Robust and Accurate Methods for Thermal Radiation Transport

Spherical Harmonics and Other Methods

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Recent progress has produced robust spherical harmonics methods

- Unicorns, a word that rhymes with orange, and a robust spherical harmonics method for x-ray radiation transport
  - *Only one of these things exists**
- I wouldn't have been able to say that spherical harmonics can be made robust as little as a year ago
  - *I'll talk about one method*
- In this talk I'll discuss…
  - *Why one might want to develop such a method,*
  - *What are the roadblocks,*
  - *What remains to be done.*
- Along the way they'll show some results
  - *Numerical and analytical*
- I'll also introduce a new way to solve the transport equation that looks to be efficient and accurate
  - *The idea is to split the transport equation based on whether particles have collided during a time step or not.*

What are we solving?

- Specifically, in this talk we will be dealing with radiation transport in high energy density (HED) systems
  - *The radiation is coupled to the material through collisions and the blackbody emission*
- In HED systems radiation transport is a significant contribution to the dynamics of the system
  - *At high enough temperatures the radiation flux and pressure can be comparable to the hydrodynamic energy flux and pressure*
  - *Ignoring radiation therefore ignores much about the evolution of the system.*
- As such, radiation transport is an important part of radiation hydrodynamics calculations where radiation in the system affects the system evolution
  - *E.g. radiating shocks, inertial confinement fusion, lightning*
- Unfortunately, the cost of solving the equations that govern the radiation transport can be prohibitively expensive
  - *The specific intensity of radiation is described by 7 independent variables (3 space, 2 direction, 1 energy, 1 time)*
  - *This makes the issue of developing inexpensive and accurate transport methods critical to high fidelity simulation of rad-hydro systems.*

What are we solving? (continued)

- In this talk we'll be solving the an equation for the transport of gray x-rays coupled to an equation describing the material internal energy

$$\frac{1}{c}\partial_t I + \Omega \cdot \nabla I + \sigma_\mathrm{a} I = \frac{c\sigma_\mathrm{a}}{4\pi} a T^4$$

$$C_\mathrm{v} \partial_t T = c\sigma_\mathrm{a} \left(E_\mathrm{r} - a T^4 \right)$$

- Where

$I(\vec{r}, \Omega, t) =$ specific intensity, $\quad T(\vec{r}, t) =$ material temperature

$E_\mathrm{r}(\vec{r}, t) = \int_{4\pi} d\Omega I(\vec{r}, \Omega, t) =$ radiation energy density

$\Omega \in \mathbb{S}_2 =$ a direction on the unit sphere

$a =$ radiation constant, $\quad c =$ speed of light

$\sigma_\mathrm{a} =$ absorption opacity (units of inverse length)

- No scattering or frequency dependence (for simplicity)

Approaches to solving the transport equation

- Methods for solving the transport equation are generally classified according to how they treat the angular variable (Ω).
- Discrete ordinates methods (S_n) solve the transport equation along particular directions and then use a quadrature rule to compute the radiation energy density.
  - *There has been a lot of work on efficient solution techniques for this method.*
  - *Ray effects can be a problem*
- Monte Carlo methods sample the phase space and track particles along trajectories and stochastically model collisions and emission
  - *Implicit Monte Carlo (IMC) is the most famous and widely used of these methods.*
  - *Can give excellent answers to the patient, though noise and overheating are issues*
  - *Unlike Monte Carlo for linear problems, the limit of an infinite number of particles is not the exact solution (linearization, temporal, and spatial errors in IMC).*
- Spherical harmonics methods (Pn) represent the angular variable using a truncated spherical harmonics expansion.
  - *Can give exponential convergence for smooth solutions*
  - *The truncated expansion leads to oscillations known as wave effects*
  - *Little work has been done on efficient solution techniques*
- Flux-limited diffusion represents the transport operator with a diffusion process
  - *Particles move from high concentrations to low concentrations*
  - *As a result particles flow like smoke*

Why (or why not) the spherical harmonics method?

- Using a orthogonal basis should be accurate in describing the radiation intensity in many cases
  - *More accurate than pointwise estimates*
- When the solution is discontinuous, however, this representation can be misleading
  - *Gibbs phenomenon (oscillations)*
- The intensity and radiation energy density should always be positive for physical reasons.
  - *The oscillations in the spherical harmonics representation can make these negative!*
  - *Worse these can drive the material temperature negative.*
- Except for low order approaches there has been no successful method to eliminate these problems (until recently):
  - *The M_n methods expand in an exponential basis rather than a polynomial basis.*
    - Above n=1 an optimization problem must be solved to find the moments.
  - *Closures for the P_1 equations have been proposed*
    - Minerbo, Kershaw, Levermore-Pomraning, etc.
- There are two techniques that can eliminate these negative solutions and oscillations.

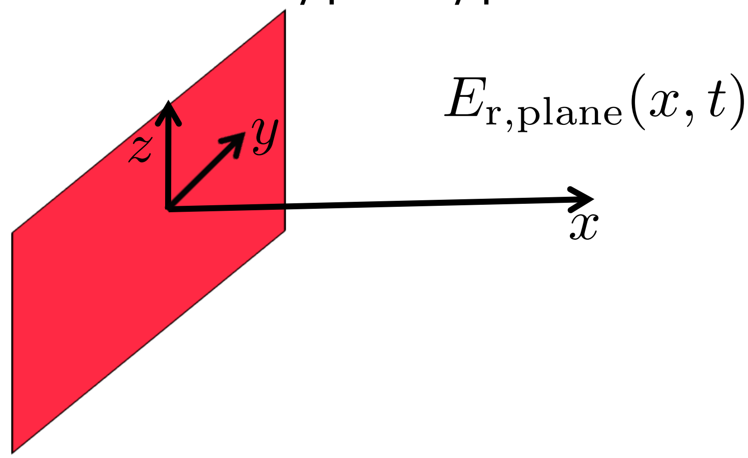
Negative Energy Densities in the P_n solutions

- One might be tempted to say, "I'll just make my *n* high enough so that I avoid these negative solutions."
- It turns out that is not possible to have a finite expansion that is bulletproof to negative solutions.
- Theorem (McClarren, et al): For any finite value of *n* there exists a transport problem where the P_n solution will have a negative energy density.
- Therefore, if we want to guarantee that our solution will never go negative we have to change the expansion or the resulting equations.
- The proof of the theorem gives us a choice of what we must change.
  - *The proof also relies on the plane to point transform by which we write the solution from a point source to the solution from a planar source.*

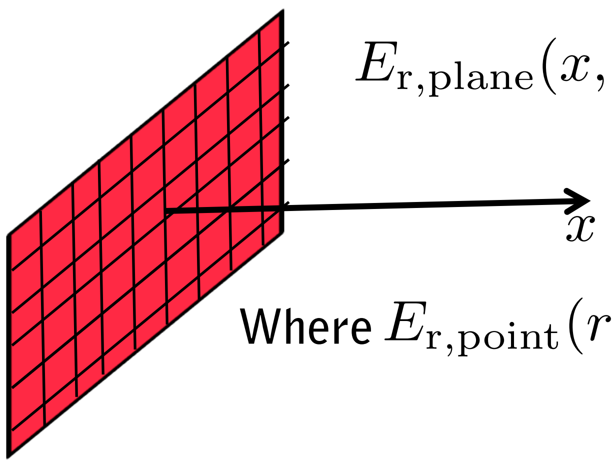
McClarren et al. On solutions to the P-n equations for thermal radiative transfer. Journal of Computational Physics (2008) vol. 227 (5) pp. 2864-2885

Plane to Point Transform

- Consider the solution due to an infinite, pulsed, planar source at x=0.



- Now we can consider the plane as being comprised of many point sources



$$E_{\mathrm{r,plane}}(x,t) = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, E_{\mathrm{r,point}}\left(\sqrt{x^2+y^2+z^2}\right)$$

Where $E_{\mathrm{r,point}}(r,t)$ is the solution at a distance *r* from a point source

Plane to Point Transform

- We can invert this formula to get the solution from a point source in terms of the planar solution:

$$E_{\mathrm{r,point}} = -\frac{1}{2r}\partial_x E_{\mathrm{r,plane}}(x)|_{x=r}$$

- This transform is only valid if the underlying equations are
  - *Linear*
  - *Rotationally invariant*
- In vacuum the solution to the P_n equations from a pulsed, planar source is a series of delta functions traveling out from the origin

$$E_{\mathrm{r,plane}} = \sum_{k=0}^{n} a_k \delta(x - v_k t)$$

- The derivative of this solution is both positive and negative
  - *Therefore, the radiation energy density due to a point source will be negative somewhere.*
  - *This will be the case for any finite n*

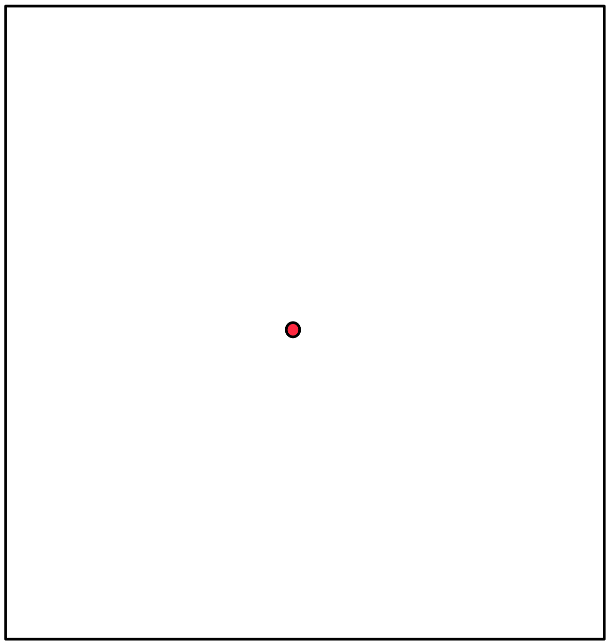
To fix the equations we have a choice

- To use the plane to point transform we needed rotational invariance and linearity.
- The delta functions in the P_n solution were a result of the P_n equations being hyperbolic (information only travels at a finite speed).
- Therefore, we need to break one of these properties to ensure positivity.
- Losing linearity seems to be the best way to go
  - *X-rays do travel with finite speed*
  - *Loss of rotational invariance can cause artifacts in the solution.*
- Discrete ordinates methods are not rotationally invariant
  - *If I rotate the coordinate system, the location of the ordinates changes*
  - *This results in ray effects*
- Diffusion methods are not hyperbolic
- Of course this is just to guarantee positive solutions
  - *We might be able to do some other tricks that make negative solutions go away when they appear.*

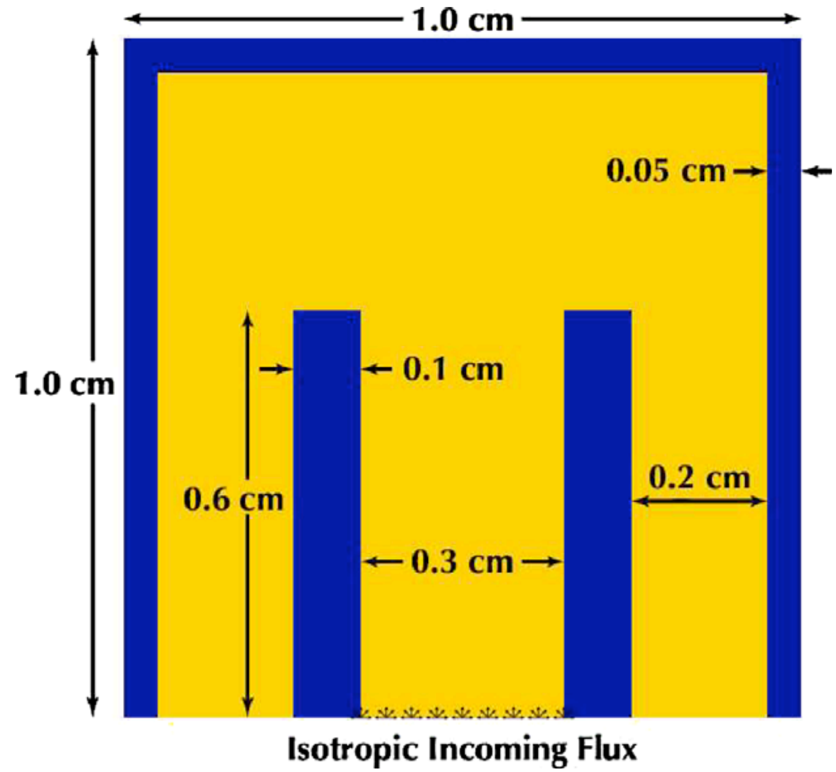
More on negative solutions

- "But my problems don't have any vacuum regions."
- Even if the problems you want to solve don't have any evacuated regions, negativity can still result
  - *On short enough time scales any material behaves like a vacuum.*
    - If I look at time scales much shorter than the time for absorption and re-emission.
  - *In multigroup problems, the some materials might look like a vacuum to the high energy photons.*
- "My problems don't have point sources"
- Shadows in the solution can also lead to negative energy densities
  - *A shadow looks like a step function in angular space, fitting this with spherical harmonics will lead to negative values.*
- In spherical geometry in the absence of point sources, negatives should not be a major problem
  - *Can't have a shadow in this geometry*
- Moreover, if I have very coarse spatial grids and time steps the negative parts of the solution might be smeared out.

P_7 Negative Solution Examples

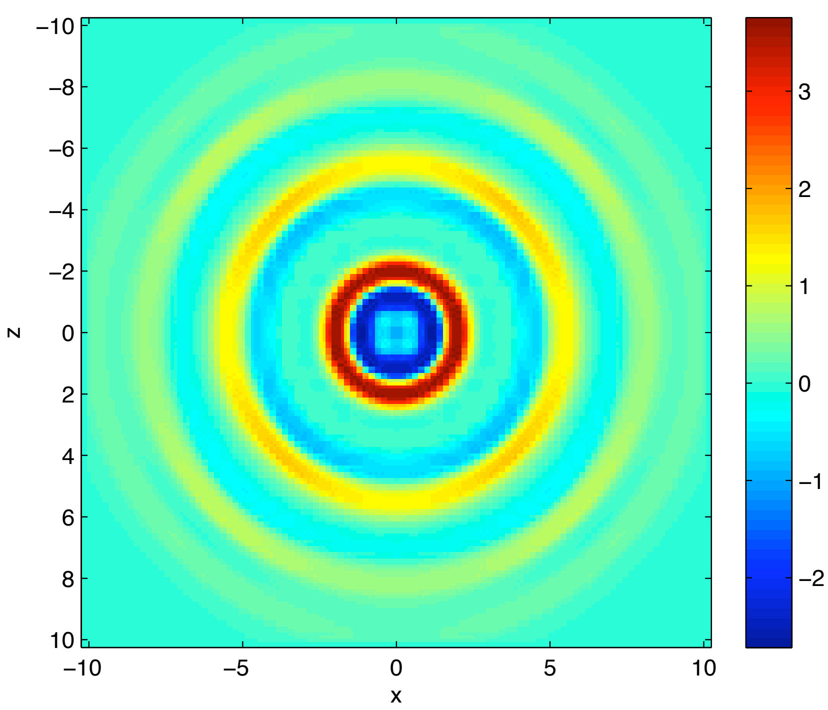


Infinite, pulsed line source



Transport down a duct

P_7 Negative Solution Examples



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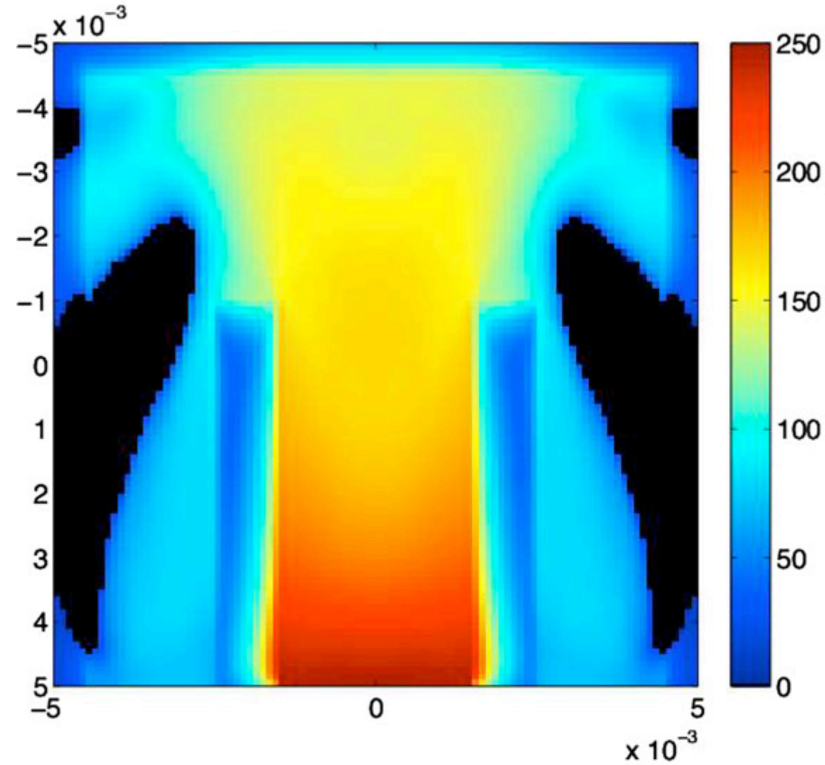


Transport down a duct

The Filtered P_n (FP_n) Method

McClarren and Hauck, "Robust and Accurate Filtered Spherical Harmonics Expansions for Radiative Transfer", J. Comput. Phys., 229, 16, 5597-5614, 2010.
McClarren and Hauck, "Simulating Radiative Transfer with Filtered Spherical Harmonics", Phys Ltr. A, 374,22, 2290-2296, 2010.

The P_n Reconstruction

- The standard P_n reconstruction of the specific intensity is

$$I \approx \sum_{l=0}^{n} \sum_{-l}^{l} Y_l^m(\Omega) I_l^m \quad \text{where} \quad I_l^m = \int_{4\pi} I(\Omega) \bar{Y}_l^m(\Omega)\, d\Omega$$

- This representation is usually derived by a straightforward expansion.
- It is possible to derive this form as the result of an variational problem
- Minimize the functional

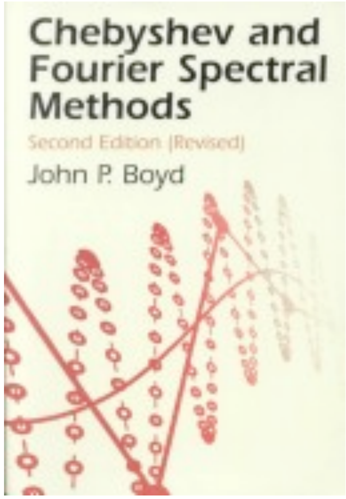
$$\mathcal{J} = \int_{4\pi} \left(I(\Omega) - \sum_{l=0}^{n} \sum_{-l}^{l} Y_l^m(\Omega) I_l^m \right)^2 \, d\Omega$$

over the I_l^m functions.
- The solution to this problem gives the standard expansion.
- This optimization problem tells us that the P_n expansion minimizes the square of the error
-

Truncating a spherical harmonic series: is it wise?

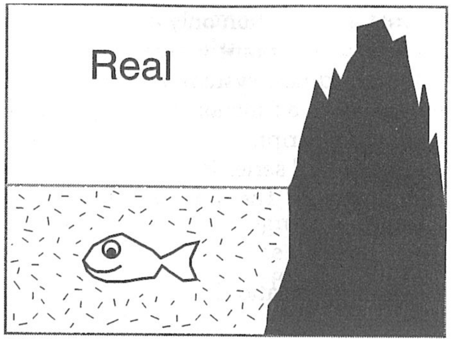
Truncating a spherical harmonic series: is it wise?

"Truncating a [spherical harmonics] series is a rather stupid idea."
John P. Boyd, *Chebyshev and Fourier Spectral Methods*



Gibbs Errors are the reason

- As alluded to earlier, the Gibbs errors near sharp features are the reasons truncating is *unwise.*
- In Boyd's book he uses this figure (from geophysics) to illustrate his point



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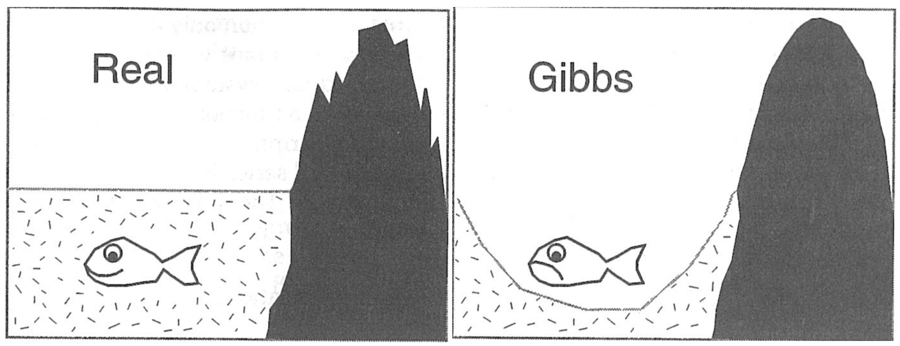

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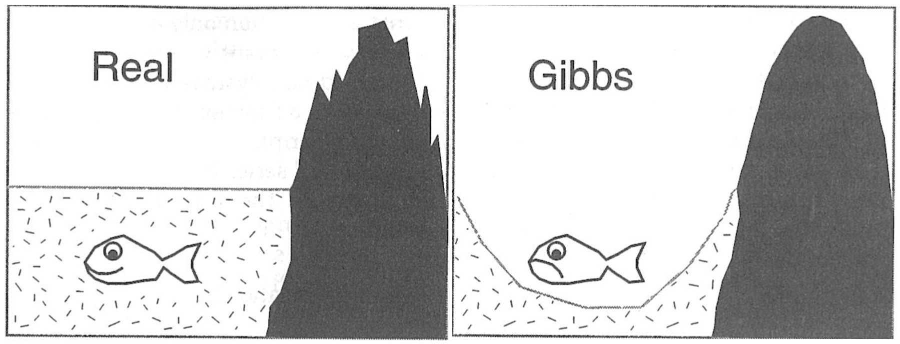


- A standard spherical harmonics expansion can't capture the flat ocean next to the mountain
  - *Making the fish rather unhappy*
- In transport these errors give us the negative solutions.
- The answer is to change the expansion so that these errors are eliminated (or at least reduced).

A modified reconstruction

- If we change the variational problem to minimize

$$\mathcal{J} = \int_{4\pi} \left[\left(I(\Omega) - \sum_{l=0}^{n} \sum_{-l}^{l} Y_l^m(\Omega) \hat{I}_l^m \right)^2 + \alpha \left(\nabla_\Omega^2 \sum_{l=0}^{n} \sum_{-l}^{l} Y_l^m(\Omega) \hat{I}_l^m \right)^2 \right] d\Omega$$

  where **α**>0 is a parameter called the filter strength.
- This new functional penalizes oscillations because it includes the derivative.
- The resulting expansion is termed a filtered spherical harmonics expansion.
- The solution to the above problem is

$$\hat{I}_l^m = \frac{I_l^m}{1 + \alpha l^2 (l+1)^2}$$

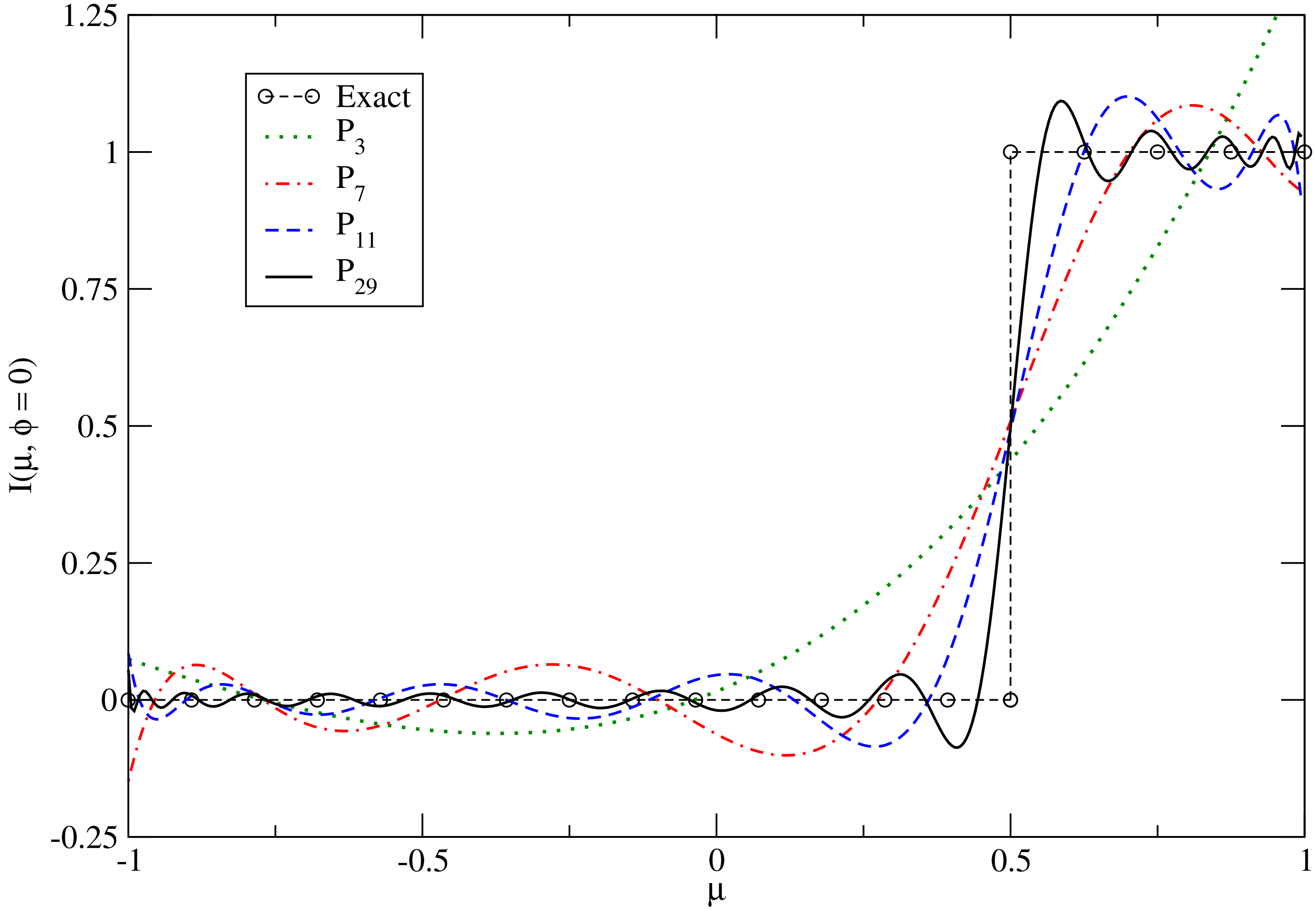
- The filtered expansion is the standard expansion where the coefficients are forced to decrease as *l* increases.

Properties of the filtered expansion

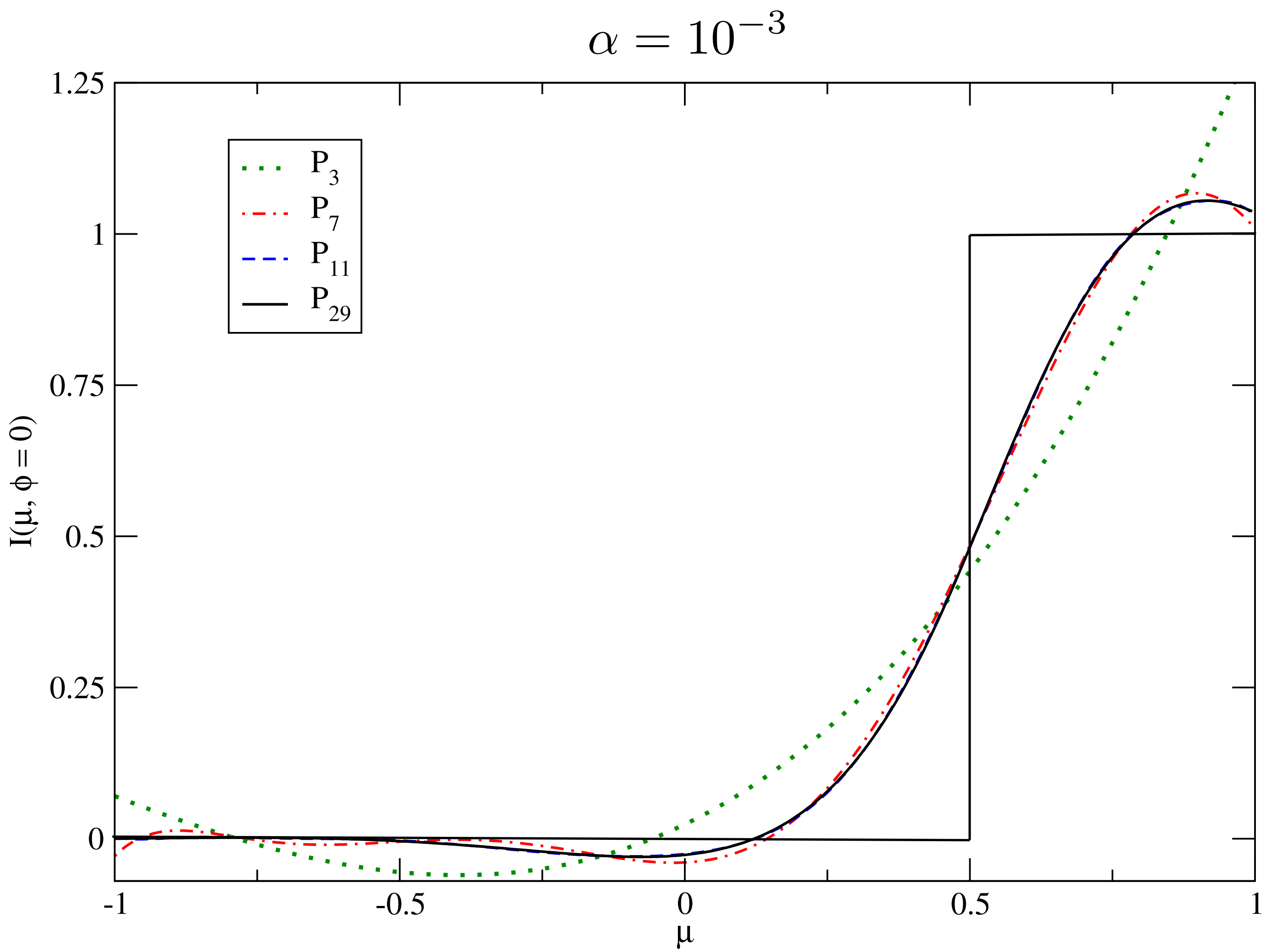
$$\hat{I}_l^m = \frac{I_l^m}{1 + \alpha l^2 (l+1)^2}$$

- In the limit of zero filter strength the standard expansion is recovered.
- We still truncate the expansion at some order
  - *The moments before the truncation will be decaying*
- The zeroth moment is not affected by the filter
  - *Number of particles is preserved.*
- The equation of how to choose the filter strength has not been addressed
  - *Picking a large filter strength would kill oscillations but might adversely affect the solution.*
- If the filter strength is not picked as a function of the moments, then negative solutions could arise
  - *The filtered expansion and resulting equations are still rotationally invariant and hyperbolic.*
  - *We'll see that this isn't necessary in most problems.*

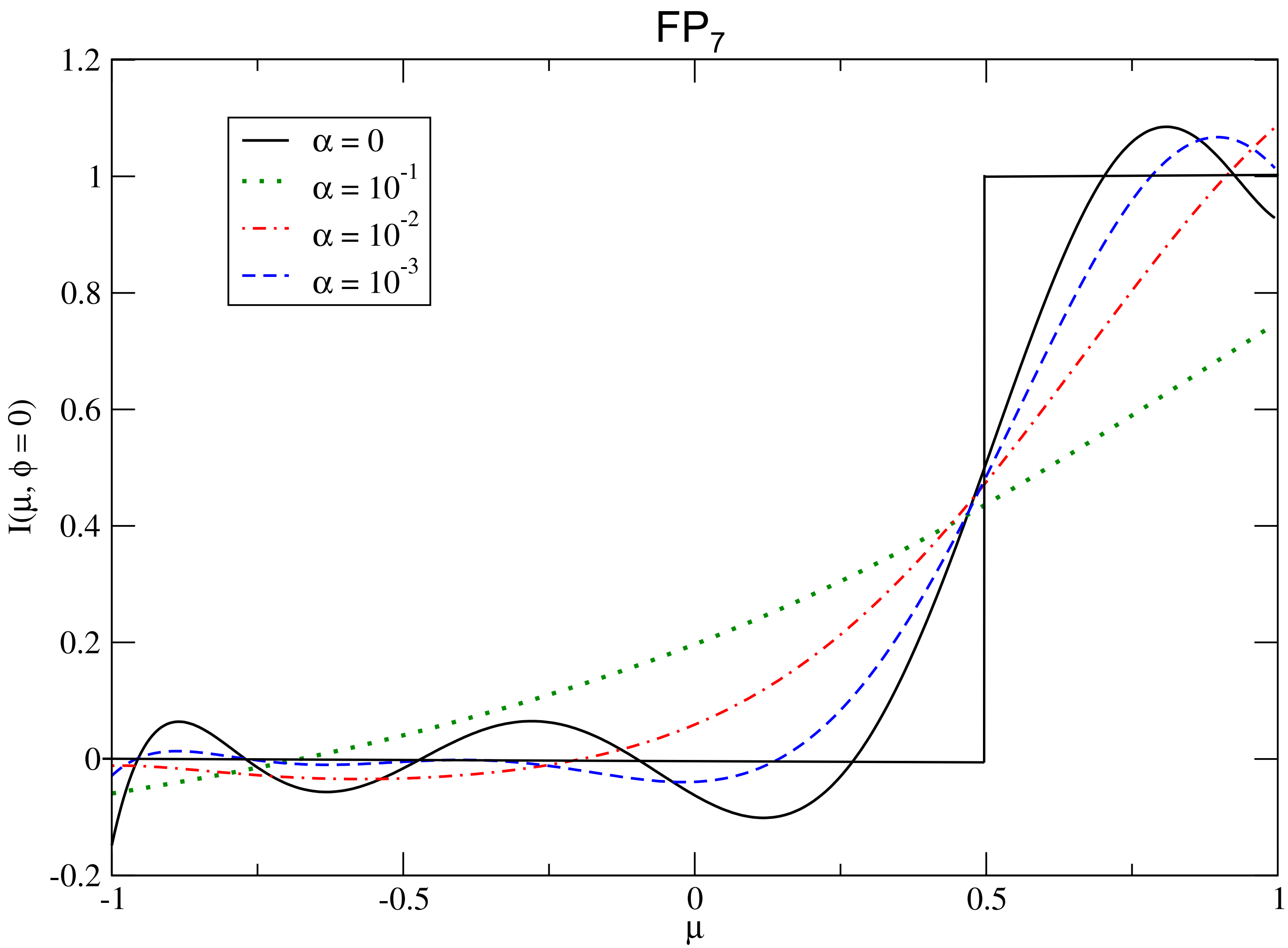
Standard Expansion Example: Shadow



Filtered Expansion Example: Shadow



Filtered Expansion Example: Shadow



Choosing the Filter Strength

- We want to choose the filter strength that
  - *Minimizes oscillations*
  - *While doing the least damage to the solution.*
- The examples demonstrated that the strength should decrease as the order of the expansion is increased.
- Also, the filter is most needed in regions of free streaming (i.e. where the material opacity is small).
  - *Absorption and re-emission by the material relaxes the intensity towards an isotropic distribution.*
- With these in mind we choose the following form

$$\alpha = \frac{\omega}{n^2(\sigma_{\mathrm{a}} L + n)^2}$$

L is a characteristic length (to make the strength dimensionless), n is the order of the expansion, and ω is a user defined, positive parameter

- This form preserves the equilibrium diffusion limit
  - *Specifically, for ϵ small and positive*

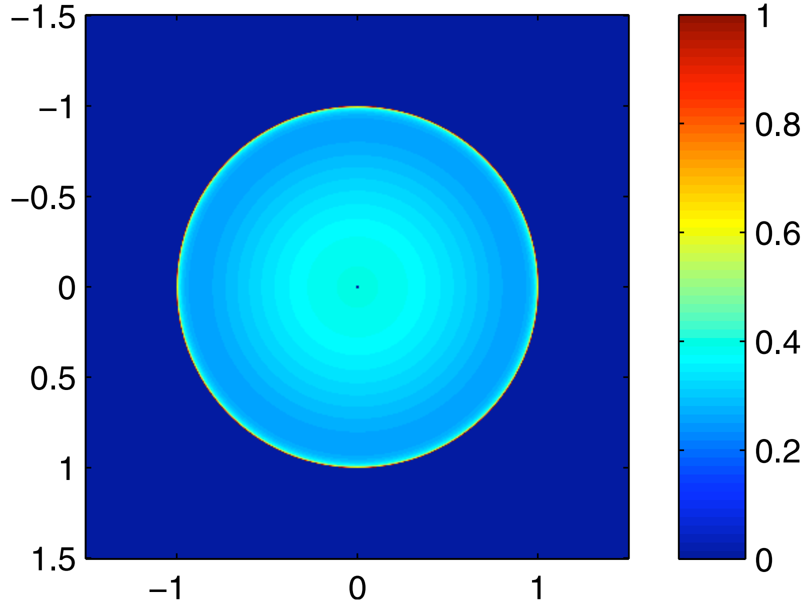
$$\sigma_{\mathrm{a}} = O(\epsilon^{-1}) \;\rightarrow\; \alpha = O(\epsilon^2)$$

Implementation

- To date the filtered Pn expansion has been implemented by adding a source term to the standard Pn equations.
- For an explicit code the source term basically acts as applying the filter to the expansion after every time step.
- When solved implicitly, the source acts as a forward peaked scattering term.
- The results I'll show here use
  - *A bilinear discontinuous Galerkin finite element spatial discretization*
  - *Second-order semi-implicit time integration*
- For the filter strength we set
  - *L=1 cm*
  - $\omega = c\Delta t / \Delta x$
- These parameters were used in all computations.

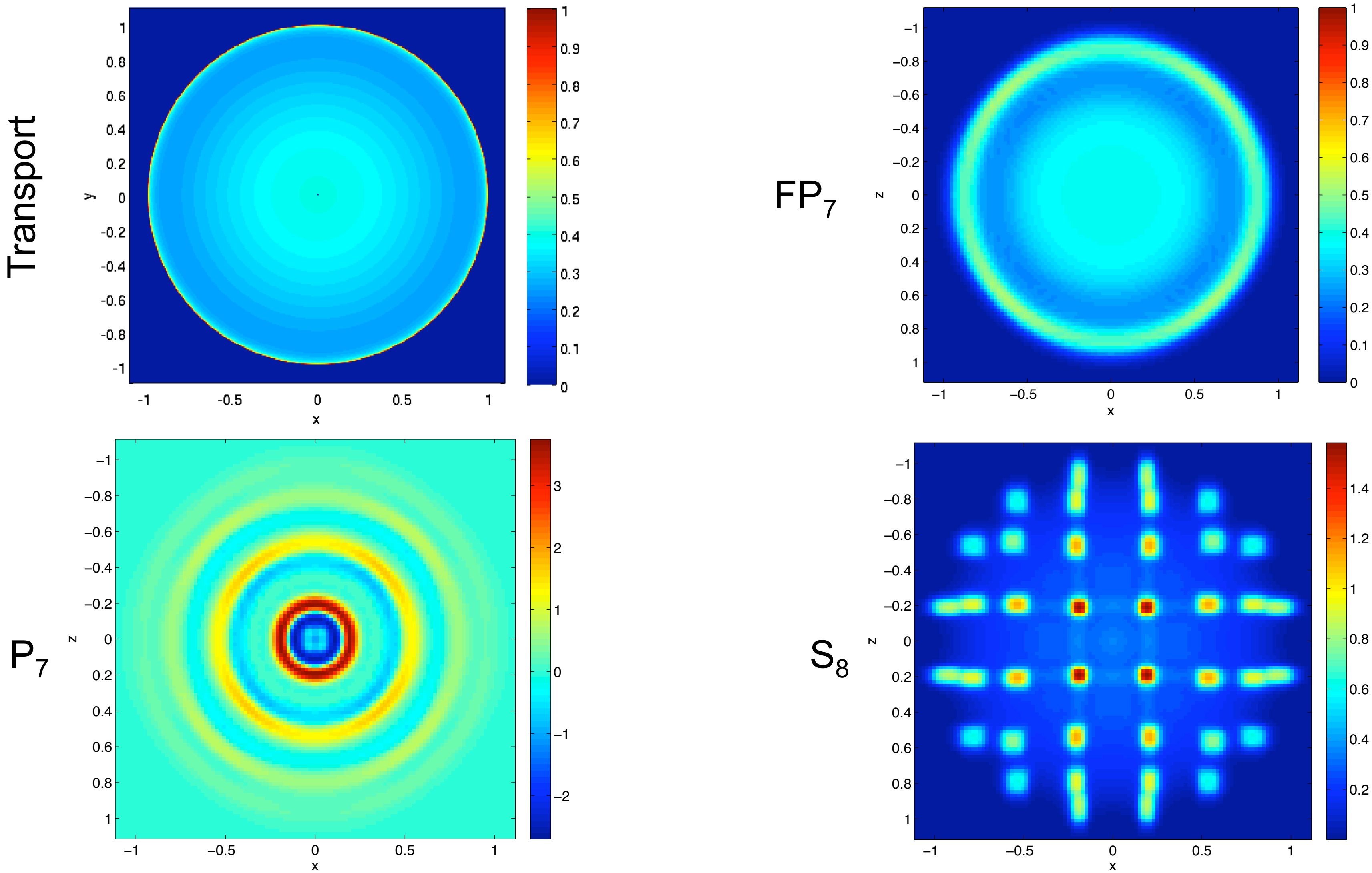
Pulsed Line Source Results

- The first problem we solve is a 2-D Cartesian problem
  - *initial condition* $I(\vec{r},\Omega,0) = \delta(x)\delta(y)$
  - *Pure scattering medium.*
- There is an analytic transport solution to this problem (Ganapol).
- This is a hard problem
  - *Delta function of uncollided particles*
  - *Smooth region of collided particles*
- Both P_n and S_n methods have a hard time with this problem.
  - *Gibbs errors and ray effect respectively*

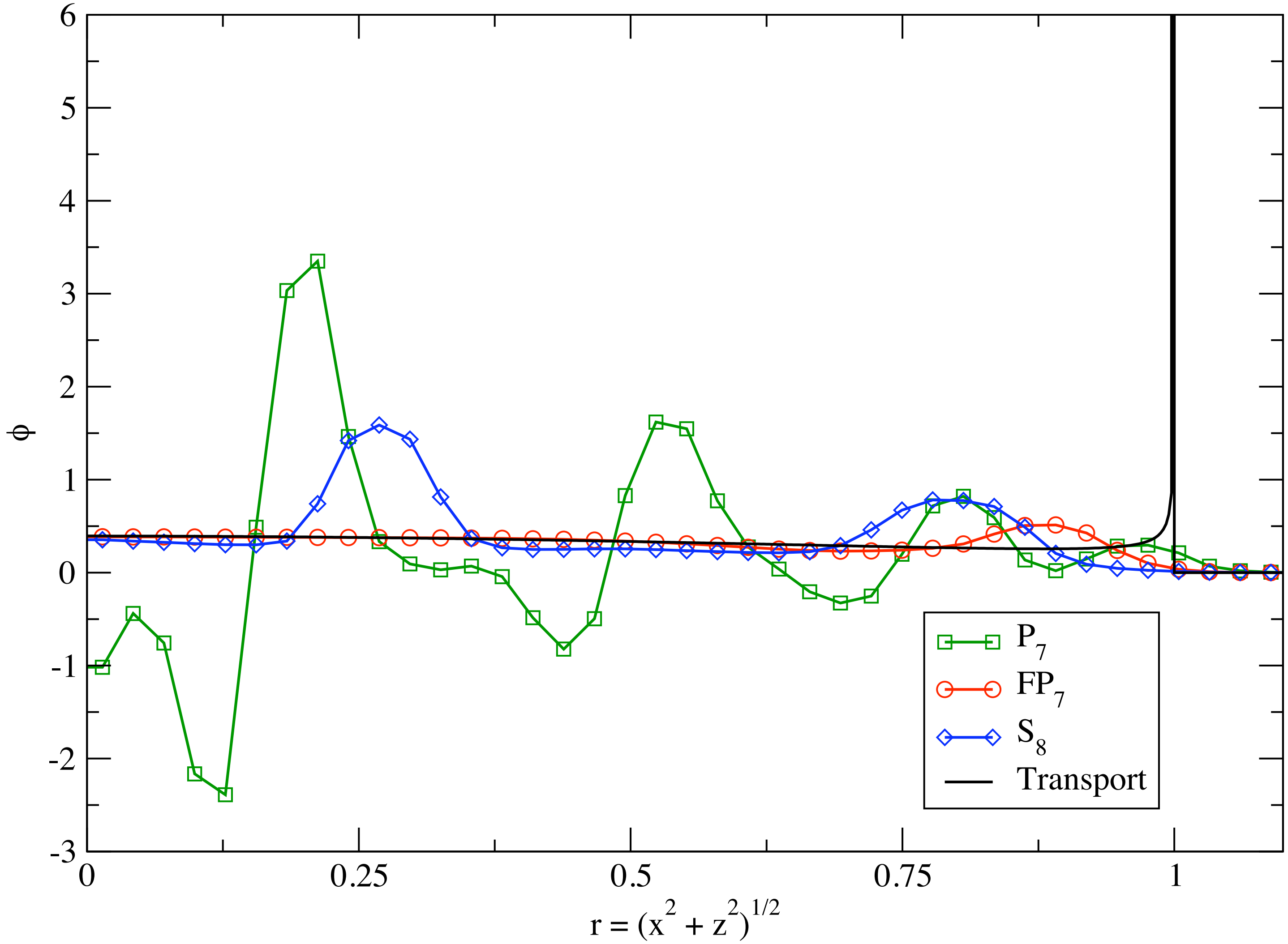


Analytic Radiation Energy Density at t = 1/c

Pulsed Line Source Results at t=1/c

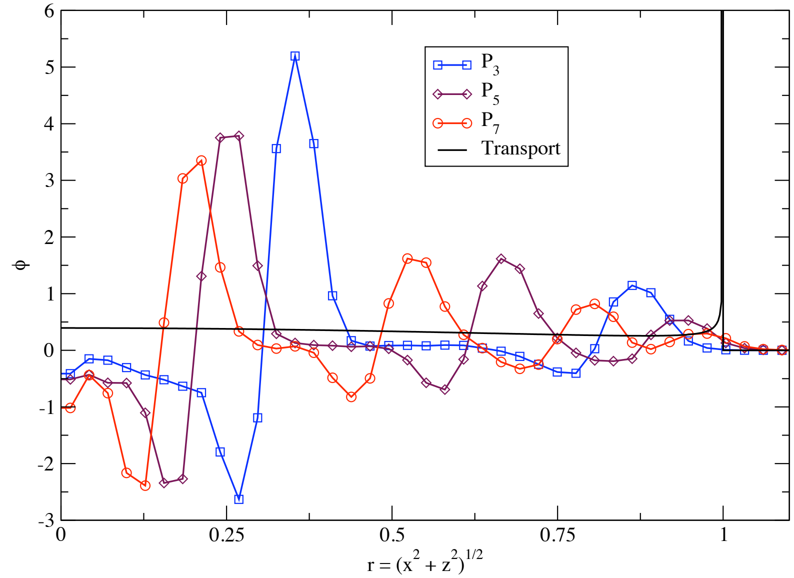


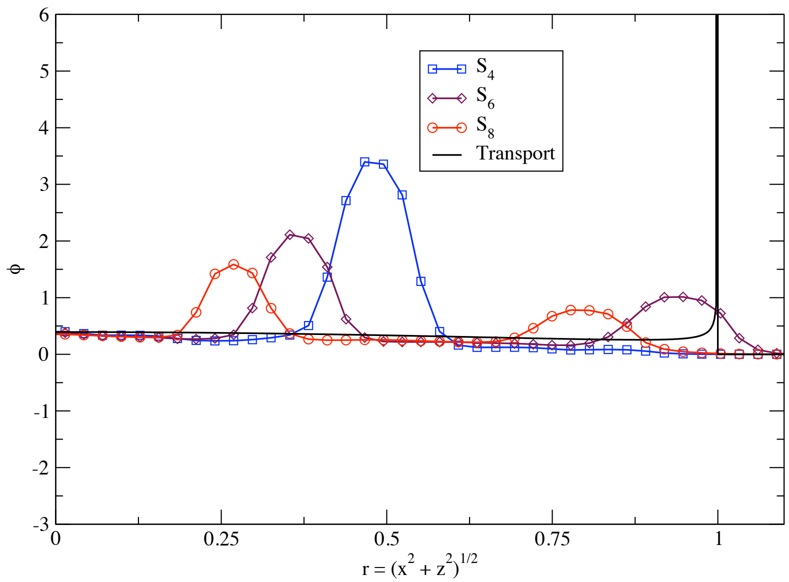
Lineout at t=1/c

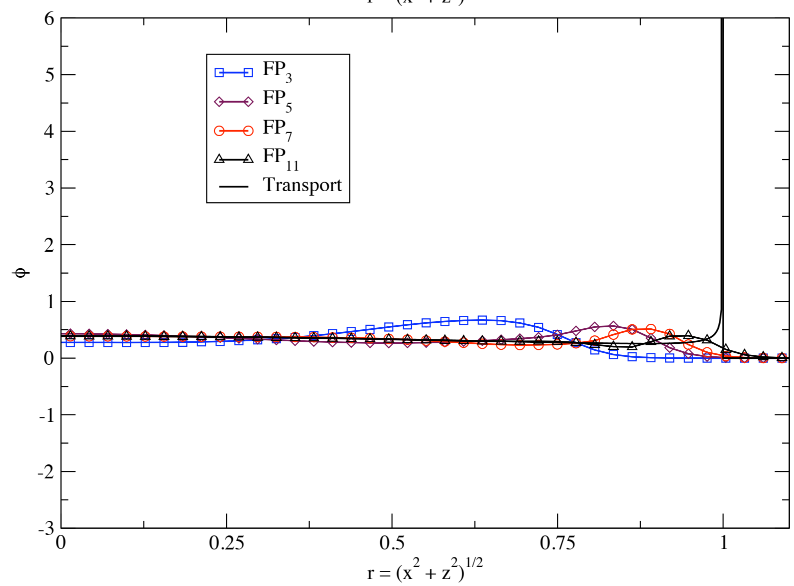


Lineout at t=1/c

- The P_n results are not converging very well
  - *The location of the oscillations is changing*
- The FP_n solutions are converging
  - *Location of hump moving to 1*
- S_n hard to tell

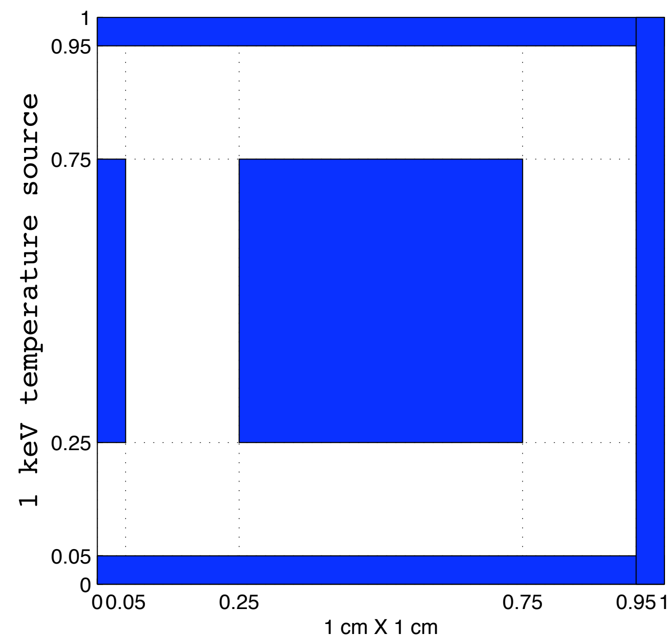






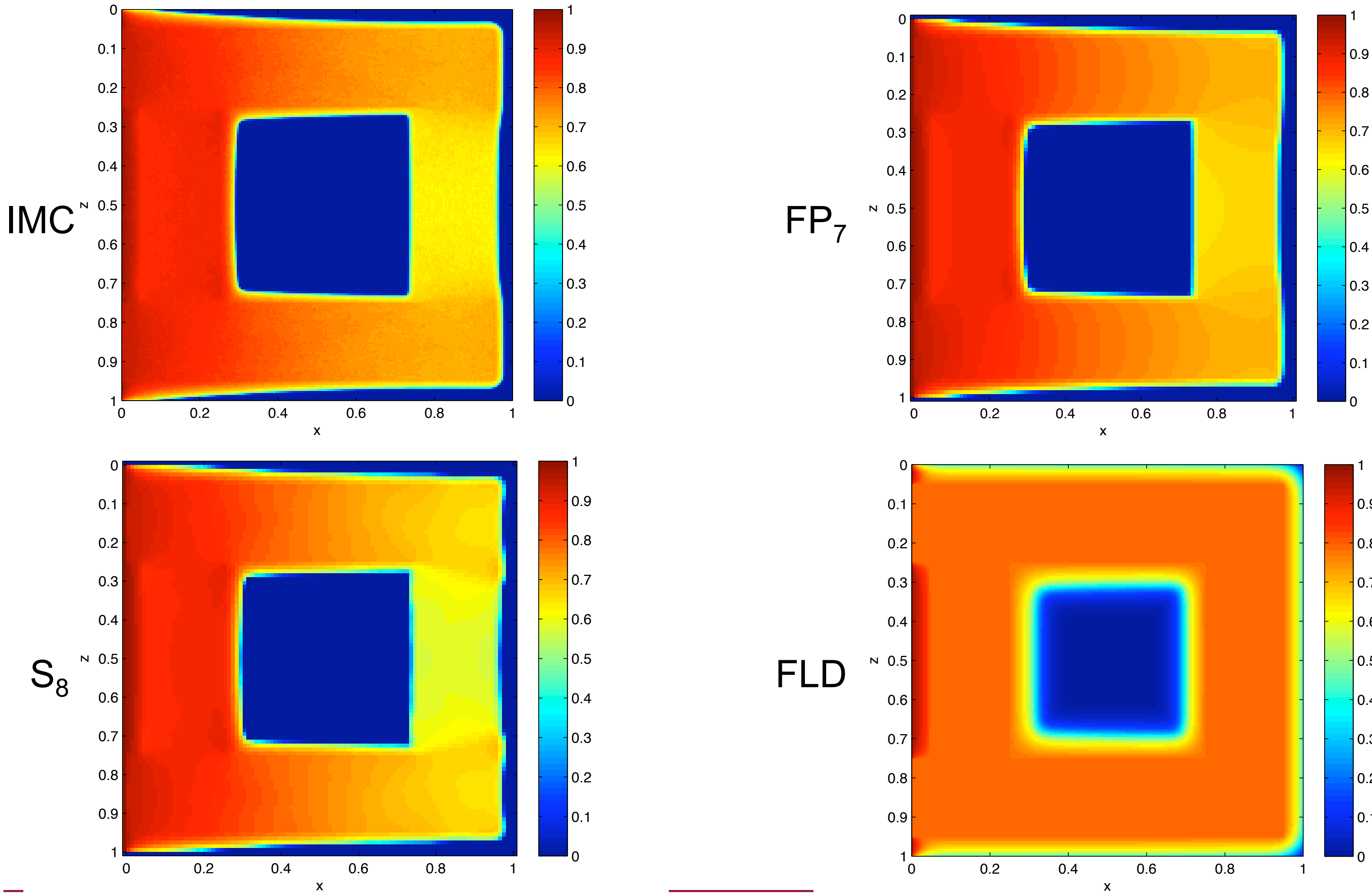
Cartesian Hohlraum problem

- A Hohlraum like configuration in x-y geometry
  - *Vacuum region (white)*
  - $\sigma_{\mathrm{a}} = 100T^{-3}$ *for T in keV (blue)*
  - *Constant specific heat*
- Using the standard P_n method
  - *The material temperature went negative*
  - *This caused the simulation to crash*
- We'll compare
  - *IMC*
  - S_n
  - FP_n
  - *FLD*
- In the solution we expect to see a shadow behind the center block
  - *Until the walls heat up*



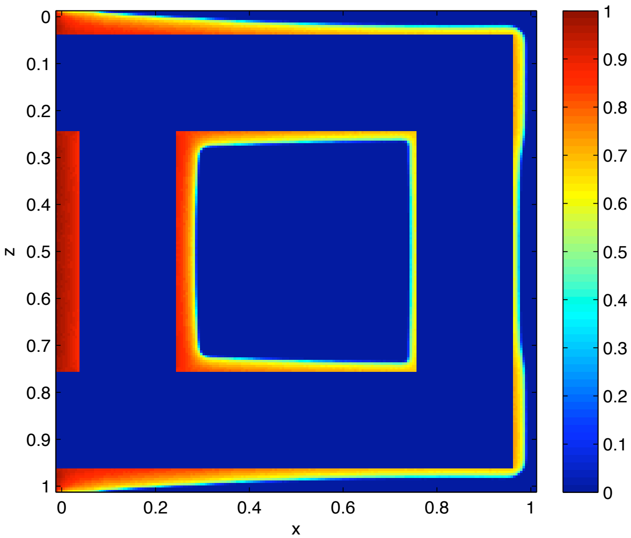
Problem Layout

T_{rad} Hohlraum Results at t=0.1 sh

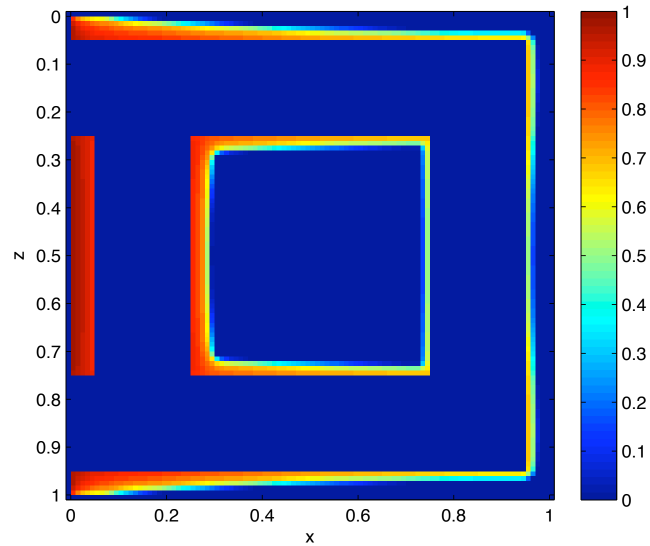


T_{mat} Hohlraum Results at t=0.1 sh

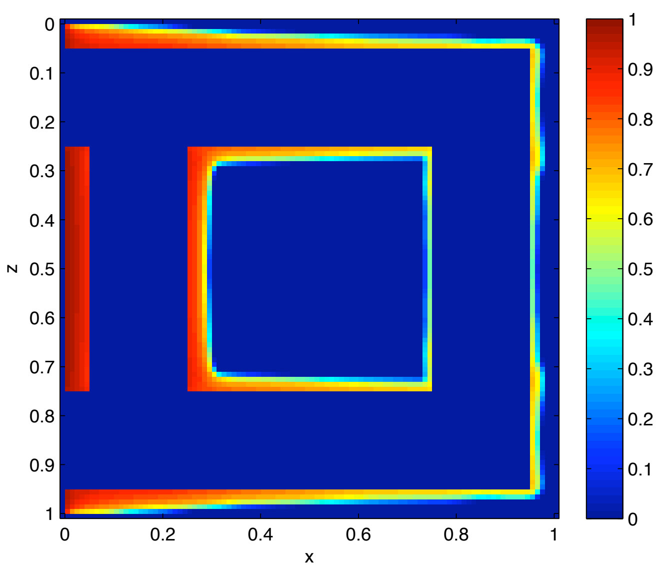
IMC



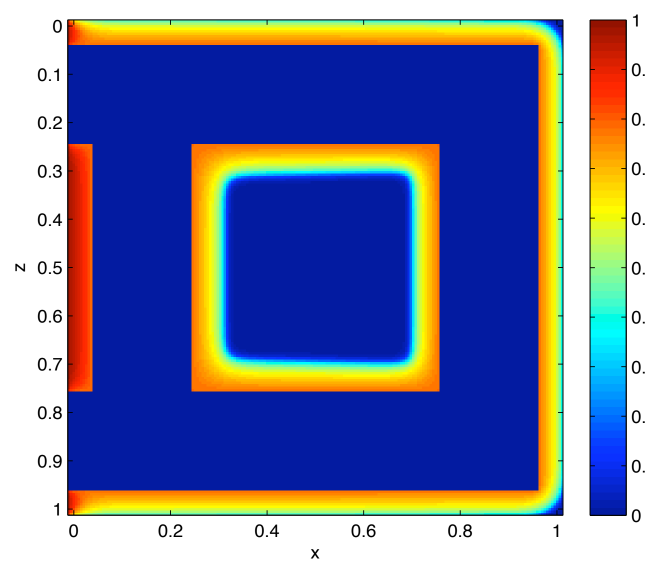
FP_7



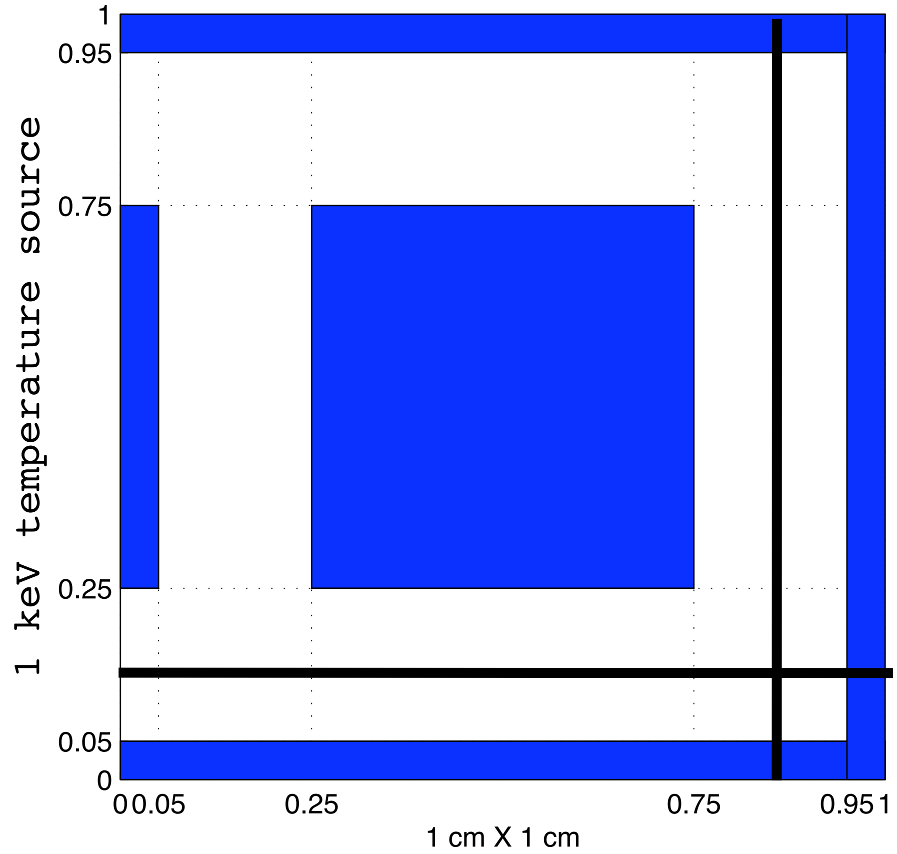
S_8



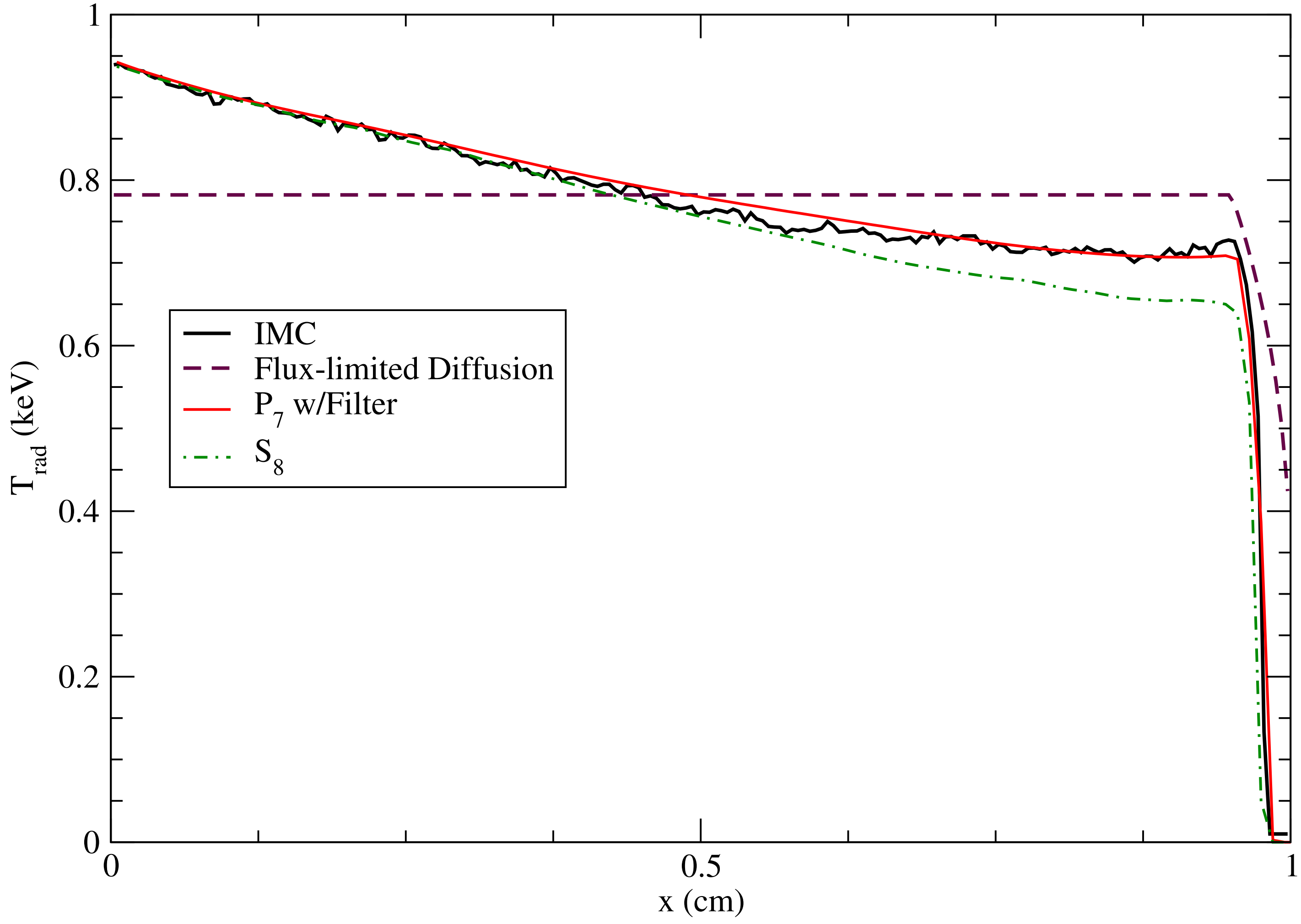
FLD



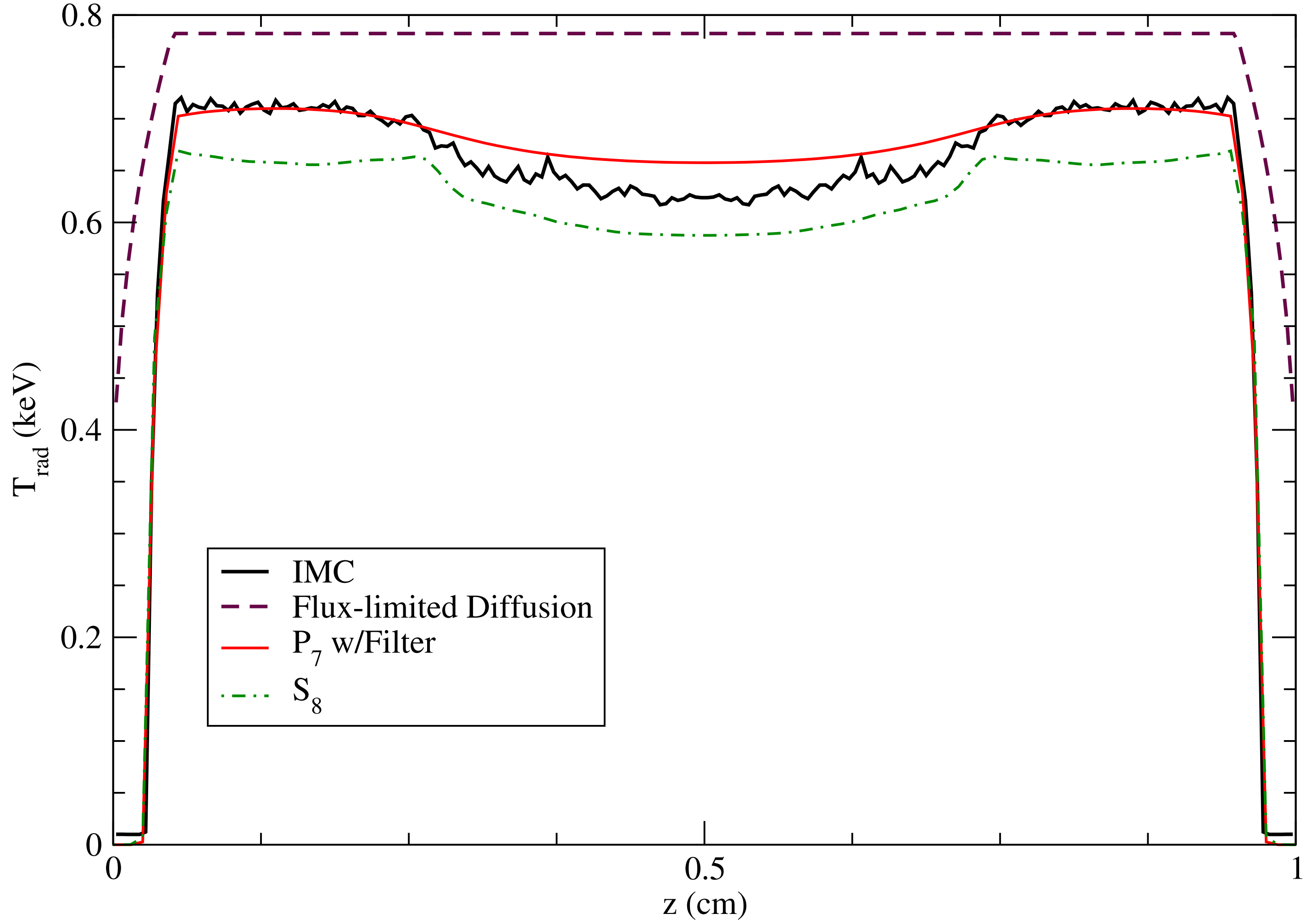
Lineouts at 0.1 sh



Lineout at y = 0.125 cm, t= 0.1 sh



Lineout at x = 0.85 cm, t= 0.1 sh



These results are encouraging

- Gibbs Errors are a problem with spherical harmonics methods
  - *Using a filter on the expansion addresses this problem*
- On two challenging problems the FP_n method performed well
  - *It was clearly the best method on the line source problem.*
  - *Gave comparable accuracy to IMC on the hohlraum problem*
- This method deserves strong consideration as a deterministic transport option.
- Still some investigation to be performed
  - *Multigroup: group dependent filters*
  - *RZ and 3D geometry*
  - *Time dependent filters*
  - *Efficient numerical methods*

A Collisional Splitting Scheme for Radiation Transport

There are two important limits of the transport equation.

- When there is no scattering or emission, the directions of particle travel don't talk to each other

$$\frac{1}{c}\partial_t I + \Omega \cdot \nabla I + \sigma_{\mathrm{a}} I = Q$$

  - *The solution at r is just an integral from the source Q to r*
- The opposite case where absorption/emission dominates leads to a diffusion equation for the material temperature

$$C_{\mathrm{v}}\partial_t T + a\partial_t T^4 = \nabla \frac{ac}{3\sigma_{\mathrm{a}}} \nabla T^4$$

- How one solves the equation in each case would be different
- In the streaming dominated case
  - *Ray tracing, integral transport, etc.*
- In the diffusion case
  - *Low order transport (P_1, S_2)*
  - *Flux-limited diffusion*
- Many problems have regions of both types or are intermediate
  - *The hohlraum problem we talked about above had both regions*
  - *Different groups might be thin or thick in a multifrequency calculation*

The common approach

- Takes a method that works well in one limit and tries to fix it in the other.
- Not a lot of success in doing this.
- Implicit Monte Carlo is efficient in optically thin media
  - *Inefficient in a diffusive medium due to tracking lots of collisions.*
  - *Discrete Diffusion MC and other approaches attempt to address this*
- Discrete Ordinates methods
  - *Have ray effects in thin regions*
  - *Ray effect mitigation techniques are not very robust*
  - *Biased quadrature sets can help.*
  - *It optically thick regions, the solutions can be more expensive.*
- Spherical Harmonics works in thick problems
  - *Gibbs errors in streaming dominated regions*
  - *Filtered expansions attempt to address this.*
- Flux-limited diffusion
  - *Can work well in thick problems*
- Other methods exist, but not works well in all problems.

Idea: Split the transport equation based on whether particles have collided or not

- Consider the transport equation with the emission source linearized over a time step

$$\frac{I^{n+1}-I^n}{c\Delta t}+\Omega\cdot\nabla I^{n+1}+\sigma_{\mathrm{a}}I^{n+1}=\frac{(1-f)\sigma_{\mathrm{a}}c}{4\pi}E_{\mathrm{r}}^{n+1}+\frac{f\sigma_{\mathrm{a}}}{4\pi}acT_n^4$$

- Now, write the intensity as $I=I_u+I_c$ and rearrange the equations

$$\Omega\cdot\nabla I_u^{n+1}+\sigma_{\mathrm{a}}^*I_u^{n+1}=\frac{f\sigma_{\mathrm{a}}}{4\pi}acT_n^4+\frac{I_u^n+I_c^n}{c\Delta t}$$

$$\Omega\cdot\nabla I_c^{n+1}+\sigma_{\mathrm{a}}^*I_c^{n+1}=\frac{(1-f)\sigma_{\mathrm{a}}c}{4\pi}\left(E_{\mathrm{r,c}}^{n+1}+E_{\mathrm{r,u}}^{n+1}\right)$$

where $\sigma_{\mathrm{a}}^*=\sigma_{\mathrm{a}}+\dfrac{1}{c\Delta t}$

- These split equations have split the transport problem into
  - *A pure absorber equation for particles that have not collided during the time step*
  - *An equation with an isotropic source for particles that have collided during the time step.*

What does this split buy me?

- The first equation can be solved using a method that is accurate and efficient for pure absorber problems
  - *Monte Carlo (won't have to track multiple collisions)*
  - *High order discrete ordinates (one transport sweep)*
  - *Ray tracing, etc.*
- The solution to the second equation should be close to isotropic
  - *Use a low order transport method (or diffusion) to solve it*
- Only one equation contributes in the limits
  - *In the free streaming limit only the uncollided equation contributes*
  - *In the diffusion limit only the collided equation matters*
- We then can get transport effects nearly for free
  - *In one sweep or history per particle*
- Can get arbitrary accuracy:
  - *Have the flexibility to solve either piece with as accurate a method as I want.*
- The split can be generalized into an arbitrary number of steps
  - *Instead of doing one collision then the collided equation, I could do more*
- This split could be easily implemented in existing codes
  - *IMC code with a DDMC option (Use IMC on uncollided, DDMC for collided)*
  - *S_n code with diffusion preconditioning*

Coupling low order to high order transport approximations is not new.

- The quasi-diffusion method (Goldin 1964) uses discrete ordinates to compute the particle pressure tensor,
  - *This particle pressure is used to close the diffusion equation.*
  - *In principle this method solves the full transport equation*
  - *Computing the pressure cannot be done in one transport sweep.*
- Diffusion-Monte Carlo methods have been proposed
  - *Simulate the particles with Monte Carlo until they enter a diffusive region, then make them "diffusion" particles.*
  - *Treating the interfaces between regions is tricky.*
- Using the discrete ordinates equations to inform diffusion has been proposed for gas cooled nuclear reactors (Larsen 2009)
  - *Under certain conditions one can compute an anisotropic diffusion tensor using one or several transport sweeps.*
- Splitting the method based on whether or not a particle has collided is new.

Example: Flux-limited Diffusion for the collided equation

- We can solve the system via the following procedure:
  - *Solve the uncollided equation via ray tracing or high order S_n*

$$\Omega \cdot \nabla I_u^{n+1} + \sigma_{\mathrm{a}}^* I_u^{n+1} = \frac{f\sigma_{\mathrm{a}}}{4\pi} acT_n^4 + \frac{I_u^n + I_c^n}{c\Delta t}$$

  - *Then compute* $E_{\mathrm{r},u}^n = \dfrac{1}{c}\displaystyle\int_{4\pi} I_u^{n+1}\, d\Omega$
  - *Then solve the diffusion equation with a flux limiter*

$$-\nabla \cdot D^n \nabla E_{\mathrm{r},c}^{n+1} + \left(f\sigma_{\mathrm{a}} + \frac{1}{c\Delta t}\right) E_{\mathrm{r},c}^{n+1} = (1-f)\sigma_{\mathrm{a}} E_{\mathrm{r},u}^{n+1}$$

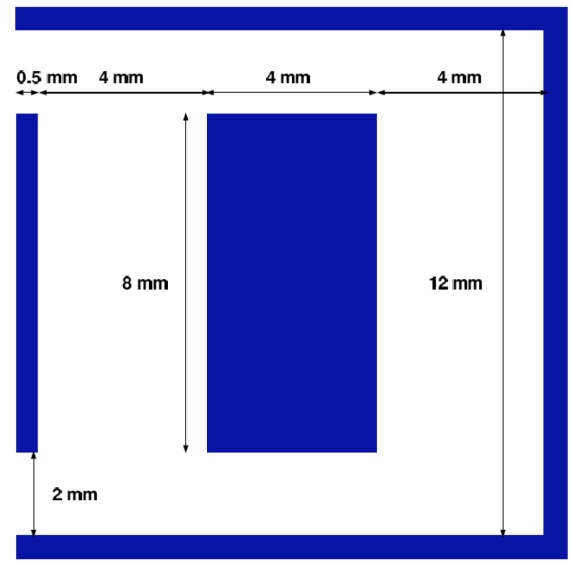
$$D^n = \left((3\sigma_{\mathrm{a}}^*)^2 + \frac{|\nabla E_{\mathrm{r}}^n|^2}{(E_{\mathrm{r}}^n)^2}\right)^{1/2}$$

  - *Finally, compute*

$$I_c^{n+1} = \frac{1}{4\pi c} E_{\mathrm{r},c}^{n+1} - \frac{1}{3\sigma_{\mathrm{a}}^* c}\Omega \cdot \nabla E_{\mathrm{r},c}^{n+1}$$

Initial 2-D Results for Linear Transport

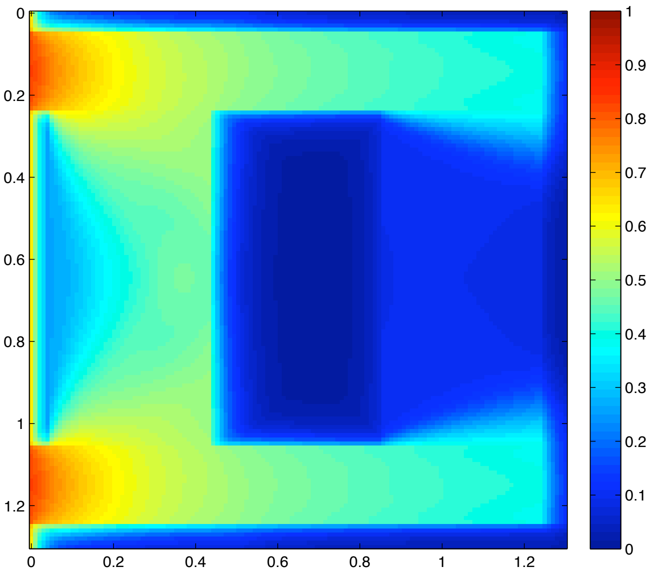
- A Hohlraum like configuration in x-y geometry
  - *Vacuum region (white)*
  - *Strong scattering (blue)*
- To solve this problem we generally need to have very high angular accuracy to capture the correct solution.
- The results demonstrate that we only need high order treatments in the uncollided part to get good answers.
- We'll compare
  - S_{20}
  - S_8
  - *FLD*
  - *Split* S_{20}/*FLD*



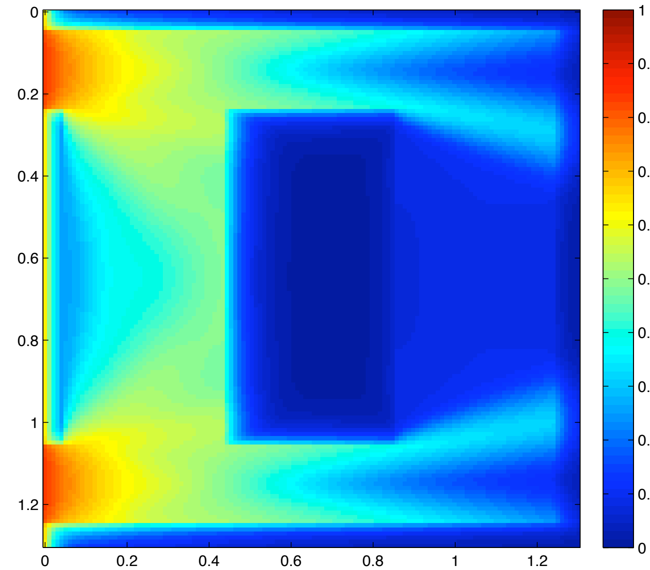
Problem Layout

2-D Results at t = 1.3/c

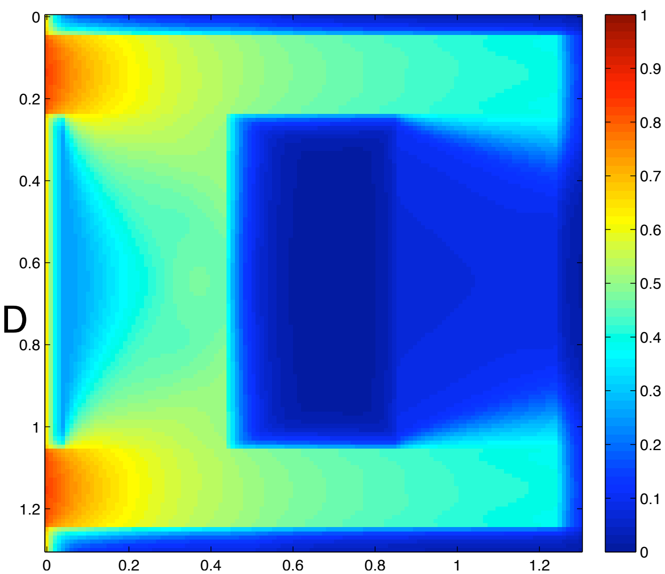
S_{20}



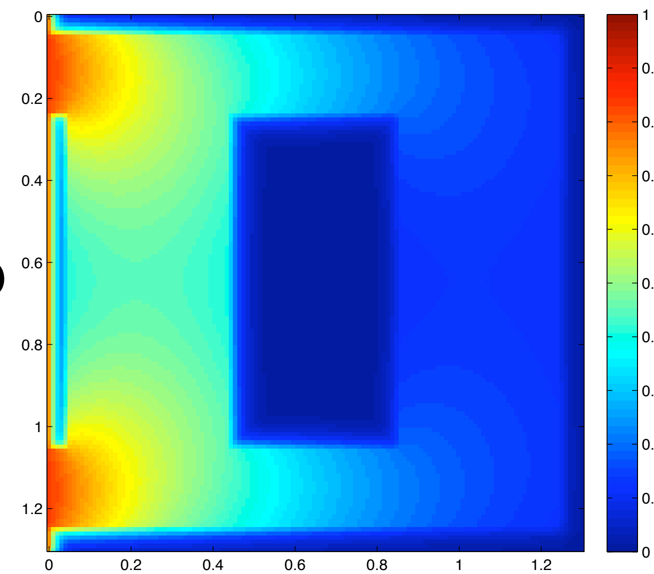
S_8



Split S_{20}/FLD



FLD



Performance on 2-D Problem

- Given that this is a simple implementation with first-order spatial discretizations,
  - *it is hard to say that this new method is going to revolutionize transport calculations.*
- We did observe, however, that the Split solution only spent 10% of the solution time solving the uncollided part
  - *This is notable because for this 10% effort all of the features of the high-order transport solution were captured.*
  - *How this will work in other problems is an open question.*
- Still a lot to look into
  - *We did not analyze how material interfaces behave*
    - These might require an asymptotic preserving method.
  - *Boundary conditions we not discussed*
    - The most straightforward implementation is to have all incoming particles treated as uncollided
    - Reflecting boundaries?
  - *Better time accuracy*
    - Higher order integration is desireable in some problems
      - *TBDF-2 and other robust scheme should apply to this technique*
    - To make the split more accurate we could use Strang splitting
  - *I only used high order S_n to solve the uncollided equation*
    - Need to look at Monte Carlo and integral techniques for this equation.

New methods for HED radiative transfer are being developed

- The spherical harmonics method, in its standard form, has robustness issues
  - *Gibbs errors lead to negative energy densities*
  - *These errors also hurt accuracy of method*
  - *Negative solutions can arise regardless of order of expansion*
- By applying a filter to the spherical harmonics expansion
  - *The robustness issues are addressed*
  - *Accuracy is greatly improved*
    - Comparable with IMC on a hohlraum problem
- Initial work looking at splitting the transport equation based on collisions during a time step look promising
  - *Split the solution during a time step into*
    - A pure absorber problem
    - A scattering problem with isotropic source
  - *Get transport effects for a fraction of the cost*
- Combining these developments could be fruitful.
- Still work to be done
  - *The future looks bright.*

Thank you for listening

The Positive P_n (PP_n) Method

Hauck and McClarren, The Positive Pn Method, SIAM Journal on Scientific Computing, in press

The Positive P_n method guarantees a positive solution

- The standard spherical harmonics reconstruction is the solution to an optimization problem

Given a set of spherical harmonic moments

$$I_l^m = \int_{4\pi} Y_l^m(\Omega) I(\Omega)\, d\Omega \quad 0 \le l \le n,\ -n \le m \le n$$

$$\text{minimize:} \quad \int_{4\pi} f(\Omega)^2\, d\Omega$$

$$\text{subject to:} \quad \int_{4\pi} f(\Omega) Y_l^m(\Omega)\, d\Omega = I_l^m \quad 0 \le l \le n,\ -n \le m \le n$$

- The solution to this problem is

$$f(\Omega) = \sum_{l=0}^{n} \sum_{m=-l}^{l} I_l^m Y_l^m(\Omega)$$

The Positive P_n method guarantees a positive solution

- We modify the optimization problem to guarantee a positive reconstruction

$$\text{minimize:} \quad \int_{4\pi} f(\Omega)^2 \, d\Omega$$

$$\text{subject to:} \quad \int_{4\pi} f(\Omega) Y_l^m(\Omega) \, d\Omega = I_l^m \quad 0 \le l \le n, \; -n \le m \le n$$

$$\text{and } f \ge 0$$

- We can't enforce the constraint everywhere (this would be an infinite number of constraints)
  - *Instead we replace the integrals with a quadrature rule and enforce positivity at each quadrature point*
- We can then use this form of *f* as a closure
- We have effectively made the P_n method nonlinear and not rotationally invariant

Numerical Issues

- The positive P_n method requires solving an optimization problem in every spatial cell for every time step
  - *These solves can be time consuming for large values of n*
  - *This problem is completely local and therefore scalable.*
- One has to choose a quadrature rule and order
  - *The quadrature rule must integrate order n spherical harmonics exactly*
  - *Using product quadrature we found using a quadrature of order 2n was most efficient*
- The value of the solution at the quadrature points does not need to be stored between time steps, only the moments.
- To guarantee that there exists a solution to the optimization problem
  - *One needs to make sure that the spatial and temporal discretizations do not introduce negative solutions.*
  - *To accomplish this we have used first order discretizations.*