# Open Problems in the Preconditioning of Moment-based Transport Equations

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# The transport equation

- We are interested in solving the transport equation for the angular flux, **Ψ** of particles (e.g. neutrons, gammas, etc.)
- The equation we need to solve is of the form

$$\Omega \cdot \nabla_x \psi(x,\Omega) + \sigma_t \psi = \int_{4\pi} d\Omega' \, \sigma_s(\Omega \cdot \Omega')\psi(x,\Omega') + Q.$$

- We have left out the time or energy dependence, because their presence doesn't affect the system solution (too much).
- This is an integro-differential equation. The spatial variables can be handled using typical methods
  - ⇒ *Finite element*
  - ⇒ *Finite difference*
  - ⇒ *Etc.*

# 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*

# There has been recent interest in moment-based methods

- Recent developments have tried to address the shortcomings of the Pn approach.
- The Pn method is a spectral method in angle. (McClarren & Hauck 2010)
  - ⇒ *As with other spectral methods, discontinuities in angle lead to Gibbs' phenomenon.*
  - ⇒ *Applying a filter to the expansion has proven effective in removing oscillations*
- High-order/Low-order methods, that use a transport method (e.g. Monte Carlo) to compute a closure that is updated using a low-order method (e.g. diffusion)
- The positive Pn method seeks to create reconstructions of the angular flux based on strictly positive reconstructions by solving an optimization problem (Hauck & McClarren 2009).

# 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.

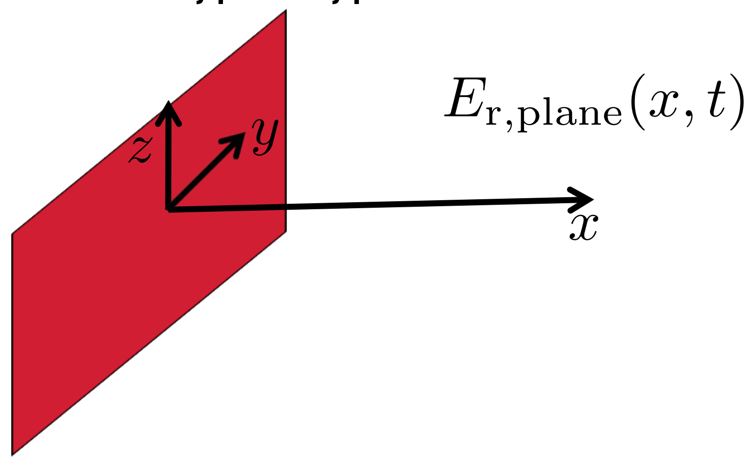
# Negative Energy Densities in the $P_n$ solutions

- 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.*

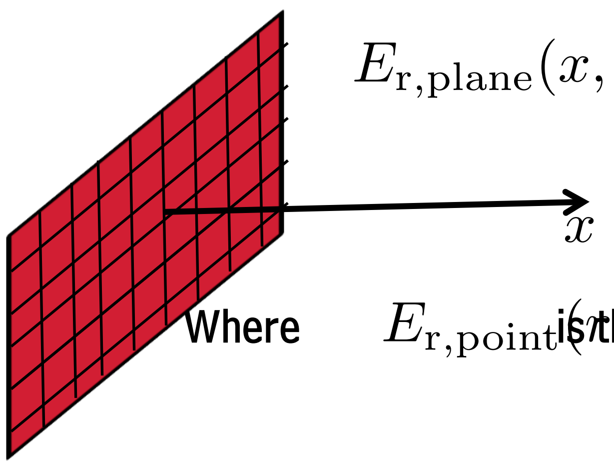
McClarren et al. On solutions to the P-n equations for thermal radiative transfer. Journal of Computational Physics (2008) vol. 227 (5) pp. 2864-2885

# 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

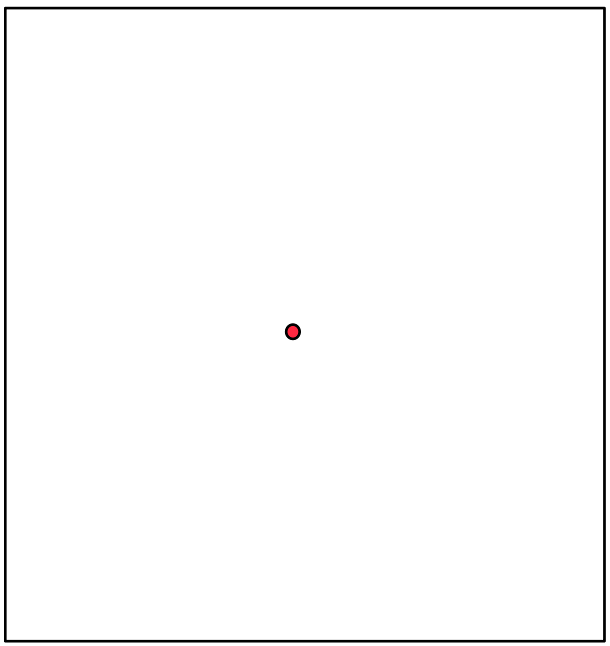


- Of course this is just to guarantee positive solutions

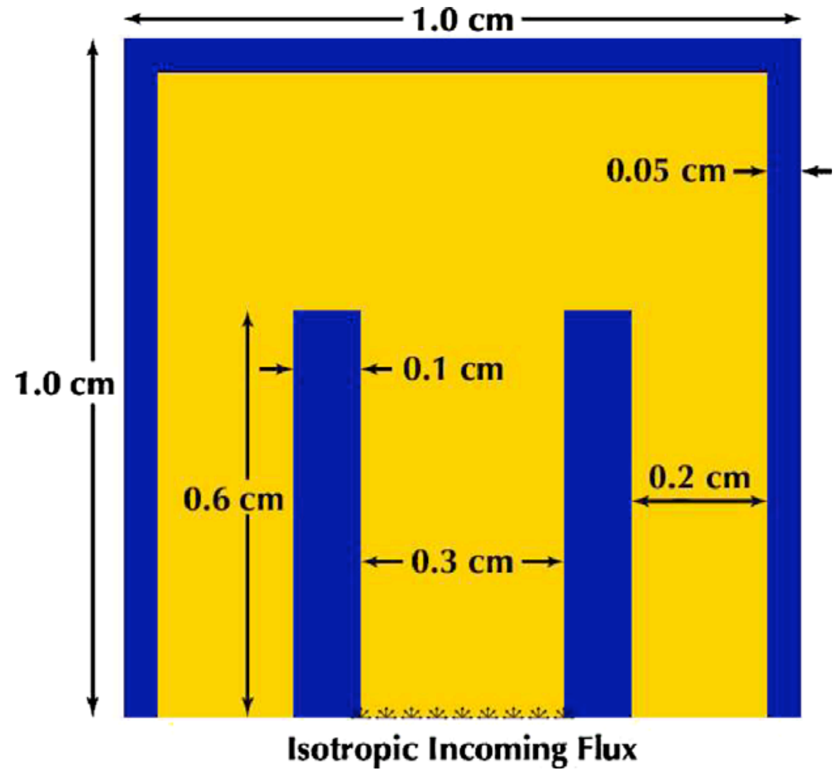
# More on negative solutions

- "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

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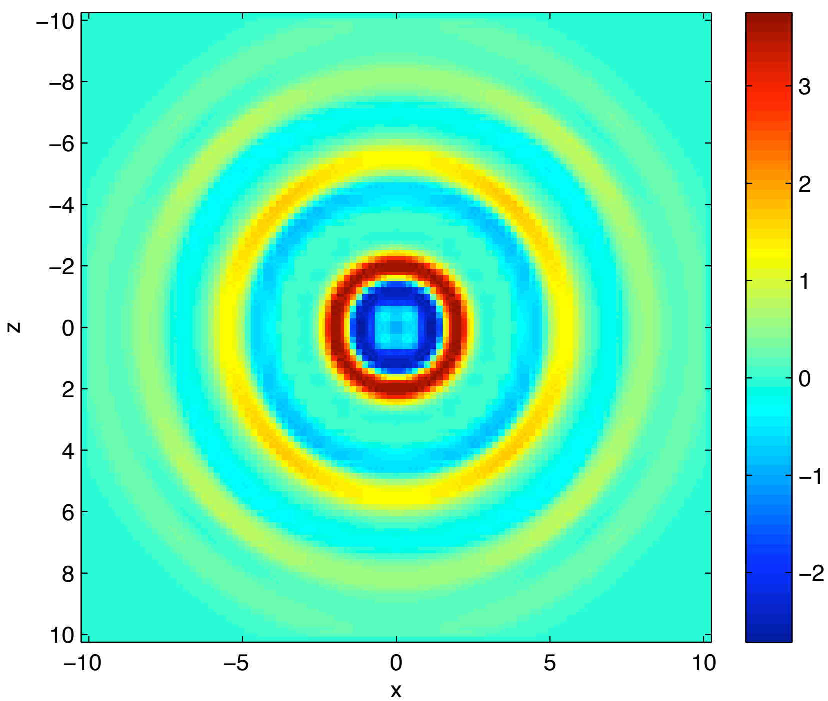


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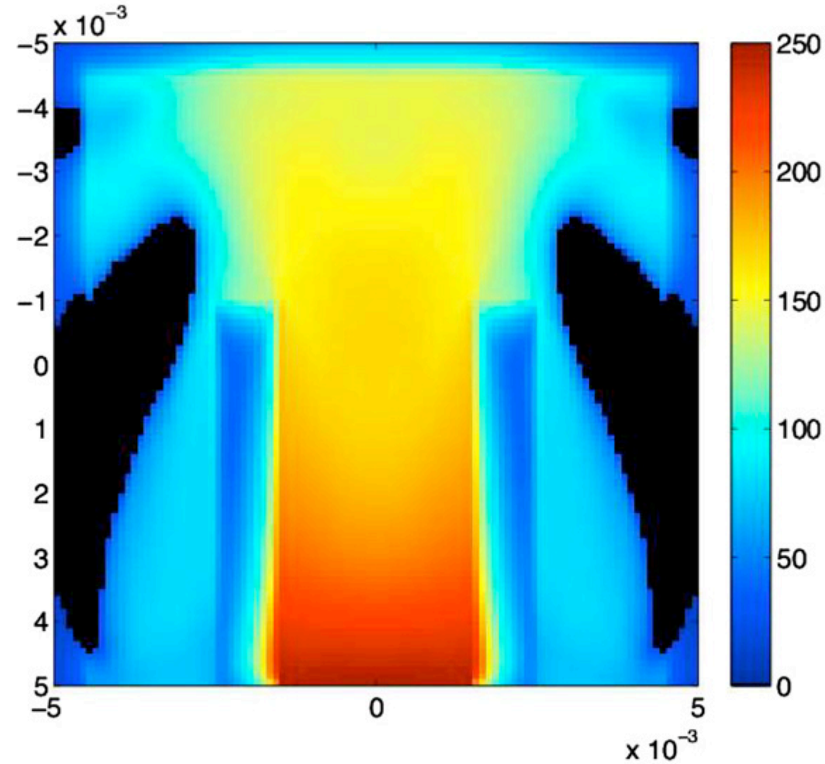


Transport down a duct

# Truncating a spherical harmonic series: is it wise?

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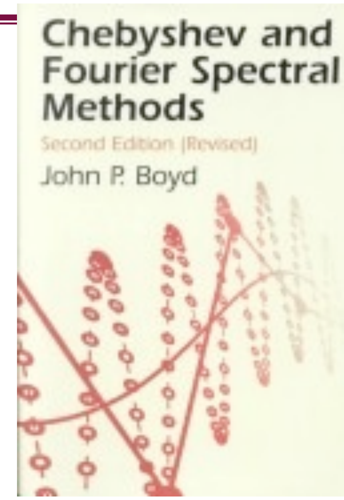
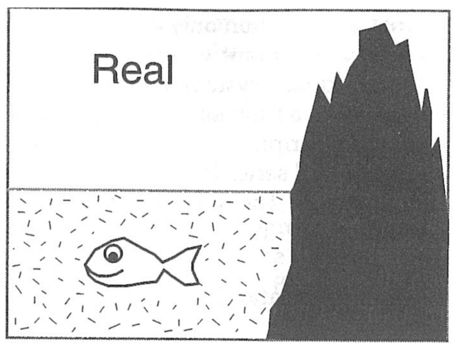



"Truncating a [spherical harmonics] series is a rather stupid idea."

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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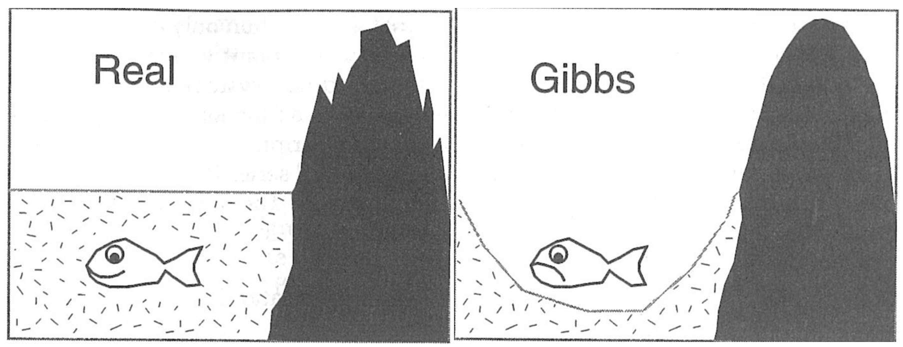

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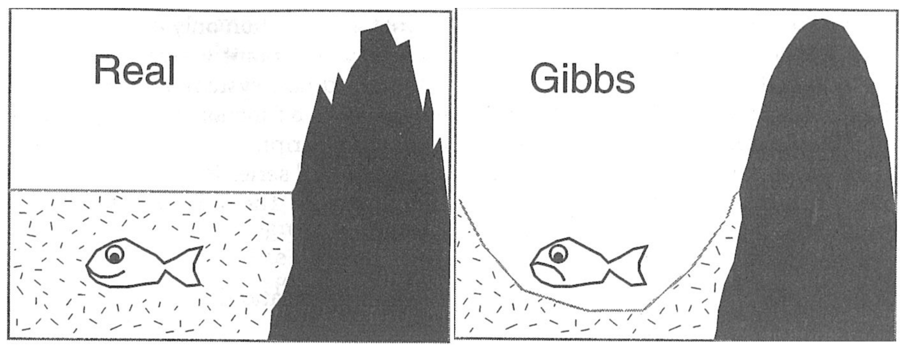
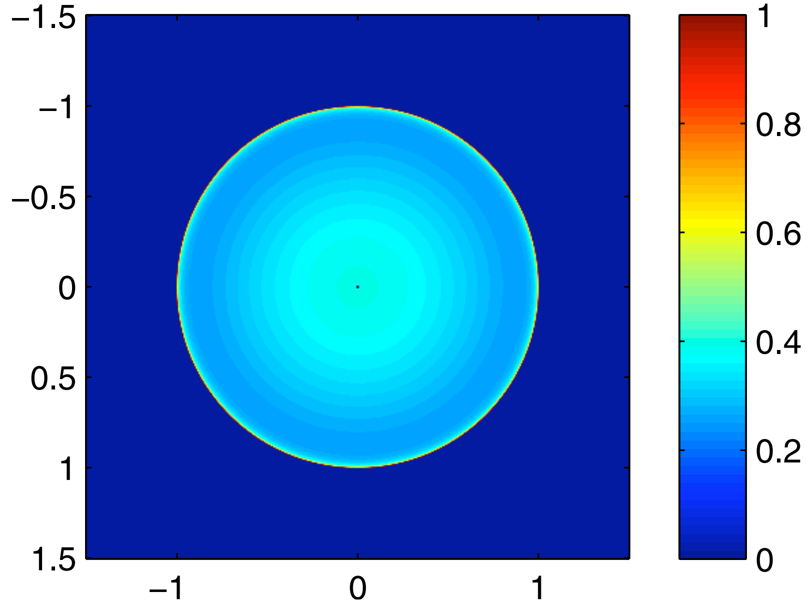



- A standard spherical harmonics expansion can't capture the flat ocean next to the mountain
  - ⇒ *Making the fish rather unhappy*
- In transport these errors give us the negative solutions.

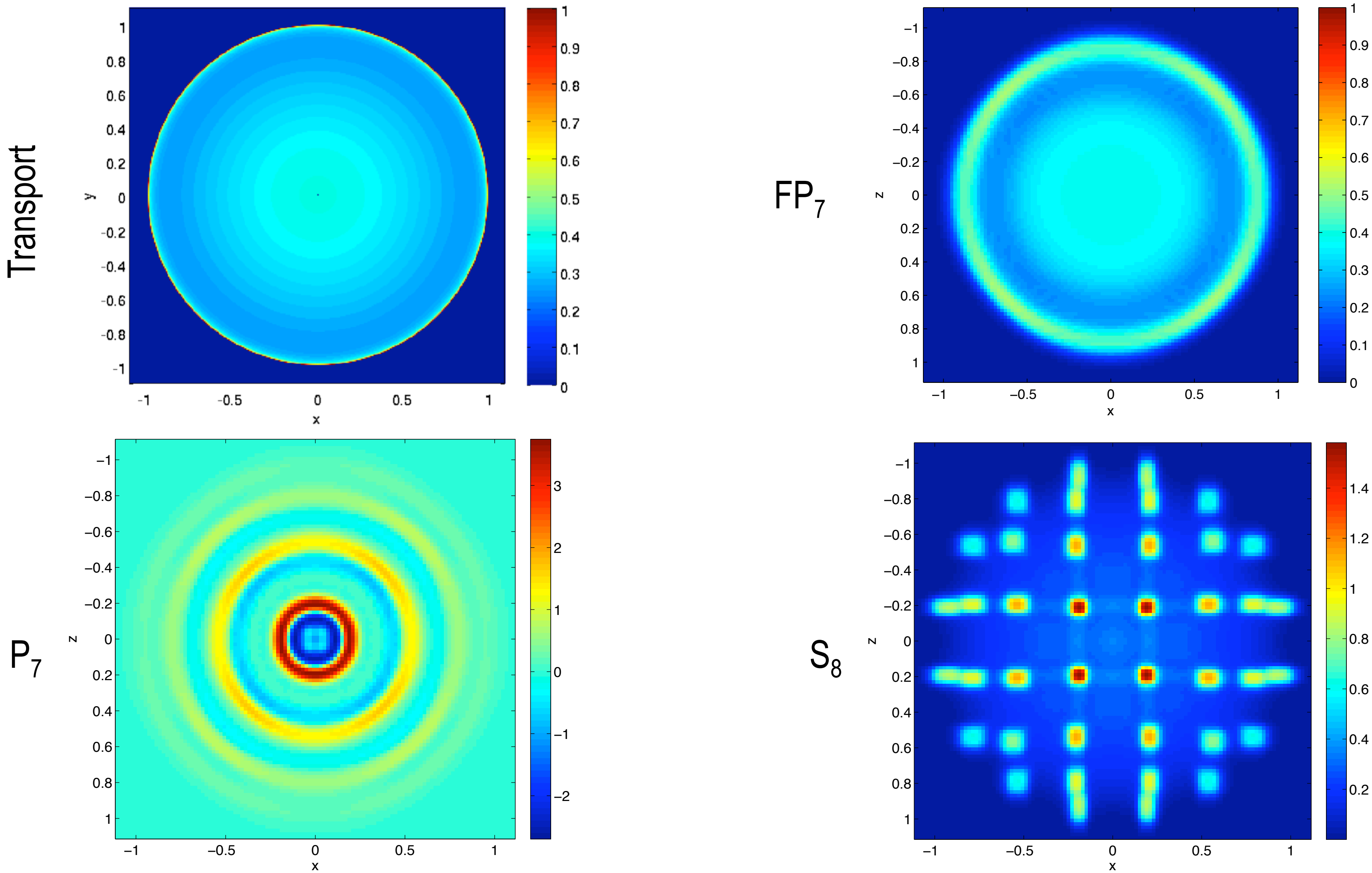
# Pulsed Line Source Results

- 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*

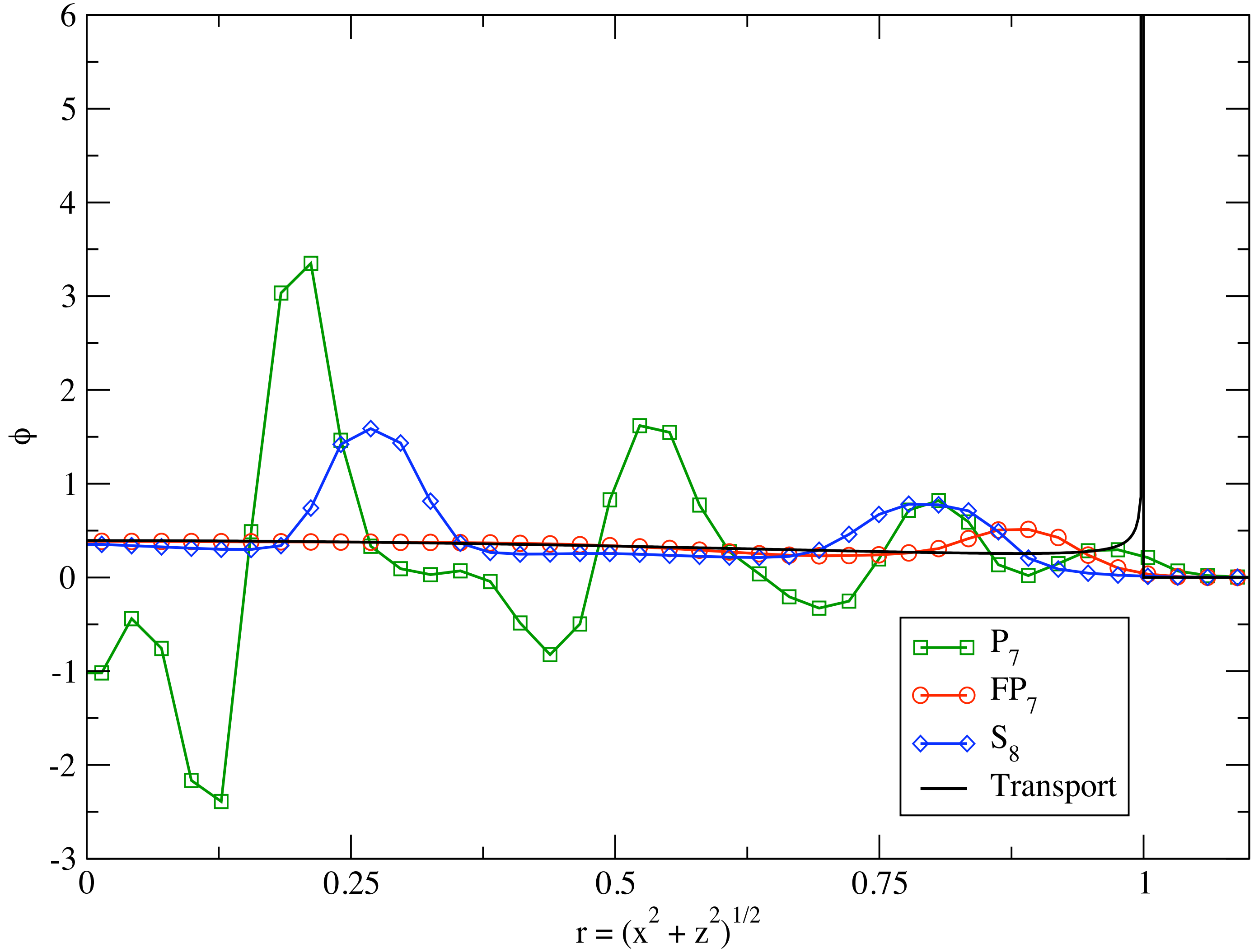



Analytic Radiation Energy Density at t = 1/c

# Pulsed Line Source Results at t=1/c

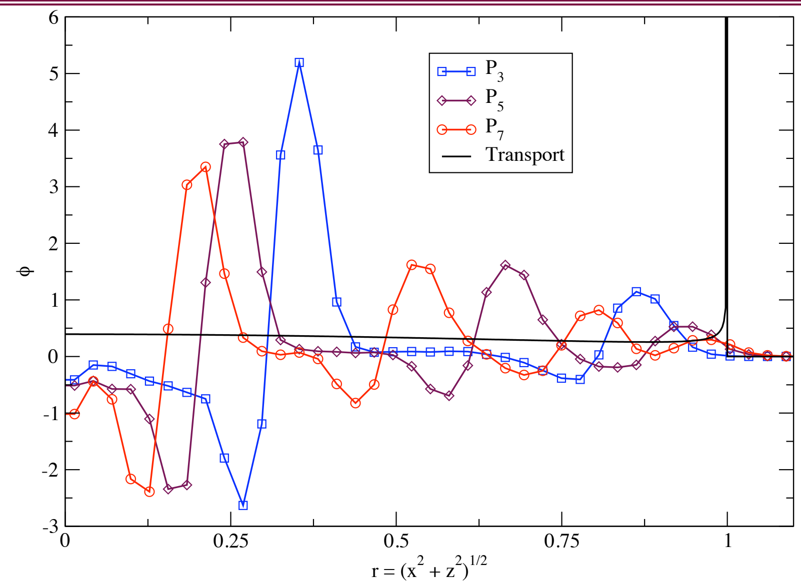


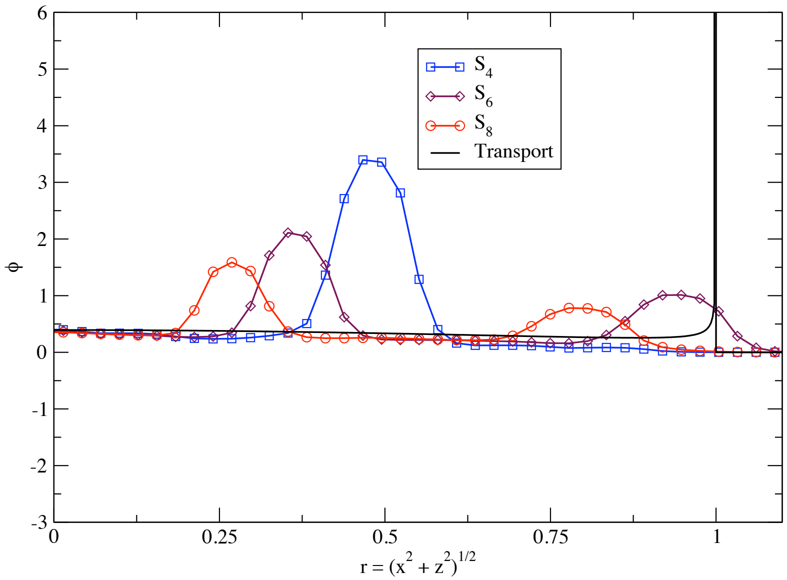
# Lineout at t=1/c

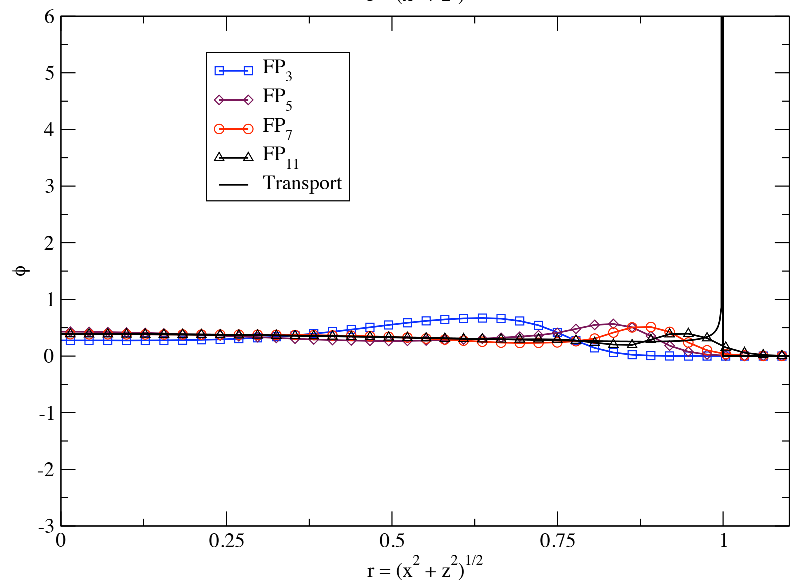


# Lineout at t=1/c

- 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



# Implicit methods are still a research topic

- Almost all of the work done on these methods has used explicit time integration
  - ⇒ *Therefore, did not require the solution of an any large, linear systems*
- In my PhD thesis I solved implicit Pn equations using GMRES with basic incomplete LU preconditioners.
- Brown, Chang, and Hanebutte derived an Sn-like form of the Pn equations that can be solved via sweeping
  - ⇒ *Has issues in convergence though.*
- In this talk I will try to show you the properties of the implicit Pn equations and hope to generate a discuss of how to precondition them.

# The Pn equations

- The Pn form of the transport equation is

$$\mathbf{A}_x \partial_x \vec{\psi} + \mathbf{A}_y \partial_y \vec{\psi} + \mathbf{A}_z \partial_z \vec{\psi} + \mathbf{C}\vec{\psi} = \mathbf{S}\vec{\psi} + \delta_{l0}\delta m 0 Q$$

- Where $\vec{\psi} = (\psi_0^0, \psi_1^{-1}, \psi_1^0, \psi_1^1, \ldots, \psi_N^N)^{\mathrm{t}}$ are the spherical harmonic moments of the angular flux.

$$\mathbf{S} = \begin{pmatrix} \sigma_{s0}^0 & & & & \\ & \sigma_{s1}^- 1 & & & \\ & & \sigma_{s1}^0 & & \\ & & & \ddots & \\ & & & & \sigma_{sN}^N \end{pmatrix} \qquad \mathbf{C} = \mathrm{diag}(\sigma_t)$$

- The streaming matrices have several important properties
  - ⇒ *Each row has 2 – 4 entries*
  - ⇒ *The diagonals are always 0*
  - ⇒ *The eigenvalues are all real.*

# Comparison to Sn

- It is useful to compare the Pn equations to the discrete ordinates (Sn) equations.
- These equations have a similar form to the Pn equations but the operators are different:

$$\mathbf{A}_x \partial_x \vec{\psi} + \mathbf{A}_y \partial_y \vec{\psi} + \mathbf{A}_z \partial_z \vec{\psi} + \mathbf{C}\vec{\psi} = \mathbf{S}\vec{\psi} + \delta_{l0}\delta m0Q$$

- Here the unknowns are the angular fluxes in a particular direction, and **C** is identical.
- In the Sn equations, however, the $A_d$ matrices are diagonal and the S matrix is full (it has a nonzero entry for every element).
- Therefore the Sn equations are typically solved by inverting the streaming operator for all of space, called a transport sweep
  - ⇒ And then iterating on the scattering operator

# Operator Form of the Equations

- In the Pn equations we have the opposite
  - ⇒ *The streaming operator is complicated*
  - ⇒ *The scattering operator is simple.*
- Writing the equations in operator form yields

$$(\mathbf{L} + \mathbf{C} - \mathbf{S})\,\vec{\psi} = \vec{Q}$$

- Which we can rewrite using $\mathbf{T} = \mathbf{C} - \mathbf{S}$

$$\left(\mathbf{T}^{-1}\mathbf{L} + \mathbf{I}\right)\vec{\psi} = \mathbf{T}^{-1}\vec{Q}$$

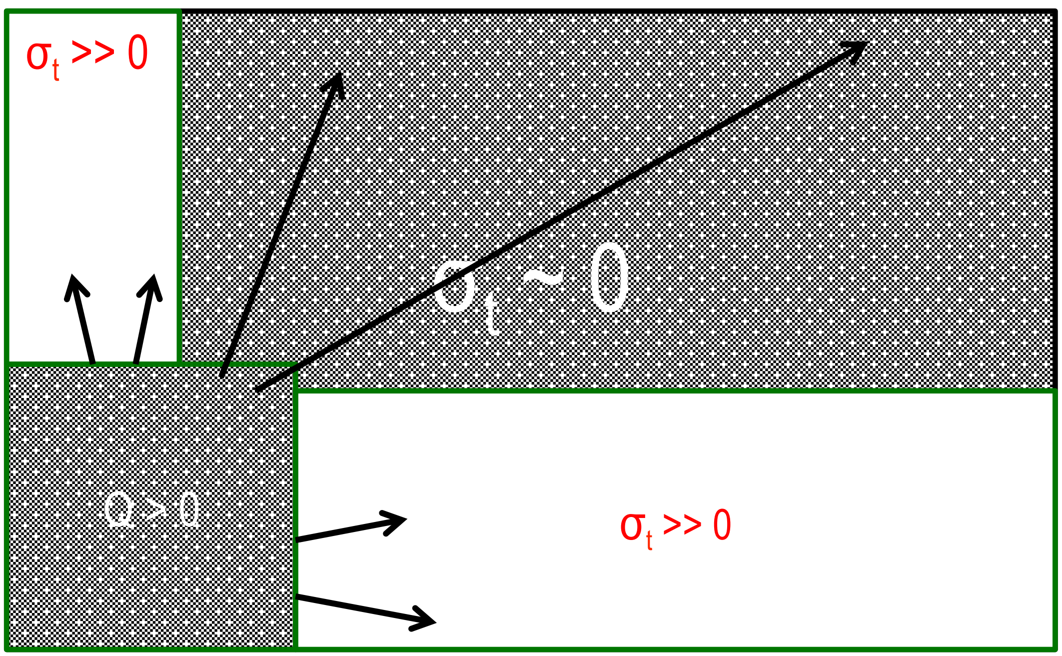
- The operator T will be invertible as long as there is some absorption.
- The streaming operator L is rotationally invariant
  - ⇒ *It moves particles in a series of waves that have a finite speed*

# The need for preconditioners

- After spatial discretization on a regular grid the matrix will have a block 7-point stencil.
  - ⇒ *The diagonal will be the identity*
  - ⇒ *The off-diagonal terms will be $T^{-1}L$ for each adjacent spatial grid cell*
- A Jacobi iteration on this matrix will move information just one grid cell.
- L is not the reason we need a preconditioner
  - ⇒ *Yes, it is not easily invertible, but it wants to move particles isotropically.*
  - ⇒ *Simple multigrid would work if it weren't for…*
- Spatial variation in the cross-sections ($\sigma_t$ and $\sigma_s$ ) causes anisotropy in the solution.
- Diffusion preconditioners may work, but this is the easy case as simple iterative schemes should converge quickly (particles don't move very far).

# Example problem

- The below problem (similar to the iron-water problem) will have anisotropic flow
  - ⇒ *The gray areas have a very small interaction between the particles and the material*
  - ⇒ *The white areas have a lot of collisions*



# How things change with Filters

- The application of a filter will look like anisotropic scattering

$$\sigma_{sl}^m \rightarrow \sigma_{sl}^m + f_l^m$$

- I don't think this will have a negative impact on the properties of the solution.

  $\Longrightarrow$ *The filter is trying to relax the angular flux to a smoother distribution.*

# Conclusions

- The spherical harmonics equations seem to have a future.
- Implicit/steady state solutions are still not practical
- Further research is needed on how best solve the equations.
- I hope that your expertise can help!