Cross Section Spatial Discretization for Nuclear Engineering Calculations

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Outline

Radiation Transport Equation

Ideally we could easily solve the (7-dimensional) Boltzmann neutron transport equation (and its variants):

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \vec{\Omega} \cdot \nabla \psi + \sigma_t \psi = \int_0^\infty \int_{4\pi} \sigma_s(\vec{\Omega}' \to \vec{\Omega}, E' \to E)\psi \; d\vec{\Omega}' dE' + Q\,, \qquad (1)$$

to answer all of the following questions:

- Where is heat being produced in the nuclear reactor?
- Am I treating this cancer effectively?
- Where is the oil/gas in this well?
- How am I compressing/heating this deuterium pellet?
- What's hiding in the shipping container?
- ...

1-D Steady State S_N Equation

Eq. (1) requires more justice than 20 minutes can give.

- Instead, let's talk about:

$$\mu_d \frac{\partial \psi_d}{\partial x} + \sigma_t(x)\psi_d = \frac{\sigma_s(x)}{2}\phi(x) + Q_d(x)\,, \tag{2}$$

the steady state, mono-energetic, 1-D Cartesian geometry, S_N approximation to Eq. (1) and how solution techniques for Eq. (2) can be improved.

In Eq. (2):

$$\begin{aligned} \psi_d &= \psi_d(x, \mu_d) \\ Q_d &= Q(x, \mu_d) \\ \phi(x) &\approx 2\pi \sum_{d=1}^{N} w_d \psi_d(x, \mu_d) \end{aligned}$$

DFEM Discretization

When we discretize Eq. (2) with discontinuous finite elements (DFEM), we get a system of equations like this:

$$\mu_d \mathbf{L}\vec{\psi}_d + \mathbf{R}_{\sigma_t}\vec{\psi}_d = \frac{1}{2}\mathbf{R}_{\sigma_s}\vec{\phi} + \vec{q}_d + \psi_{in}\vec{f}$$

where we define the following (focusing only on $\mu_d > 0$):

$$\begin{aligned}
\psi_d(s) &\approx \widetilde{\psi}(s) \\
\widetilde{\psi}(s) &= \sum_{j=1}^{P+1} \psi_j B_j(s) \\
B_j(s) &= \prod_{\substack{k=1 \\ k\neq j}}^{N_P} \frac{s - s_k}{s_j - s_k}
\end{aligned}$$

$$\begin{aligned}
\mathbf{L}_{ij} &= B_i(1)B_j(1) - \int_{-1}^{1} \frac{dB_i}{ds} B_j(s)\, ds \\
\mathbf{R}_{\sigma,ij} &= \frac{\Delta x}{2} \int_{-1}^{1} \sigma(s) B_i(s) B_j(s)\, ds \\
\vec{f}_i &= B_i(-1) \\
\vec{q}_{d,i} &= \frac{\Delta x}{2} \int_{-1}^{1} B_i(s) Q_d(s)\, ds
\end{aligned}$$

Cell-wise Constant Cross Sections

If cross section is truly cell-wise constant, there is no approximation in assuming

$$\mathbf{R}_\sigma = \sigma\mathbf{M}$$

- Good examples: shielding calculations, material detection problems

There are many problems of interest where this is not the case

- Cross sections are functions of temperature, density, fuel burn-up, etc.
- Neutronics examples: coupled reactor physics, fuel depletion problems, ...
- Radiative transfer: ICF, astrophysics, ...

Radiative Transfer with Constant Opacities

Initial dissertation topic

- S_N coupled to Euler equations

First step

- Test radiative transfer in MATLAB

Expected result

- Replicate published calculation

Actual result

- Radiation profile within visual norm acceptance criteria
- Temperature profile is not
- Why? WHY?

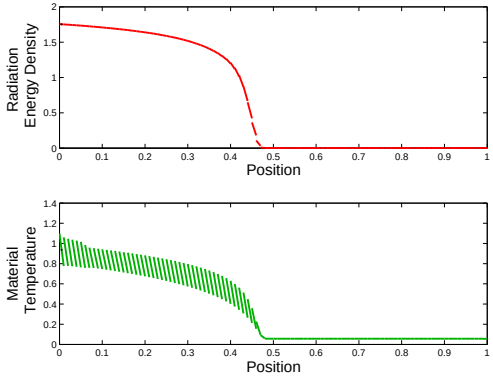


Figure: Cell-wise constant opacity solution to Marshak wave problem with $\sigma_a = \sigma_t = T^{-3}$.

Relationship Between Neutronics and Radiative Transfer

- The 1-D grey radiative transfer equations are:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial x} + \sigma_t I = \frac{\sigma_s}{4\pi}\phi + \frac{\sigma_a}{4\pi}acT^4$$

$$C_v\frac{\partial T}{\partial t} = \sigma_a\left(\phi - acT^4\right)$$

- Temperature equation is driven by an interaction term, $\sigma_a\phi$
- Radiative transfer is more complicated and computationally intense than neutronics.

Idea

Find a neutronics problem that exhibits behavior similar to radiative transfer temperature profile and demonstrate that the temperature profile is not a result of my own mistake.

Numerical Schemes to Compare

- **CXS DFEM**: Equally-spaced points as DFEM interpolation points, exact integration, evaluate **R** using cell-wise constant (volume average) cross section
- **SL Gauss**: Gauss quadrature as DFEM interpolation points, evaluate **R** using self-lumping quadrature
- **SL Lobatto**: Lobatto quadrature as DFEM interpolation points, evaluate **R** using self-lumping quadrature
- **SL Newton-Cotes**: Equally-spaced points as DFEM interpolation points, evaluate **R** using self-lumping quadrature

What is Lumping?

- Matrix lumping, or just lumping, is a mathematical technique that can be applied to all equations solved with DGFEM (and interpolatory basis functions)
- Done to improve the "robustness" of numerical schemes
- In radiation transport, we define robustness as solution positivity and resistance to oscillations
- Lumping- make diagonal matrices
- Two ways to lump
  1. Collapse an exactly integrated matrix's entries to the main diagonal
  2. Use quadrature restricted to the DFEM interpolation points

Self-Lumping Concept

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

Self-lumping (SL) **M**

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

Trivial to extend quadrature integration to include spatial variation of cross section

Self-lumping (SL) $\mathbf{R}_\sigma$

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

Test Problem

- Source-free pure absorber with:

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

- Vacuum BC on the right and beam of incident flux, $\psi_{in,d}$, on the left side in the direction μ_d. Analytic ψ is:

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

- Interaction rate, $IR(x)$, driven only by beam:

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

- In results that follow, we consider $\mu_d = 1$ and $x \in [0, 1\ [cm]]$

State of the Practice Solution

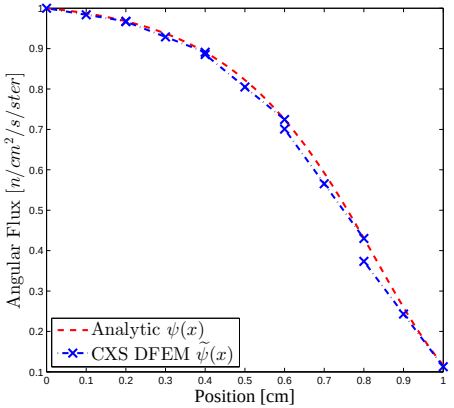


Figure: Angular flux profile.

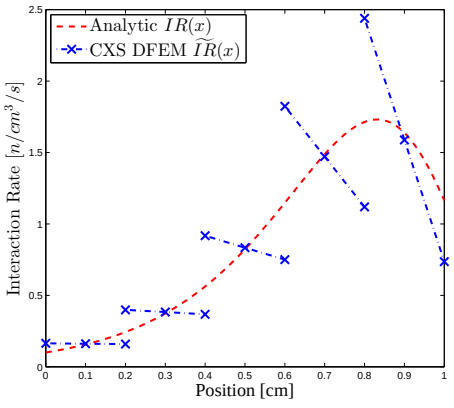


Figure: Interaction rate profile.

Neutronics problem that exhibits blading seen in radiative transfer!!

Surely this is well documented, right?

No. Angular flux profile is smooth. Simplified plotting can hide the blading.

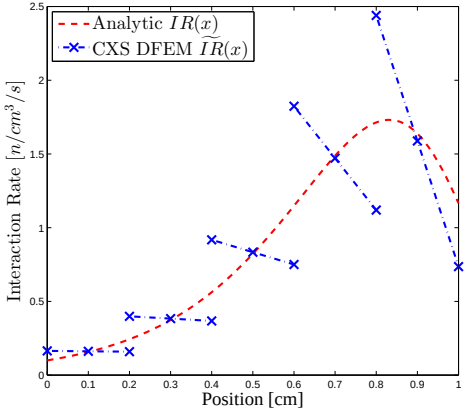


Figure: $\widetilde{IR}(x)$.

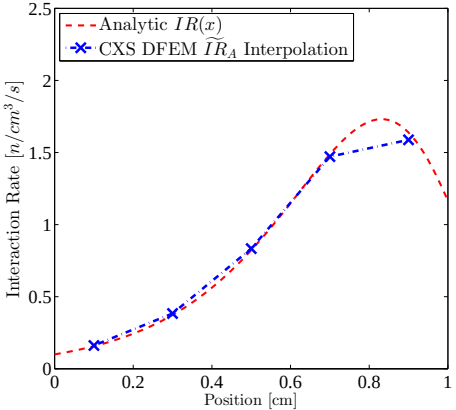


Figure: Interpolated $\widetilde{IR}$.

Something Wrong with DFEM?

No. Consider the analytic solution that uses the cell-wise average cross section.

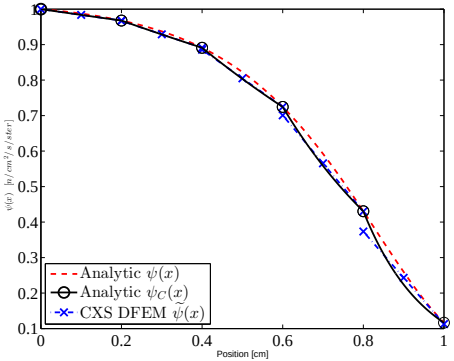


Figure: Angular Flux.

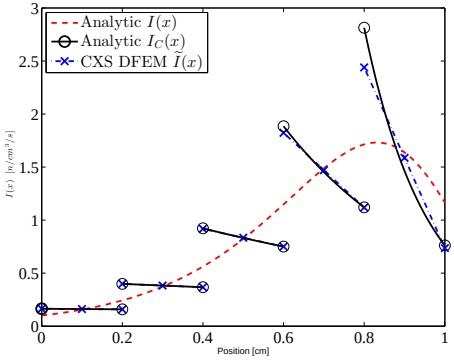
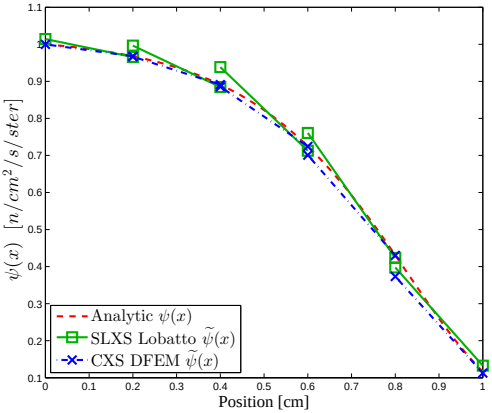


Figure: Interaction Rate.

Is there a solution to this problem?

Yes. Self-lumping schemes do not exhibit blading. Consider linear SL Lobatto solution:



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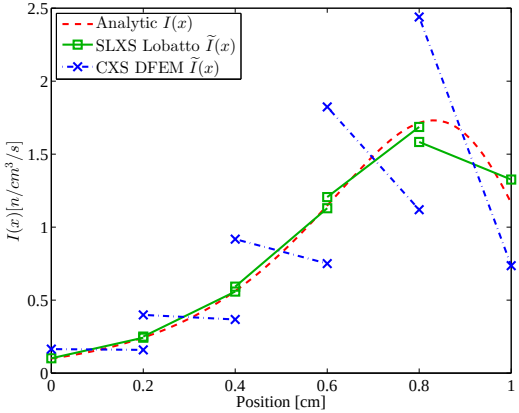


Figure: Interaction Rate.

$\left\|\psi - \widetilde{\psi}\right\|_{L^2}$ Convergence

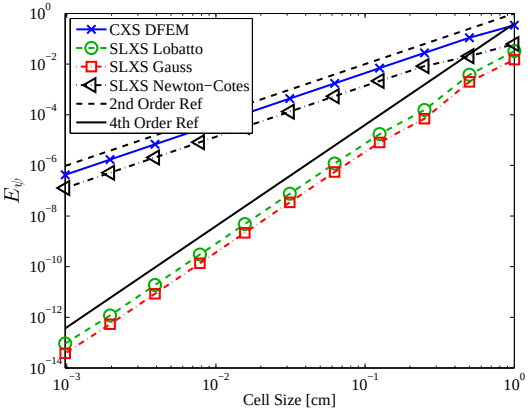
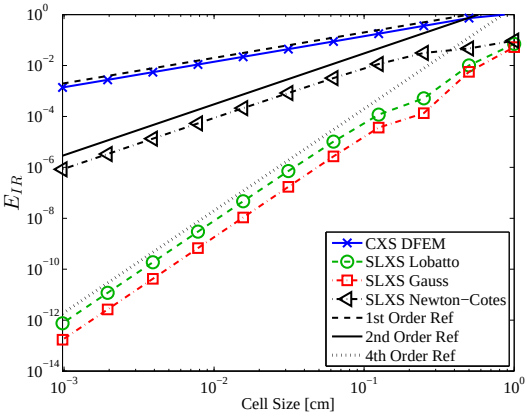


Figure: Cubic DFEM error convergence for $\psi(x)$.

Summary of Convergence Orders

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

$\left\| IR - \widetilde{IR} \right\|_{L^2}$ Convergence



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Marshak Wave Problem with Self-Lumping

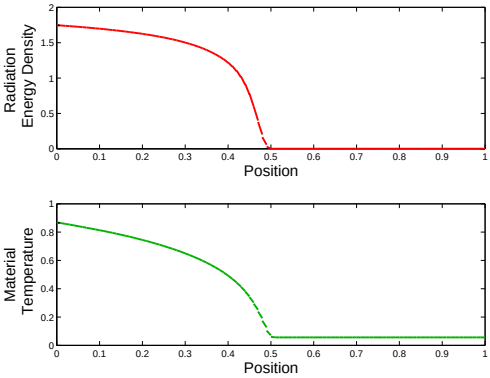

Figure: Linear SL Lobatto solution.

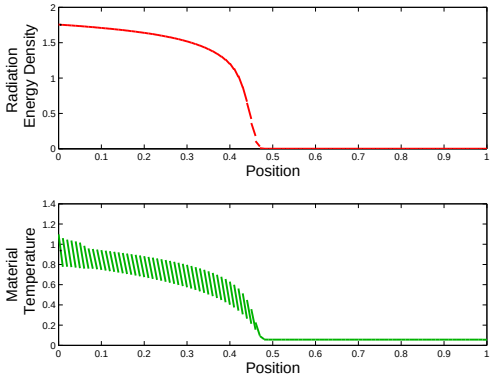

Figure: Linear, constant cross section (with mass matrix lumping) solution.

Thanks!

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