(T_*),\ D_* = \left.\frac{dB}{dT}\right|_{T=T_*} \\
B &\approx B_* + D_*(T - T_*)
\end{aligned}
$$

2. Expand Planckian in P degree trial space

$$
B(\widetilde{T}) \approx \sum_{j=1}^{N_P} B(T_j) b_j(s)
$$

3. Linearize (for given temperature iterate) radiation equation using temperature equation
4. Ignore material properties contributions to Jacobian
5. Assume SDIRK time integration
6. Newton-Picard iteration for temperature

SDIRK- S-stable Diagonally Implicit Runge-Kutta

Solves problems of the form:

$$\begin{aligned} g(t=0) &= g_0 \\ g'(t) &= f(t,g) \end{aligned}$$

With the following relations

$$g_{n+1} = g_n + \Delta t \sum_{i=1}^{N_{stage}} b_i k_i \tag{3}$$

$$k_i = f\left(t_n + c_i \Delta t \ , \ g_n + \Delta t \sum_{j=1}^{i} a_{ij} k_j \right)$$

Eq. (3) can also be interpreted as:

$$g_i = g_n + \Delta t \sum_{j=1}^{i} a_{ij} f\left(t_n + \Delta t c_j, g_j\right),$$

a_{ij}, b_i, c_i are all constants inherent to a given scheme

TRT Time Discretization

Manipulating analytic equations, k of stage s are:

$$\begin{aligned} k_{I,s} &= c\left[\frac{1}{4\pi}\sigma_s(T_s)\phi_s + \sigma_a(T_s)B(T_s) + S_I(t_s) - \mu_d\frac{\partial I_s}{\partial x} - \sigma_t(T_s)I_s\right] \\ k_{T,s} &= \frac{1}{C_v(T_s)}\left[\sigma_a(T_s)\left(\phi_s - 4\pi B(T_s)\right) + S_T(t_s)\right] \end{aligned}$$

SDIRK stage 1 intensity and temperature relations:

$$I_1 = I_n + a_{11}\Delta tc\left[\frac{1}{4\pi}\sigma_s\phi_1 + \sigma_a B + S_I - \mu_d\frac{\partial I_1}{\partial x} - \sigma_t I_1\right]$$

$$T_1 = T_n + \frac{a_{11}\Delta t}{C_v}\left[\sigma_a\left(\phi_1 - 4\pi B\right) + S_T\right]$$

Manipulate Temperature Equation

Linearize temperature equation

$$T_1 = T_n + \frac{a_{11}\Delta t}{C_v}\left[\sigma_a\left(\phi_1 - 4\pi\left(B_* + D_*\left(T_1 - T_*\right)\right)\right) + S_T\right]$$

Manipulate and arrive at

$$T_1 = T_* + \left(1 + \frac{4\pi a_{11}\Delta t}{C_v}\sigma_a D_*\right)^{-1} \dots \left(T_n - T_* + \frac{a_{11}\Delta t}{C_v}\left[\sigma_a\left(\phi_1 - 4\pi B_*\right) + S_T\right]\right) \quad (4)$$

Linearize Radiation Equation

Insert Eq. (4) into linearized stage 1 intensity equation:

$$I_1 = I_n + a_{11}\Delta tc\left[\frac{1}{4\pi}\sigma_s\phi_1 + \sigma_a\left(B_* + D_*(T_1 - T_*)\right)\right]\dots$$
$$+ a_{11}\Delta tc\left[S_I - \mu_d\frac{\partial I_1}{\partial x} - \sigma_t I_1\right].$$

Manipulate extensively to achieve

$$\mu_d\frac{\partial I_1}{\partial x} + \sigma_{\tau,1} = \frac{1}{4\pi}\sigma_s\phi_1 + \frac{1}{4\pi}\nu_1\sigma_a\phi_1 + \xi_1 \tag{5}$$

Spatially Analytic Linearized TRT Radiation Equation

$$\nu_1 = \frac{4\pi a_{ii} \Delta t \sigma_a D_*}{C_v + 4\pi a_{11} \Delta t \sigma_a D_*} \tag{6a}$$

$$\sigma_{\tau,1} = \frac{1}{a_{11} \Delta t c} + \sigma_t \tag{6b}$$

$$\xi_1 = \sigma_a B_* + S_I + \frac{1}{a_{11} \Delta t c} I_n + \dots$$
$$\sigma_a D_* \left(1 + \frac{4\pi a_{11} \Delta t}{C_v} \sigma_a D_* \right)^{-1} \left(T_n - T_* + \frac{a_{11} \Delta t}{C_v} \left(S_T - 4\pi \sigma_a B_* \right) \right) \tag{6c}$$

Multi-Stage SDIRK Requires Minor Adaptation

Only one term added to temperature equation:

$$T_i = T_n + \boxed{\Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j}} + \frac{a_{ii}\Delta t}{C_v}\left[\sigma_a\left(\phi_i - 4\pi\left[B_* + D_*(T_i - T_*)\right]\right) + S_T\right]$$

$$T_i = T_* + \left(1 + \frac{4\pi a_{ii}\Delta t}{C_v}\sigma_a D_*\right)^{-1} \left(T_n - T_* + \boxed{\Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j}} + \frac{a_{ii}\Delta t}{C_v}\left[\sigma_a\left(\phi_i - 4\pi B_*\right) + S_T\right]\right)$$

Performing the radiation equation linearization still yields:

Multi-Stage SDIRK Requires Minor Adaptation

Transport equation linearization still yields:

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

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

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

$$\xi_i = \sigma_a B_* + S_I + \frac{1}{a_{ii}\Delta t c} I_n + \boxed{\frac{1}{a_{ii} c}\sum_{j=1}^{i-1} a_{ij} k_{I,j}} + \ldots$$

$$\sigma_a D_* \left(1 + \frac{4\pi a_{ii}\Delta t}{C_v}\sigma_a D_*\right)^{-1} \left\{ T_n - T_* + \boxed{\Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j}} + \frac{a_{ii}\Delta t}{C_v}\left(S_T - 4\pi\sigma_a B_*\right) \right\}$$

Spatially Discretized Equations

Nearly identical result for spatially discretizing then manipulating:

$$\vec{k}_I = c\mathbf{M}^{-1}\left[\frac{1}{4\pi}\mathbf{R}_{\sigma_s}\vec{\phi} + \mathbf{R}_{\sigma_a}\vec{B} - \mathbf{R}_{\sigma_t}\vec{I} - \mu_d \mathbf{G}\vec{I} + \mu_d I_{in}\vec{f} + \vec{S}_I\right]$$

$$\vec{k}_T = \mathbf{R}_{C_v}^{-1}\left[\mathbf{R}_{\sigma_a}\left(\vec{\phi} - 4\pi\vec{B}\right) + \vec{S}_T\right]$$

$$\vec{I}_i = \vec{I}_n + \Delta t\sum_{j=1}^{i-1} a_{ij}k_{I,j} + \Delta t a_{ii} c\mathbf{M}^{-1}\left\{\frac{1}{4\pi}\mathbf{R}_{\sigma_s}\vec{\phi}_i + \right.$$

$$\left.\mathbf{R}_{\sigma_a}\left(\vec{B}_* + \mathbf{D}_*\left(\vec{T}_i - \vec{T}_*\right)\right) - \mathbf{R}_{\sigma_t}\vec{I}_i - \mu_d\mathbf{G}\vec{I}_i + \mu_d I_{in,i}\vec{f} + \vec{S}_I\right\}$$

$$\vec{T}_i = \vec{T}_n + \Delta t\sum_{j=1}^{i-1} a_{ij}k_{T,j} +$$

$$\Delta t a_{ii}\mathbf{R}_{C_v}^{-1}\left[\mathbf{R}_{\sigma_a}\left(\vec{\phi}_i - 4\pi\vec{B}_* - 4\pi\mathbf{D}_*\left(\vec{T}_i - \vec{T}_*\right)\right) + \vec{S}_T\right]$$

Definitions

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

- **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

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

- **I** - $N_P \times N_P$ identity matrix
- $\mathbf{D}_*$ - diagonal matrix of Planck derivatives

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

"Fission" Terms

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

$$\begin{aligned}
\overline{\overline{\xi}}_{d,i} = \frac{1}{c\Delta t a_{ii}}\mathbf{M}\vec{I}_n + \frac{1}{c a_{ii}}\mathbf{M}\sum_{j=1}^{i-1} a_{ij}k_{I,j} + \mathbf{R}_{\sigma_a}\vec{B}_* + \vec{S}_I \dots \\
+ \mathbf{R}_{\sigma_a}\mathbf{D}_*\left[\mathbf{I} + 4\pi\Delta t a_{ii}\mathbf{R}_{C_v}^{-1}\mathbf{R}_{\sigma_a}\mathbf{D}_*\right]^{-1}\Bigg\{\vec{T}_n - \vec{T}_* + \Delta t\sum_{j=1}^{i-1} a_{ij}k_{T,j} \\
+\Delta t a_{ii}\mathbf{R}_{C_v}^{-1}\left[\vec{S}_T - 4\pi\mathbf{R}_{\sigma_a}\vec{B}_*\right]\Bigg\}
\end{aligned}$$

MIP Diffusion Coefficient

Modified Interior Penalty (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 $\mathbf{R}_{\widetilde{\Sigma}_t}$ we'll argue that we have a consistently defined diffusion coefficient

Equivalence for $\widetilde{\Sigma}_t$

By definition:

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

Likewise

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

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

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

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

Designed Optically Thick and Diffusive 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, $a = c = 1$, $x \in [0, 100]$, $t \in [0, 5]$, $\Delta t_{max} = 0.1$, $C_v = 0.05$, $\sigma_a = \frac{5000}{T^2}$, and $\sigma_s = 0$.

Iterative Strategy	Average Iterations
Diffusion Synthetic Acceleration	2.5
Source Iteration Alone	4460.7

Quick estimate of scattering ratio

$$\frac{\widetilde{\widetilde{\Sigma}}_s}{\widetilde{\widetilde{\Sigma}}_t} = \frac{\nu \sigma_a}{\sigma_T}$$

using $T = \max\left[\widetilde{T}(x, t_{end})\right] \approx 4$, $\sigma_a = 313$, $\sigma_T = 323$:

$$\begin{aligned} \nu &= 0.99999376 \\ \frac{\widetilde{\widetilde{\Sigma}}_s}{\widetilde{\widetilde{\Sigma}}_t} &\approx 0.97 \end{aligned}$$

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)
}
```

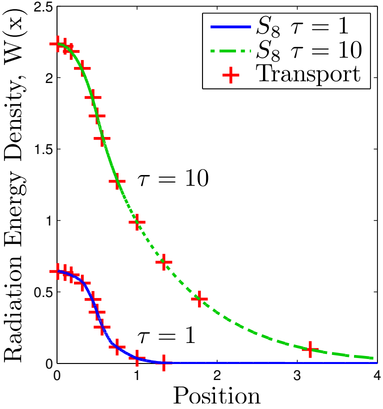
Su-Olson Description

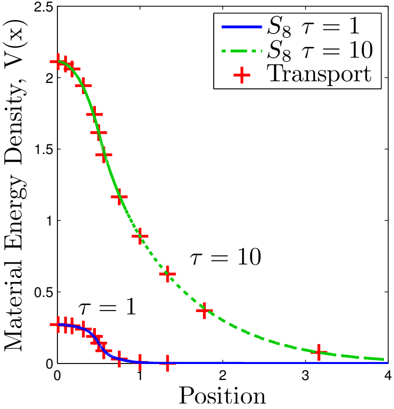
- Initially cold (absolute zero) half space
- Volumetric source near origin for a finite period of time
- Constant opacity
- $C_v = \alpha T^3$
  - C_v assumption causes TRT equations to be linear in I and T^4/material internal energy density
  - Iteratively challenging if fundamental unknown is temperature,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

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

We choose $\sigma_a = 1,\ \sigma_s = 0,\ a = c = 1,\ \alpha = 4,$ and $\epsilon = 10^{-8}$. 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_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

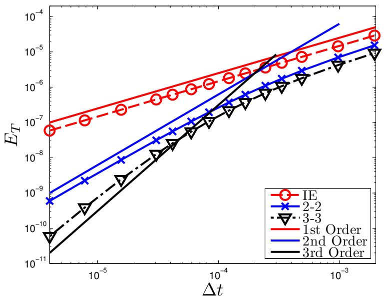
$$\begin{aligned} I_d(x,\mu_d,t) &= M(\mu_d)F(t)W_I(x) && (7)\\ T(x) &= F(t)W_T(x) && (8)\\ \phi(x) &= C_M F(t) W_I(x) && (9)\\ C_M &= \sum_{d=1}^{N_{dir}} w_d M(\mu_d) && (10) \end{aligned}$$

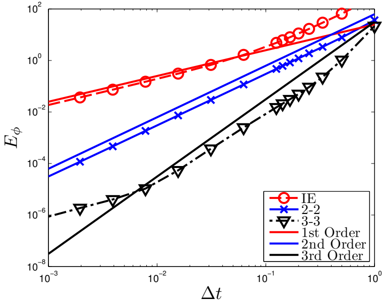
SDIRK Order of Convergence

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

10 equally-spaced cells, quartic SLXS Gauss

SDIRK Order of Convergence





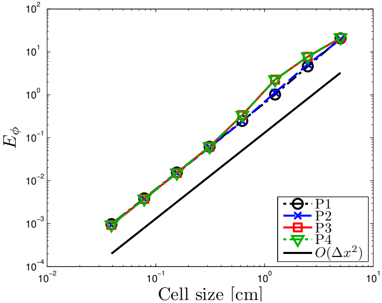
Variable Material Properties Problem- MMS2

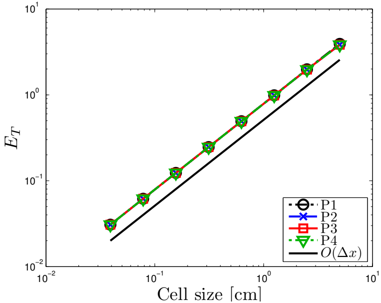
$$
\begin{aligned}
M(\mu_d) &= \frac{1}{4\pi} \\
W_I(x) &= 9\cos\left(\frac{\pi x}{10} - \frac{\pi}{2}\right) + 3 \\
W_T(x) &= 5\cos\left(\frac{\pi x}{10} - \frac{\pi}{2}\right) + 5 \\
F(t) &= 1 + .02t \\
C_v &= 0.2 + 0.01\,T^3 \\
\sigma_a &= \frac{10^4}{T^3} \\
\sigma_s &= 0.5
\end{aligned}
$$

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

Must Account for Spatially Varying Material Properties

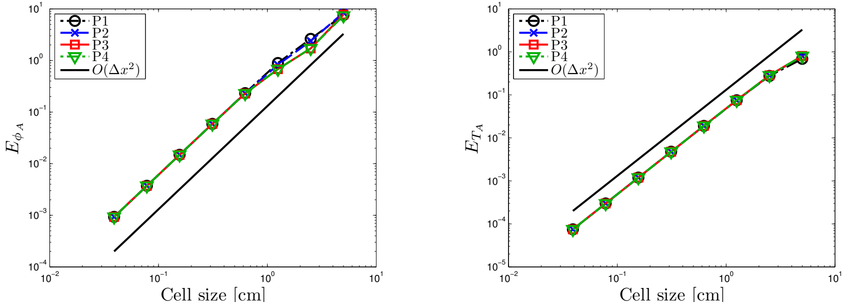
SL Gauss, $P \in [1, 4]$. Limited L^2 convergence.





This Is Not a Pure Absorber Test Problem

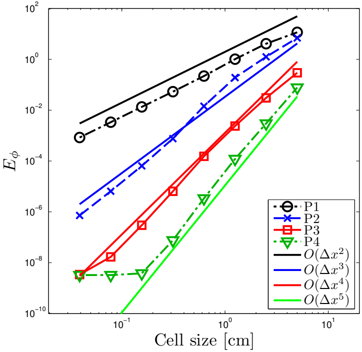
SL Gauss, $P \in [1, 4]$.



In a neutron transport pure absorber test problem, cell-wise constant cross section assumption yields poor L^2 convergence, but very accurate cell average interaction rates.

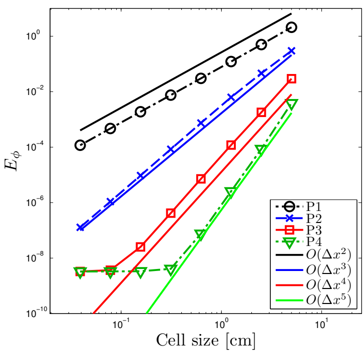
SLXS E_ϕ Convergence

SLXS Lobatto



$\propto P+1$

SLXS Gauss



$\propto P+1$

Plateauing of Errors

Caused by point-wise relative change convergence criteria. For temperature:

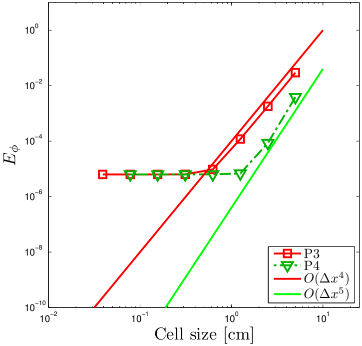
$$
\begin{aligned}
\text{err\_t} &= \max_{c=1}^{N_{cells}} \left[\max_{j=1}^{N_P} \left[\left| \frac{\Delta T_j}{T_{j,*}} \right| \right] \right] \\
\text{converged} &= \text{err\_t} < \epsilon_T
\end{aligned}
$$

All MMS results generated with $\epsilon_T = 10^{-11},\ \epsilon_\phi = 10^{-13}$.

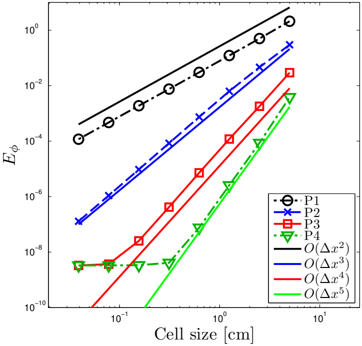
Looser Tolerances

SLXS Gauss E_ϕ convergence if ...

$\epsilon_T = 10^{-8},\ \epsilon_\phi = 10^{-10}$

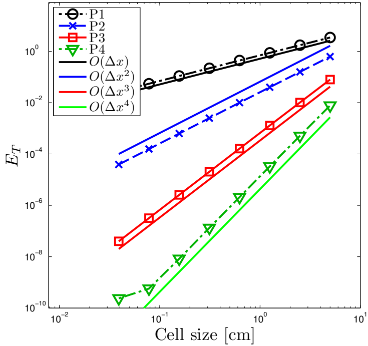


$\epsilon_T = 10^{-11},\ \epsilon_\phi = 10^{-13}$



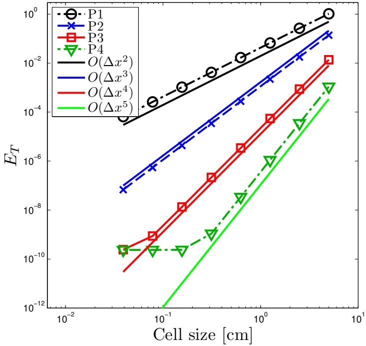
SLXS E_T Convergence

SLXS Lobatto



$\propto P$

SLXS Gauss



$\propto P+1$

Marshak Wave Problem

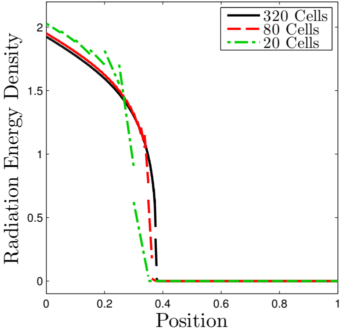
Unit current incident intensity on left face. Vacuum right boundary condition. Initially cold slab. No analytic solution.

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

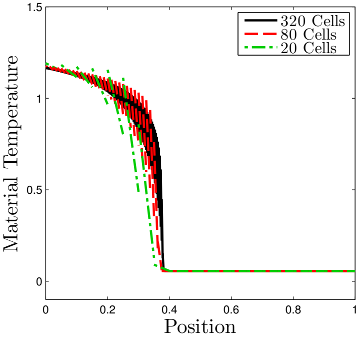
Blading with Cell-Wise Constant Assumption

Linear TL, volumetric average opacity

Radiation energy density

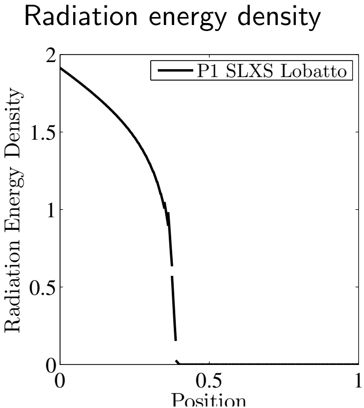


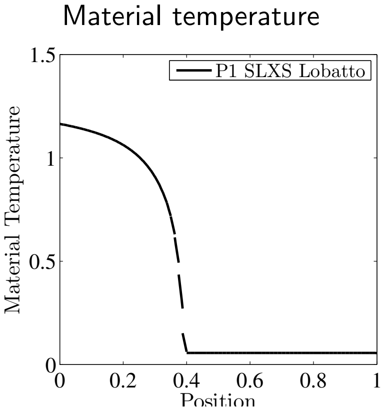
Material temperature



SLXS Treatment

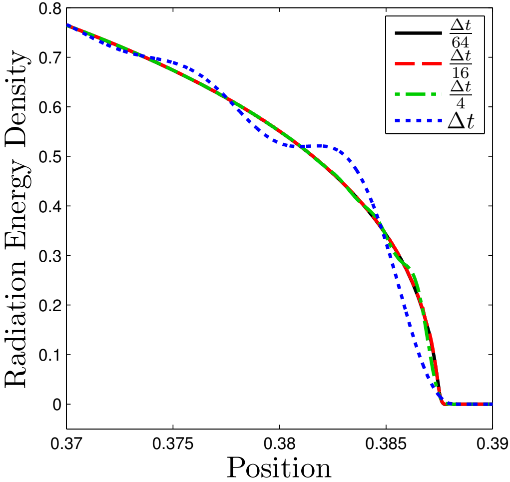
Linear SLXS Lobatto



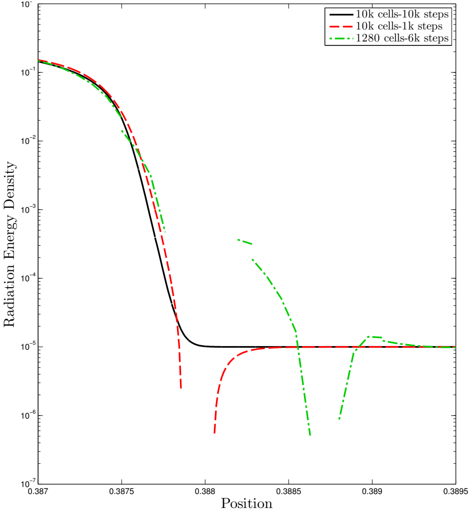


Time Resolution Cannot Be Neglected

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

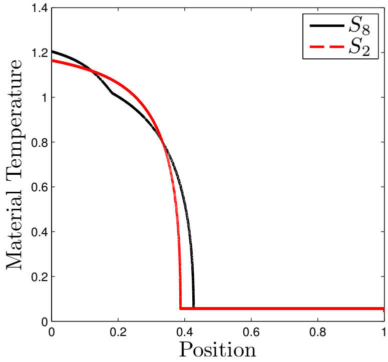


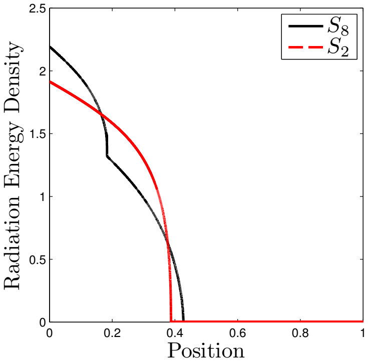
Extreme Zoom of S_2 Radiation Energy Density



- Log scaly y-axis

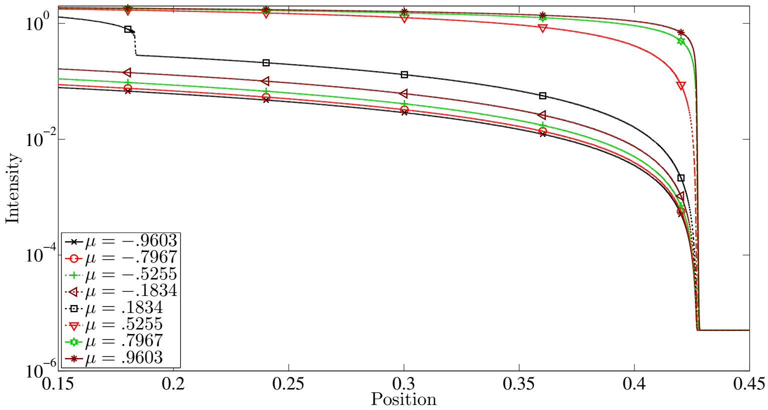
S_2 vs S_8



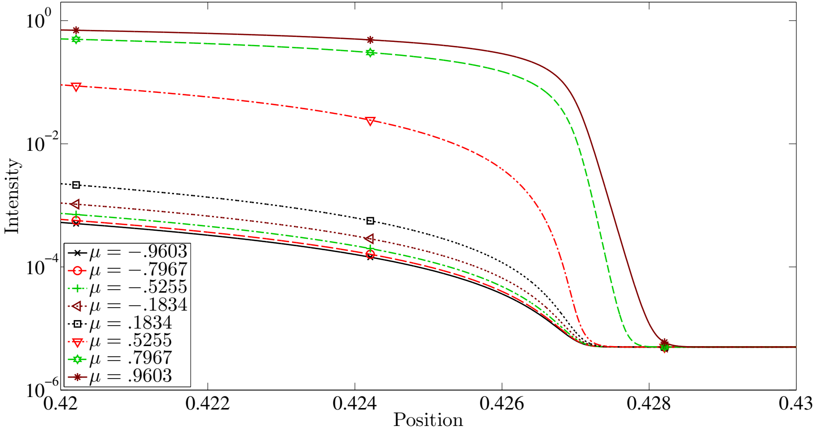


5000 mesh cells, P4 SLXS Gauss, 5k time steps, 2-2 scheme

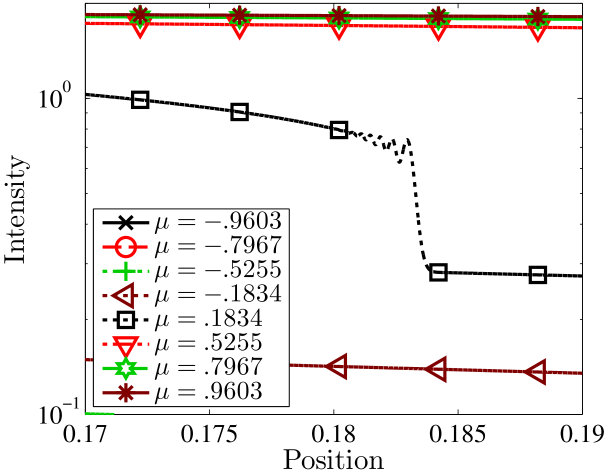
S_8 Angular Intensity



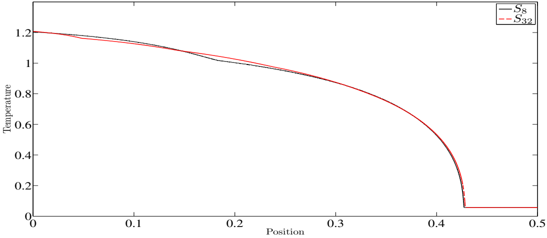
Wavefront Boundary Layers

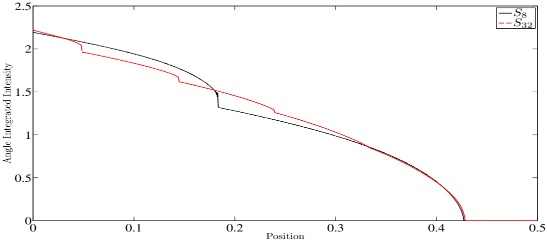


Need More Resolution for Interior Boundary Layer



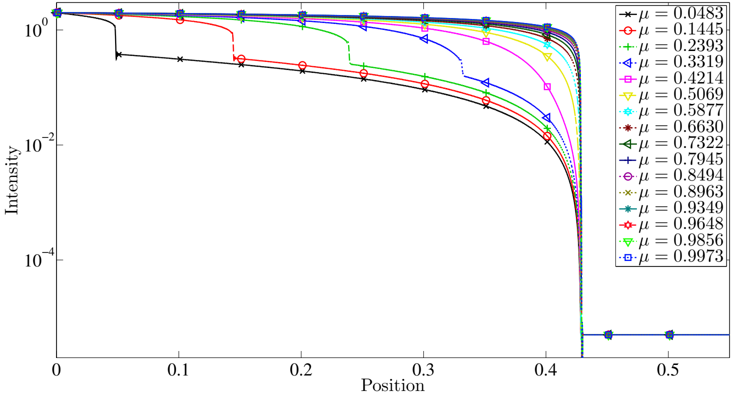
S_8 vs S_{32} Solutions





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

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



Conclusions

In this research we have

1. Developed a matrix lumping framework that is effective for arbitrary order DFEM trial space degree
2. Demonstrated the need to consider spatial variation of material properties
3. Applied MIP diffusion operator to TRT acceleration
4. Applied higher order DFEM to grey TRT
5. Examined the asymptotic accuracy of higher order DFEM for coupled grey TRT problems
6. Generated high order, 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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Test Problem

Source-free pure absorber, left incident flux, $\psi_{in,d}$, vacuum right BC.

Defining h:

$$h = \frac{\sigma_t \Delta x}{\mu_d}$$

Analytic solution is

$$\psi(x, \mu_d) = \psi_{in,d} \exp[-h]$$

Convergence of $\left\|\widetilde{\psi}-\psi\right\|_{L^2}$ as a function of h

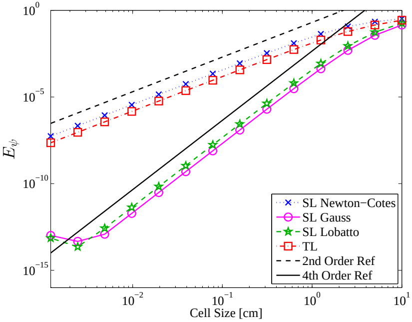


Figure: $P = 3$.

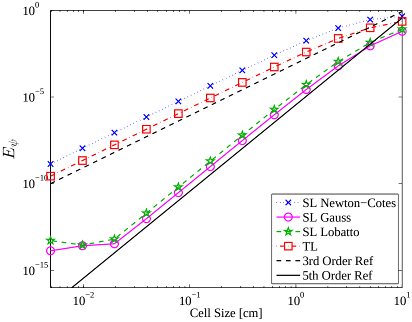


Figure: $P = 4$

Summary of Constant Cross Section Discoveries

Positivity

- SL Gauss is strictly positive for even P
- SL Lobatto and SL Newton-Cotes: strictly positive for odd P
- TL not robust for $P > 1$

Accuracy

- TL and SL Newton-Cotes converge $\left\|\widetilde{\psi} - \psi\right\|_{L^2}$ 2nd order for odd P, 3rd order for even P
- SL Lobatto and SL Gauss converge $\left\|\widetilde{\psi} - \psi\right\|_{L^2} \propto P + 1$

Equivalence

- SL Gauss equivalent to Exact DFEM for all P
- TL $=$ SL Lobatto $=$ SL Newton-Cotes for $P = 1, 2$

Test Problem

- Spatially varying cross section of the form:

$$\sigma_t(x) = c_1 e^{c_2 x}$$

- Incident flux, $\psi_{in,d}$ on the left, vacuum on the right, no sources.
- Analytic Solution

$$\psi(\mu_d, x) = \psi_{in,d} \exp\left[\frac{c_1}{\mu_d c_2}\left(1 - e^{c_2 x}\right)\right]$$

Additional Numerical Schemes

- **CXS DFEM**: Equally-spaced interpolation points, analytic integration. Approximate cross section by cell average value
- **SLXS Lobatto**: Lobatto interpolation points, self-lumping extended to account for cross section variation
- **SLXS Gauss**: Gauss interpolation points, self-lumping extended to account for cross section variation
- **SLXS Newton-Cotes**: Equally-spaced interpolation points, self-lumping extended to account for cross section variation

We will no longer consider the TL scheme.

Convergence Results

We examine the convergence of E_ψ and $E_{\psi_{out}}$ for a pure absorber with

$$\sigma_t(x) = 0.1 \; 10^{2x}$$

and $x \in [0, 1 \; cm]$. We define the error quantities as:

$$\begin{aligned} E_\psi &= \left\| \widetilde{\psi}_d(x) - \psi(x, \mu_d) \right\|_{L^2} \\ E_{\psi_{out}} &= \sqrt{\sum_{i=1}^{N_{cells}} \Delta x_i \left(\widetilde{\psi}_{out,i} - \psi(x_{i+1/2}) \right)^2} \end{aligned}$$

L^2 Convergence

New Result: SLXS Lobatto and SLXS Gauss are accurate methods for spatially varying cross section problems

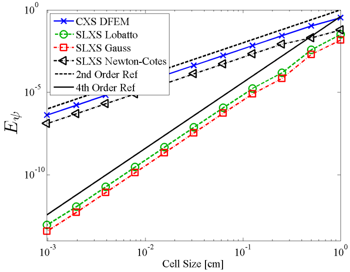


Figure: $P = 3$ convergence plot.

Summary of Convergence Orders

- SLXS Gauss: $\propto P + 1$
- SLXS Lobatto: $\propto P + 1$, less accurate than SL Gauss
- SLXS Newton-Cotes: 2 if odd P, 3 if even P
- CXS DFEM: 2 regardless of P

Interaction Rate

- Analytic interaction rate

$$IR(x) = \sigma_t(x)\psi(x,\mu_d)$$

- CXS DFEM approximation

$$\widetilde{IR}(x) = \hat{\sigma}_t\widetilde{\psi}(x)$$

- SLXS schemes: Only point-wise knowledge of $\sigma_t(x)$ in DFEM equations
  - Integrals: evaluate $\widetilde{IR}(x)$ with quadrature restricted to interpolation points
  - Plotting purposes:

$$\widetilde{IR}(x) = \sum_{j=1}^{P+1} \sigma_{t,j}\psi_j b_j(s)$$

New Result: SLXS Lobatto and SLXS Gauss Accurately Approximate $\widetilde{IR}(x)$

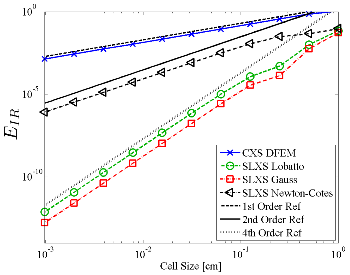


Figure: Cubic DFEM

Summary of Convergence Orders

- SL Gauss: $P+1$
- SL Lobatto: $P+1$
- SL Newton-Cotes: 2 for odd P, 3 for even P
- CXS DFEM: 1, regardless of trial space degree

E_{IR_A} Convergence

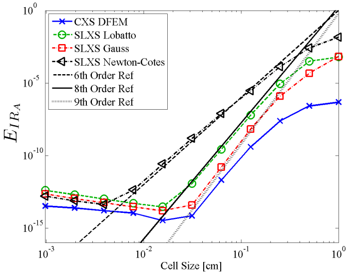


Figure: Quartic DFEM

Summary of Convergence Orders

- SL Gauss: $2P + 1$
- SL Lobatto: $2P$
- SL Newton-Cotes: $P + 1$ for odd P, $P + 2$ for even P
- CXS DFEM: $2P + 1$, regardless of trial space degree

CXS DFEM Accuracy Calculating IR_A

- How can CXS DFEM converge E_{IR_A} so accurately?
- Local Conservation

$$\text{Particles In} - \text{Particles Out} = \text{Total Interactions}$$

- Particles In: Outflow from Previous Cell
- Particles Out: Outflow from Current Cell
- CXS DFEM converges angular flux outflow $\propto 2P+1$
- $\therefore$ CXS DFEM accurately calculates

$$\text{Total Interactions} = \Delta x \left(\widetilde{IR}_A \right)$$

CXS DFEM Interaction Rate Profile

New to Dissertation

Observation and explanation of blading phenomena

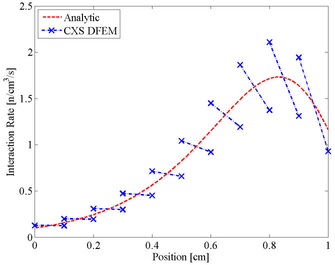


Figure: $\widetilde{IR}(x)$ profile.

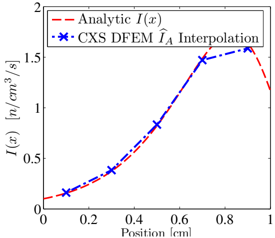


Figure: Interpolated $\widetilde{IR}_A$ profile.

Something Wrong with DFEM?

No. Consider the analytic solution to a problem that has the cell-wise average cross section.

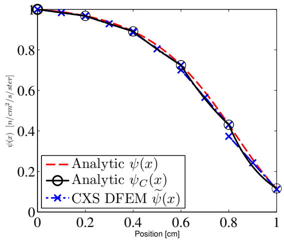


Figure: Angular Flux.

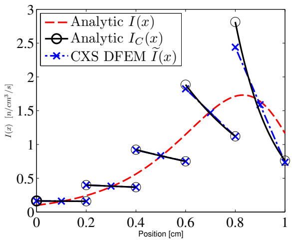


Figure: Interaction Rate.

Linear SL Lobatto Solution

New to Dissertation

New: Self-lumping schemes do not exhibit blading

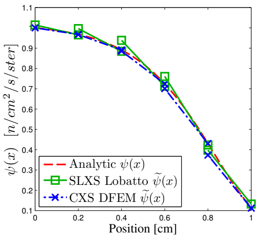


Figure: Angular Flux.

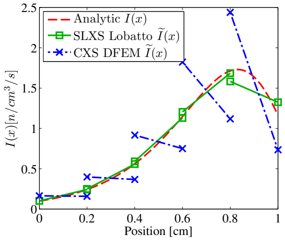


Figure: Interaction Rate.

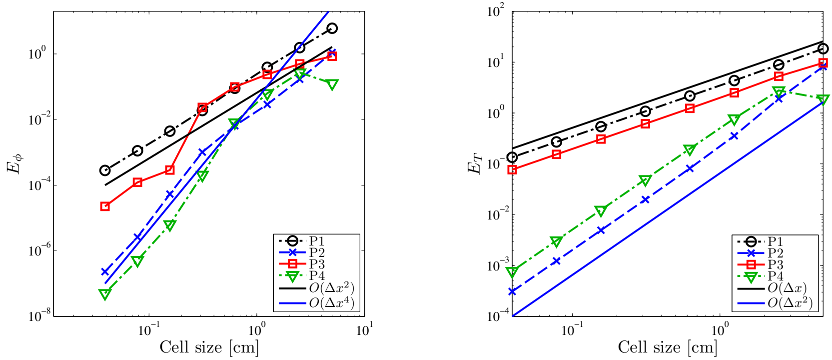
Constant Material Properties- MMS1

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

Used S_8 quadrature, 2-2 SDIRK scheme

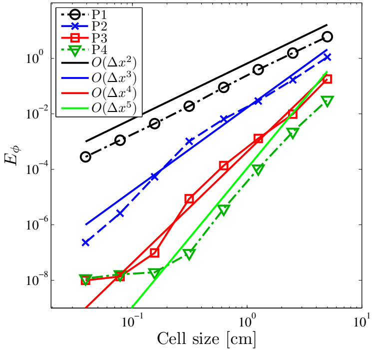
TL- MMS1 Results

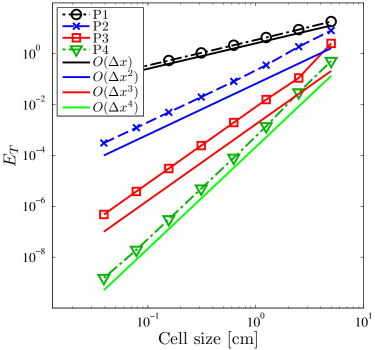
TL does not get better applied to a harder problem



SL Lobatto- MMS1 Results

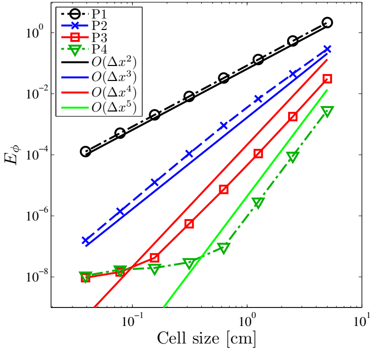
SL Lobatto loses an order in T

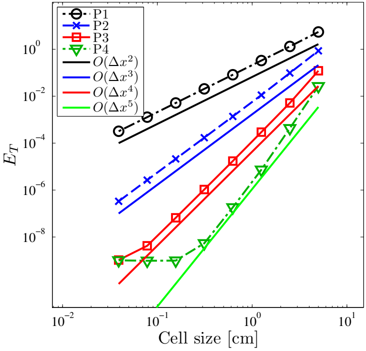




SL Gauss- MMS1 Results

SL Gauss picks up an order for T?



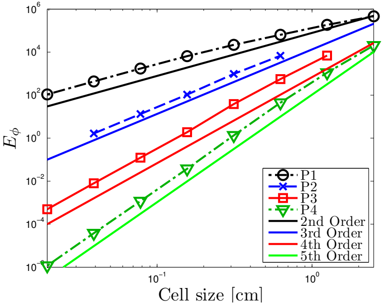


Steady-state problem

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

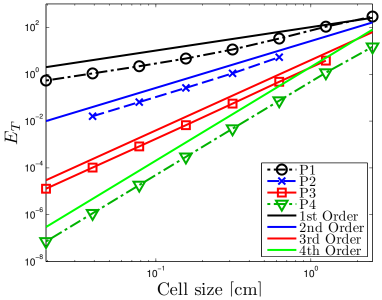
SLXS Lobatto L^2 Convergence

E_ϕ



$\propto P+1$

E_T

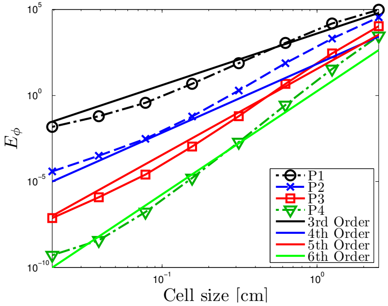


$\propto P$

No surprises

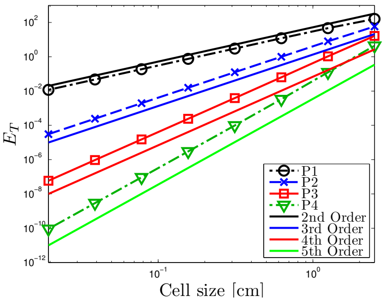
SLXS Gauss L^2 Convergence

E_ϕ



$\propto P+2$

E_T

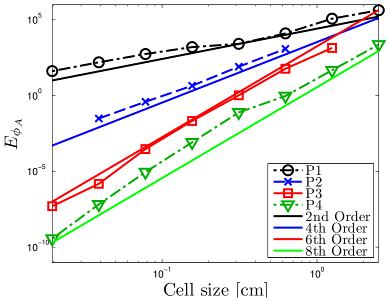


$\propto P+1$

Where did the extra order in E_ϕ come from?

E_{ϕ_A} Convergence

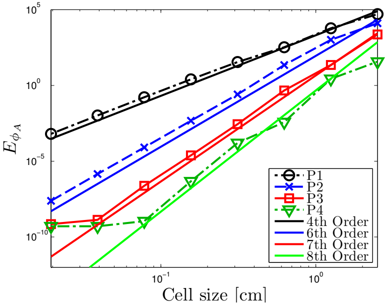
SLXS Lobatto



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

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

SLXS Gauss

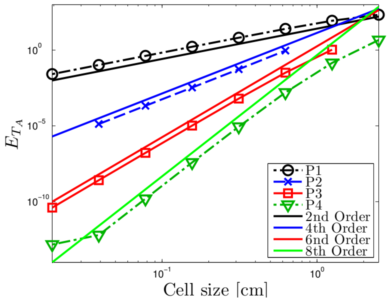


TRT $E_{\phi_A} < 2P + 2$

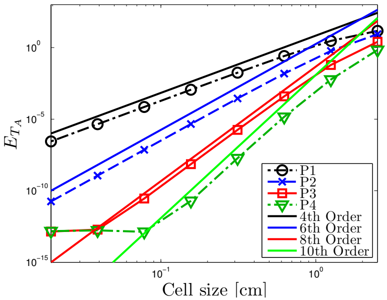
Neutronics $E_{\psi_A} \propto 2P + 1$

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 $E_{\psi_A} \propto 2P + 1$