Measuring Angular Discretization Error During TRT Simulations with Energy Collapsed, Single Group Calculations

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Abstract

The SN method uses a quadrature rule to evaluate the integral of . This discrete treatment of angle leads to errors called "ray effects." These effects are well documented [1] and are especially harmful when the radiation transport is coupled to hydrodynamics. This angular error can be reduced by increasing the angular quadrature, but this is computationally expensive, especially when there are many energy groups. We present a way to estimate angular discretization error during a simulation. This method uses the multigroup solution to calculate grey cross sections, which are then used in a grey simulation with a relatively more refined angular quadrature on the same timestep. We evaluate how effective this method is at determining the angular discretization error and it's potential as a refinement metric.

Overview

Transport Equations

- The thermal radiative transfer (TRT) equations, without scattering:

$$\frac{1}{c}\frac{\partial I(x,\nu,\Omega,t)}{\partial t} + \Omega\cdot\nabla I(x,\nu,\Omega,t) + \sigma_{\mathrm{a}}(x,\nu,T)I(x,\nu,\Omega,t) = \sigma_{\mathrm{a}}(x,\nu,T)B(\nu,T) \quad (1)$$

$$\frac{dU_m}{dt} = \int_0^{\infty}\int_0^{4\pi}\sigma_a I d\Omega d\nu - \int_0^{\infty}\sigma_a B d\nu + S_m. \quad (2)$$

- These two equations are non-linearly coupled by the material temperature, T.
- All groups travel at the speed of light, c

Angular Discretization

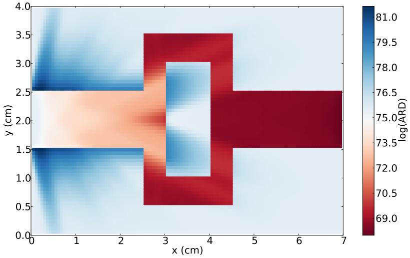
- The S_N method discretizes the angular domain and uses a quadrature rule to evaluate angle-integrated quantities:

$$I = \sum_{n=1}^{M} w_n I_n \tag{3}$$

- The transport equation becomes a set of equations for each discrete angle, coupled by scattering
- Using too few angles leads to errors in the angle-integrated intensity (usually non-physical oscillations)
- Errors caused by lack of angular resolution are called "ray effects"
- Ray effects occur regardless of the linearization applied to the S_N TRT equations

Ray Effects

- Ray effects can lead to errors when coupled to other physics (e.g. seeding Rayleigh Taylor instabilities)
- Increasing the quadrature order decreases ray effects
- Scattering reduces ray effects (intensity is more homogeneous in angle)
- Number of unknowns in 3D goes as $N^2 + 2N$, where N is quadrature order



1: Example of ray effects in total ARD for multigroup S_8 simulation at 3.2×10^{-9} s

Overview

Error Estimate

- If there was a computationally inexpensive way to estimate angular error, we could adapt quadrature dynamically
- To estimate the error on a time step, a relatively coarse angular discretization is used to converge the material temperature
- The converged multigroup intensity is used to calculate grey opacities (energy collapsed)

$$\overline{\sigma} = \frac{\int_0^\infty \sigma(x,\nu,T) I(x,\nu,\Omega) d\nu}{\int_0^\infty I(x,\nu,\Omega) d\nu} \approx \frac{\sum_{g=1}^{G} \sigma_{\mathrm{g}} I_g}{\sum_{g=1}^{G} I_g}. \tag{4}$$

- Grey cross sections are often calculated assuming a shape of the intensity, using the converged intensity potentially avoids this error

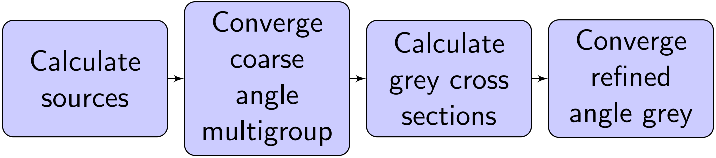
Error Estimate

- The collapsed grey opacities are used in a refined angle (relative to the multigroup solution) simulation on the same timestep
- We call the grey solution obtained with collapsed opacities the *collapsed grey* solution
- The angular error is estimated to be the difference between the absorption rate density (ARD) in the collapsed grey and mulitgroup solutions:

$$\epsilon = \sum_{n=1}^{N} \frac{\left| \overline{\sigma_n} I_{n,grey} - \sum_{g=1}^{G} \sigma_{n,g} I_{n,g} \right|}{\overline{\sigma_n} I_{n,grey}} \quad (5)$$

Implementation

- This error estimate method was implemented in the PDT code [3] at Texas A&M University
- PDT allows group dependent angular quadrature
- An additional group is created with energy bounds that cover the whole domain
- The solution procedure is:

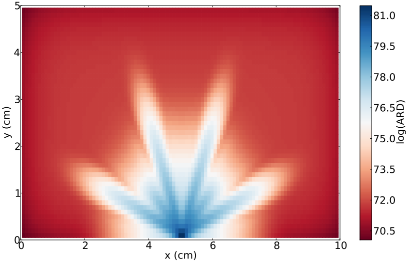


- The temperature is updated with the mutigroup solution–the grey solution is not used to advance the simulation

Overview

Simple Point Source Problem

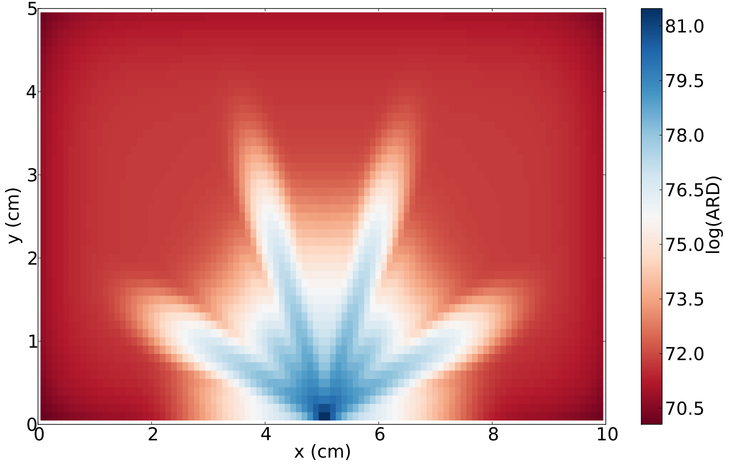
- A simple source is used to test ability to measure the error accurately
- Problem is multigroup but all groups are the same opacity
- Only error is in angle, not related to cross section collapse
- Problem has opacity of $1.0\frac{1}{cm}$, point source of 0.5 keV at half way down the x-axis, vacuum boundaries



2: Point source problem at at 1.13×10^{-10} s

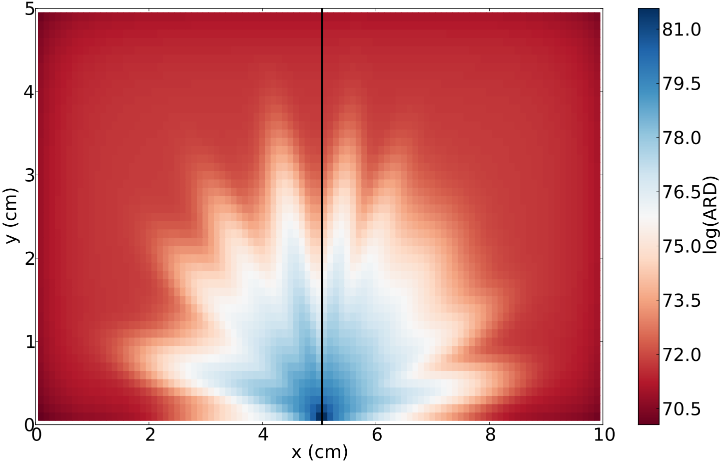
Simple Point Source Problem–Results

- Total ARD for multigroup S_4 simulation at 1.13×10^{-10} s



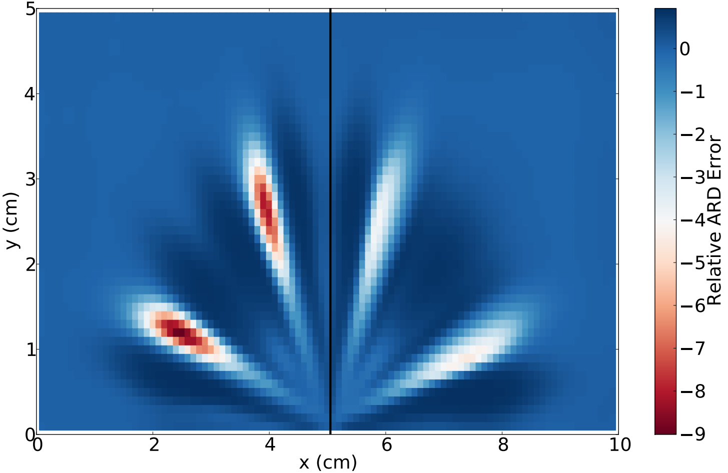
Simple Point Source Problem–Results

- Total ARD for the collapsed grey S_8 (left) and a multigroup S_{16} simulation (right) at 1.13×10^{-10} s



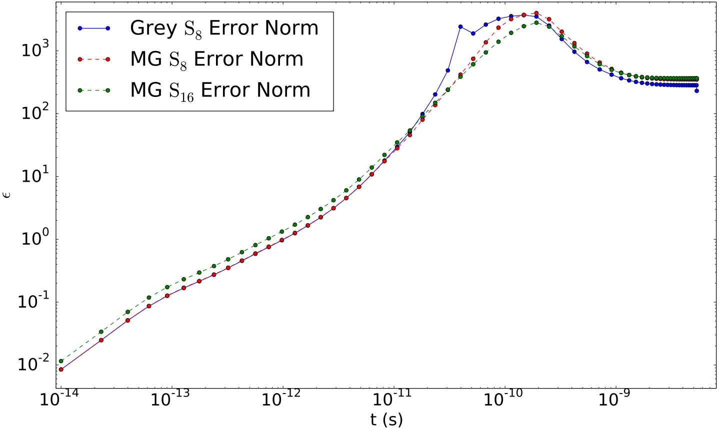
Simple Point Source Problem–Results

- Relative error in the multigroup S_4 ARD as measured by the collapsed grey S_8 (left) and a multigroup S_{16} simulation (right) at 1.13×10^{-10} s



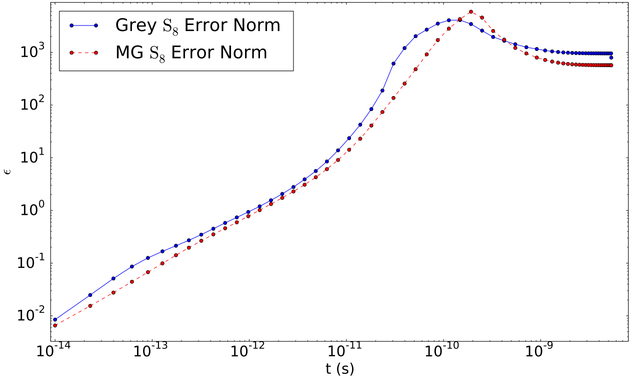
Simple Point Source Problem–Results

- Error vs. time for the simple source problem as measured by the collapsed grey S_8 simulation and a multigroup S_8 simulation



Multigroup Point Source Problem–Results

- A multigroup version of the point source problem was run using 10 groups (opacities in appendix)
- Error vs. time for the multigroup simple source problem as measured by the collapsed grey S_8 simulation and a multigroup S_8 simulation

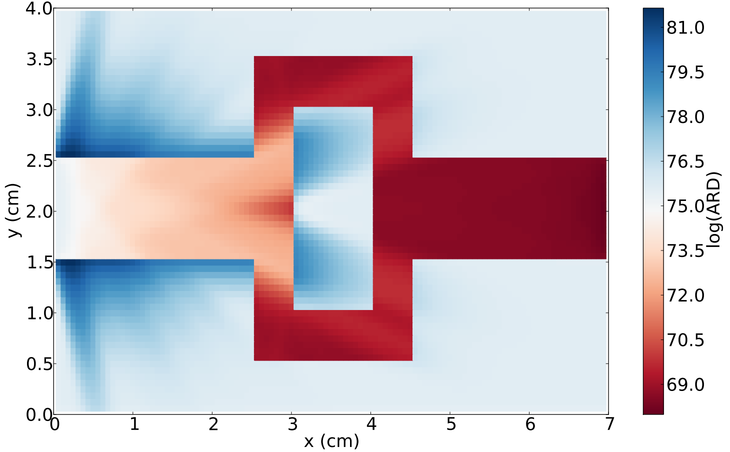


Crooked Pipe Problem–Setup

- Source and geometry are the same as given by Graziani[2] with XY instead of RZ
- Opacity has 10 groups, thick at low frequencies, thin at high frequencies
- Multigroup transport uses S_8, collapsed grey uses S_{16}

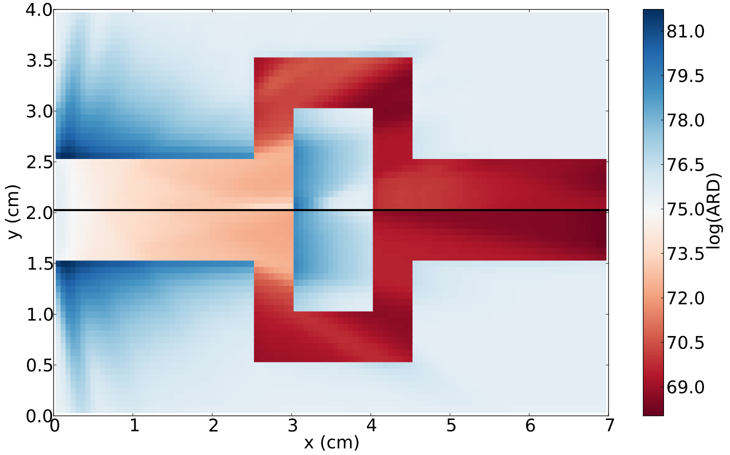
Crooked Pipe Problem–Results

- Total ARD for multigroup S_8 simulation at 3.2×10^{-9} s



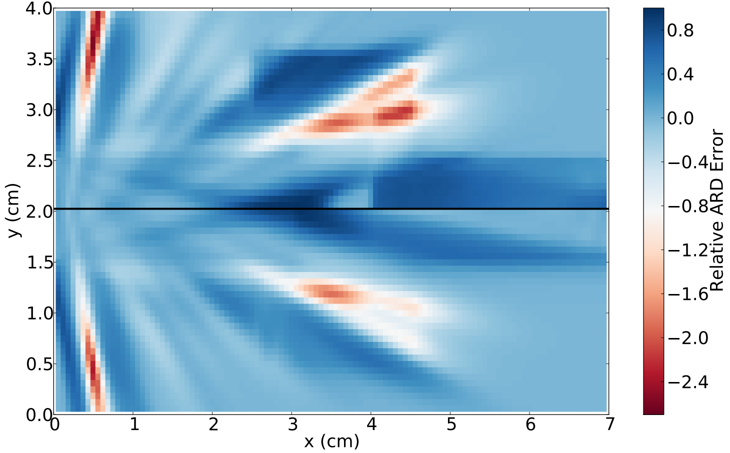
Crooked Pipe Problem–Results

- Total ARD for the collapsed grey S_{16} (top) and the full multigroup S_{16} simulation (bottom) at 3.2×10^{-9} s



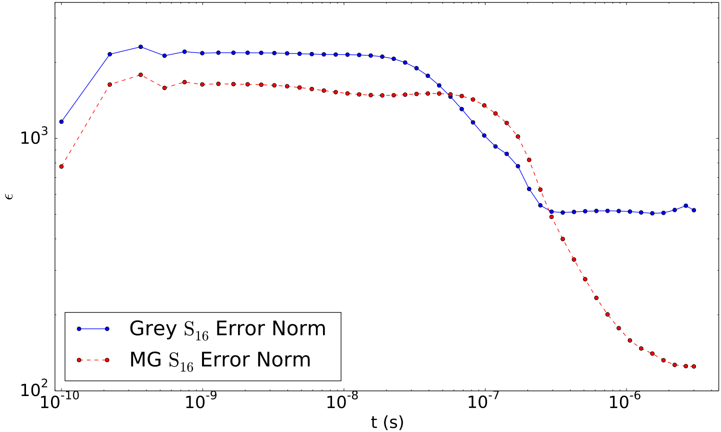
Crooked Pipe Problem–Results

- Relative error in the multigroup S_8 ARD as measured by the collapsed grey S_{16} (top) and a multigroup S_{16} simulation (bottom) at 3.2×10^{-9} s



Crooked Pipe Problem–Results

- Error vs. time for the crooked pipe problem as measured by the collapsed grey S_{16} simulation and a multigroup S_{16} simulation



Timing

- For the point source problem, S_4 has 12 unknowns and S_8 has 40 unknowns
- For the crooked pipe problem, S_8 has 40 unknowns, S_{16} has 144

Point Source	
Angular Discretization	Runtime (hours)
S_4	0.702
S_4 with S_8 grey	1.65
S_8	0.961

Crooked Pipe	
Angular Discretization	Runtime (hours)
S_8	1.694
S_8 with S_{16} grey	3.700
S_{16}	3.883

Discussion

Ray Effects

- The higher order angular solution still has ray effects, but those rays are in different places
- This could over-predict the error (see the measured error near the y-axis in the crooked pipe results)
- The error estimate decreases as the problem heats up

Runtime

- More groups affects the number of iterations required for convergence (more off-diagonal entries in matrix)
- The number of angles does not increase the number of off-diagonal entries, but does increase sweep time
- This error estimate may be relatively inexpensive if a large number of groups are used

Overview

Conclusions and future work

Conclusions

- The temporal shape of the error is roughly predicted by the collapsed-grey method
- The collapsed-grey method correctly indicates where spatial error is large
- Currently, the refined angular estimate takes longer than the more refined solution in angle

Future Work

- Run on problems with group-to-group coupling
- Examine more ways to improve the speed of the error estimate
- Develop a metric for relaxing and refining angle based on error estimate

Acknowledgments

- Anthony Barbu (Texas A&M)
- Daryl Hawkins (Texas A&M)

Overview

Crooked Pipe Opacity

- Opacity is meant to resemble real material: thick at low frequency, thin at high frequency

Group	Energy bounds (eV)	Value (cm^2/g)
σ_0	1.0×10^9 - 1.0×10^6	0.25
σ_1	1.0×10^6 - 1.0×10^3	0.5
σ_2	1.0×10^3 - 500.0	1.0
σ_3	500.0 - 200.0	2.0
σ_4	200.0 - 100.0	4.0
σ_5	100.0 - 50.0	8.0
σ_6	50.0 - 10.0	16.0
σ_7	10.0 - 1.0	20.0
σ_8	1.0 - 0.5	20.0
σ_9	0.5 - 1.0×10^{-5}	20.0

1: Group bounds and opacity values for the crooked pipe problem

Thomas Brunner.
Forms of approximate radiation transport.
Technical Report SAND2002-1778, Sandia National Laboratory, Albuquerque, New Mexico 87185, 2002.

F. Graziani and J. LeBlanc.
The crooked pipe test problem.
Technical Report UCRL-MI-143393, Lawrence Livermore National Laboratory, 100, 2000.

Carolyn N. McGraw, Marvin L Adams, W. Daryl Hawkins, Michael P Adams, and Timmie Smith.
Accuracy of the Linear Discontinuous Galerkin Method for Reactor Analysis with Resolved Fuel Pins.
In *Proc. International Conference on the Physics of Reactors*, Kyoto, Japan, Oct. 2014. American Nuclear Society.
Submitted.