Improved Discrete Ordinates Solutions Using Angular Filtering

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Deterministic Transport Methods

- Two common deterministic methods for treating the angular variable in transport problems are the discrete ordinates (S_n) and spherical harmonics (P_n) methods.
- Each of these methods has it's drawbacks:
  - S_n has ray effects, areas in the solution where no particles get to because of the finite number of angles.
  - P_n has wave effects that can cause the solution to go negative and oscillate when the solution is not smooth in angle.
- These artifacts come from the fact the underlying types of each method.
  - S_n is a collocation method in angle. Without enough points, issues can arise.
  - P_n is a global, spectral method in angle. This leads to Gibbs' oscillations.

Deterministic Transport Methods

- As such, standard refinement in angle for each scheme cannot remove the limitations of the method.
- For S_n, adding more and more angles to your discretization is often necessary.
  - Even this won't work if the problem has little scattering and the sources are localized.
  - That said, there has been interesting work in developing obscenely high order quadrature sets that can be locally refined (the LDFE methods of Jarrell and Adams and the QR sets of Abu-Shumays)
- In P_n increasing n will not remove oscillations as long as the solution is non-smooth in angle.
- From my perspective, we should be asking how we can break free of the shackles of each method's foundation.

Breaking the Shackles

- For P_n this would be mean giving up spectral convergence in favor of robustness.
  - It turns out this is not much of a sacrifice. You won't get spectral convergence for non-smooth solutions anyway.
- In the case of S_n , it might mean allowing angles to ”talk” to each other in the absence of scattering.
  - This blasphemy sounds horribly non-physical, and in a sense it is.
  - Nevertheless, away from localized sources, in the absence of scattering we don't believe the S_n answer anyway.
- Both of these approaches hew to the maxim: “It's better to be approximately right than exactly wrong.”

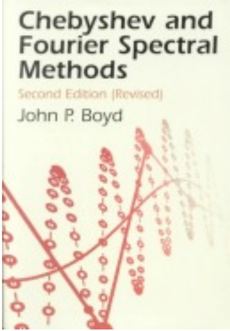
Filtered Spherical Harmonics Methods

- There has been work to remove oscillations by treating the standard spherical harmonics expansion using filters.
- RGM and Cory Hauck showed that spherical spline filters could give answers comparable to Monte Carlo solutions when used on a P_7 expansion on some challenging test problems.
- Radice, Abdikamalov, et al. built upon this work to show that the Lanczos filter is also an effective filter for these solutions.
- The implementation of filters can be done in such a way that it is
  - Extensible to any order of expansion
  - Preserves the equilibrium diffusion limit
  - Preserves the convergence of P_n to the transport solution as $n \to \infty$.
- These works used explicit time-stepping algorithms, and implicit implementations are a work in progress.

The drawbacks of P_n are well-studied in the spectral methods literature

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

John P. Boyd
Chebyshev and Fourier Spectral Methods



Gibbs Errors

- The reason a truncated expansion is a bad idea is the introduction of Gibbs' errors.
- These are oscillations in the solution near sharp features in the solution.

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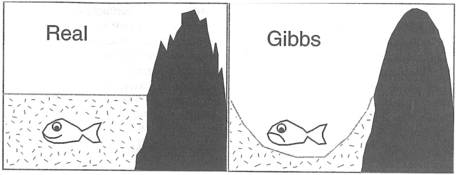
- These are oscillations in the solution near sharp features in the solution.
- An cartoon from Boyd's book helps illustrate why these are bad:

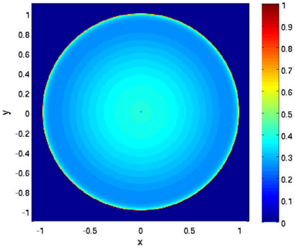


- What filters do, is ensure that that the expansion coefficients are decaying before the series is truncated.

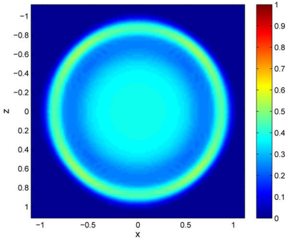
The Fruits of Filtered P_n

- A illustrative example of the power of filtering can be seen in the line source problem.
- This problem has a delta-function initial condition in a 2-D, purely scattering medium.
- The time-dependent solution is a delta-function wave front of uncollided particles followed by a smooth region of scattered particles.
- Experience has shown that almost no deterministic method can do a reasonable job on this problem.

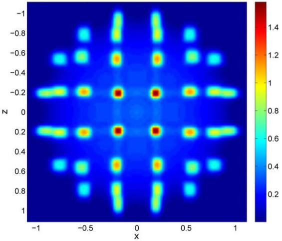
Line source solutions at ct = 1



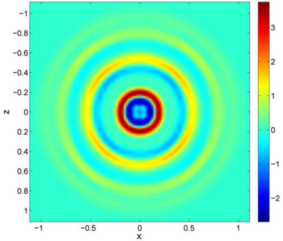
(a) Transport



(b) FP_7

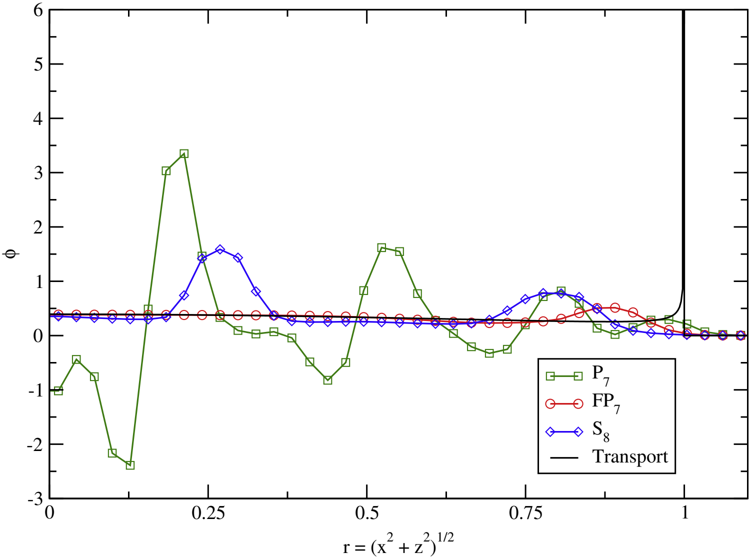


(c) S_8



(d) P_7

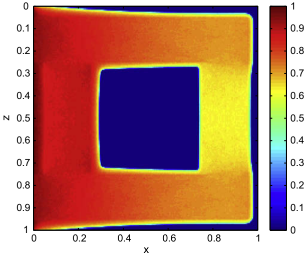
Line source solutions at ct = 1



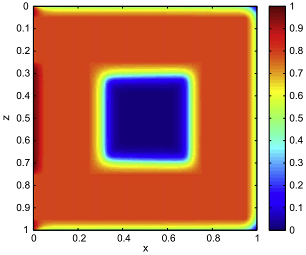
The Fruits of Filtered P_n

- There are similar results on many problems.
- For example, in a radiative transfer problem on a Cartesian hohlraum, the filtered method tracks the implicit Monte Carlo solution without the noise.
- See the relevant papers for more information
  1. McClarren, R. G., & Hauck, C. D. (2010). Journal of Computational Physics, 229(16), 5597-5614.
  2. McClarren, R. G., & Hauck, C. D. (2010). Physics Letters A, 374(22), 2290-2296.
  3. Radice, D., Abdikamalov, E., Rezzolla, L., & Ott, C. D. (2013). Journal of Computational Physics, 242, 648-669.

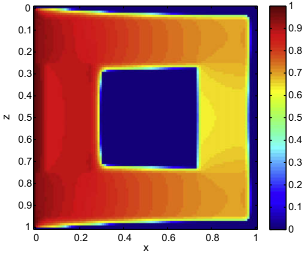
Cartesian Hohlraum problem



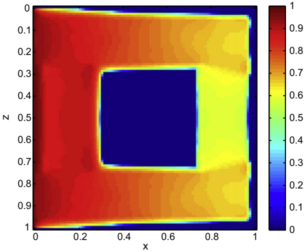
(a) Implicit Monte Carlo



(b) Flux-limited Diffusion



(c) FP_7



(d) S_8

Can we apply Filters to S_n

- The filters can be interpreted in two ways.
    - As adding artificial viscosity in angle. That is adding a small amount of diffusion in angle.
    - As adding forward-peaked scattering to the problem. Particles scatter as they travel.
- Therefore we should be able to use a filter to correct the fact that under resolved S_n solutions need the angles to talk to each other to remove ray effects.

Applying the P_n prescription

- The most straightforward way to apply a filter is to
    1. Take our S_n solution,
    2. Convert it to a P_n representation,
    3. Filter the P_n moments,
    4. Reconstruct the discrete ordinates from the filtered P_n representation.
- This will have the effect of smoothing the S_n representation of the angular flux.

Applying the P_n prescription

- In performing this filtering we want several properties.
- First, if no filtering is done, then the procedure should return the initial angular flux.
- In diffusive regions, filtering should not affect the asymptotic limit of the S_n method.
- As the S_n order goes to ∞ it should not affect the limit.
- We can accomplish all of these.

Galerkin Quadratures

- For a given quadrature set, and a set of discrete ordinates, $\vec{\psi}$,
- A set of moments, $\vec{\phi}$, can be obtained by multiplying $\vec{\psi}$ by a discrete-to-moment matrix $\mathbf{D}$.
- The set of moments depends on the quadrature set and $\mathbf{D}$.
- Also, one maps from moments to discrete ordinates using a moment-to-discrete matrix, $\mathbf{M}$ as $\vec{\psi} = \mathbf{M}\vec{\phi}$.
- In most cases the mapping from ordinates to moments is not invertible, (i.e., $\mathbf{MD} \neq \mathbf{I}$).
- However, Galerkin quadrature sets (Morel, NSE 1989) are defined to have this property.
- We will use this property to define our filtered S_n method.

Applying the Filter

- Using Galerkin quadratures, in each spatial zone of an S_n code we will apply the filter.
- For a spherical harmonic moment of order lm we define the filter as

$$(\mathbf{F}\vec{\phi})_l^m = \frac{\phi_l^m}{1 + \alpha l(l+1)}$$

- Where α is given by

$$\alpha = \frac{\omega}{N(\sigma_s + N)^2}$$

  where ω is a filter strength parameter and N is the quadrature order.
- This prescription for α turns off the filter in the diffusion limit and has the effect of causing the filter strength to go to zero as $N \to \infty$.

Filtering Algorithm

- Using Galerkin quadratures, in each spatial zone of an S_n code we take the current iterate of the angular flux and
  1. Compute the moments as $\vec{\phi} = \mathbf{D}\vec{\psi}$.
  2. Apply the filter, $\hat{\phi} = \mathbf{F}\vec{\phi}$
  3. Create the filtered angular flux ordinates, $\hat{\psi} = \mathbf{M}\hat{\phi}$.
- Note that if the filter strength is zero ($\mathbf{F} = \mathbf{I}$), then the filtering procedure does nothing.
- We still have not shown how we include the filter in our S_n solution technique.

Naïve Implementation

- Given a standard source-iteration approach to solving the S_n equations:
$$\mathbf{L}\vec{\psi}^{l+1} = \mathbf{MSD}\vec{\psi}^{l},$$
where $\mathbf{L}$ is the discretized streaming plus removal operator, and $\mathbf{S}$ is the scattering operator,
- We can obtain the filtered solution by adding a source to the RHS, and changing the solution used in the scattering term:
$$\mathbf{L}\vec{\psi}^{l+1} = \mathbf{MSD}\hat{\psi}^{l} - \mathbf{L}\left(\hat{\psi}^{l} - \vec{\psi}^{l}\right),$$
- Therefore (if?) when the iterations converge the solution will be $\hat{\psi}$.

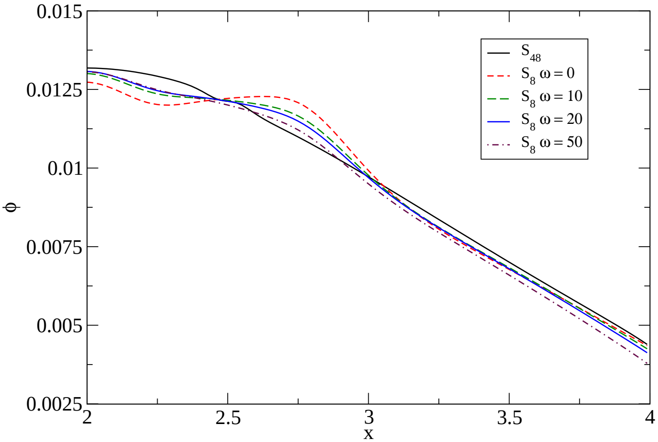
Numerical Results

- We have implemented our scheme using a first-order upwind method (commonly called the step method).
- All of our meshes are highly resolved because we are using a low-order spatial method.
- On the following problems we used source-iteration to solve the discretized equations.
- We do not have a prescription for choosing the parameter ω. We ran several different values.
- We did notice slower convergence for larger values of ω. This is most likely the result of their being a large difference between ψ and $\hat{\psi}$ in these problems.

Simple Test Problem

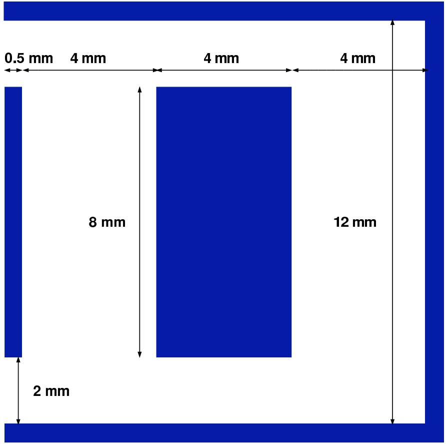
- We solve a similar problem to one from a previous paper on ray-effect mitigation techniques (Morel, Wareing, Lowrie and Parsons 2003).
- The problem has a localized source in a larger medium.
- In this problem $\sigma_\mathrm{t} = 0.75$, $\sigma_\mathrm{s} = 0.5$,
- The domain is a 4 by 4 square with a source of strength 0.25 of dimensions 0.5 by 0.5 in the middle of the geometry.
- We look at the solution along the top quarter of the domain ($y = 4$ and $x \in [2, 4]$).

Solutions for several values of ω with S_8.

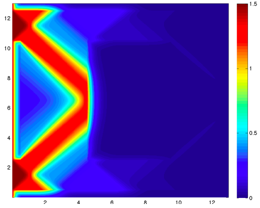


Hohlraum Problem

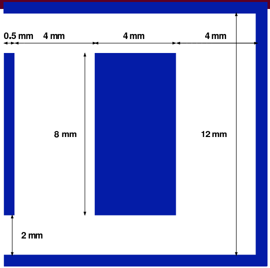
- 2-D Cartesian hohlraum layout from Brunner.
- Blue regions have $\sigma_a = 10$
- White regions have $\sigma_t = \sigma_s = 1$.
- Source at left edge.



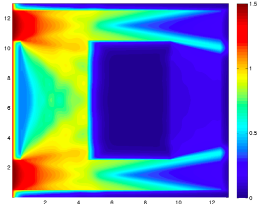
The Hohlraum Problem



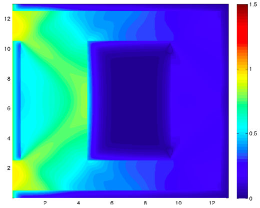
(a) S_2 No Filter



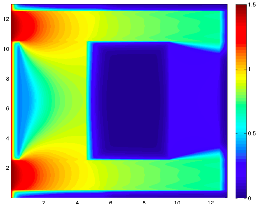
(b) Layout



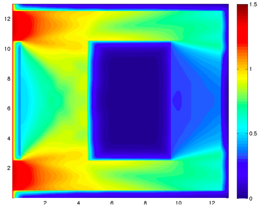
(c) S_8 No Filter



(d) S_2 $\omega = 100$



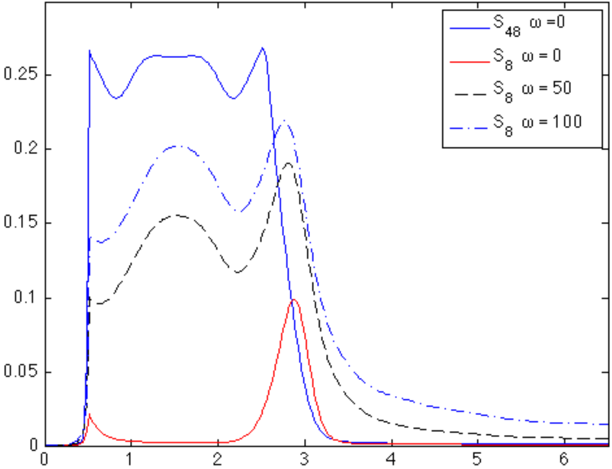
(e) S_{48}



(f) S_8 $\omega = 100$

T. A. Brunner. Tech. Rep. SAND2002-1778, Sandia National Laboratories, Jul 2002.

Solutions for several values of ω with S_8 at $x = 12$.



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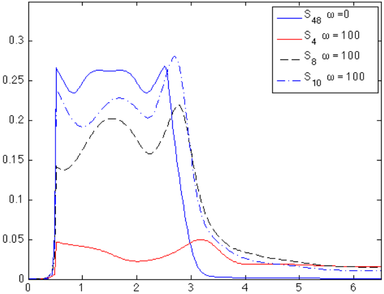
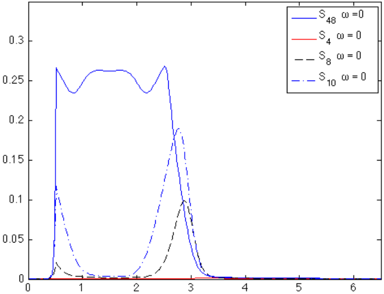
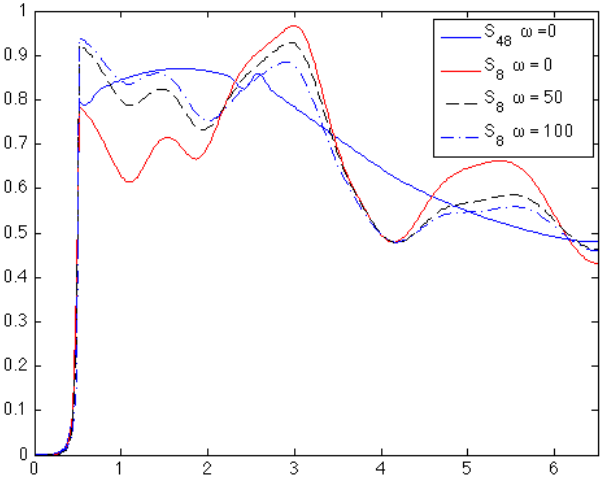
Convergence for filtered and unfiltered solutions.

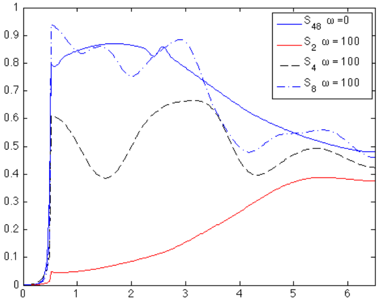


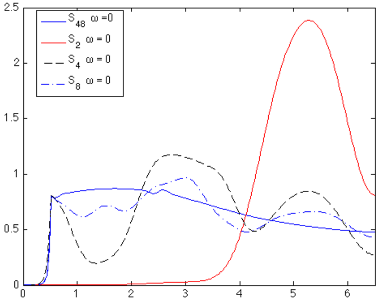


Solutions for several values of ω with S_8 at $x = 4$.

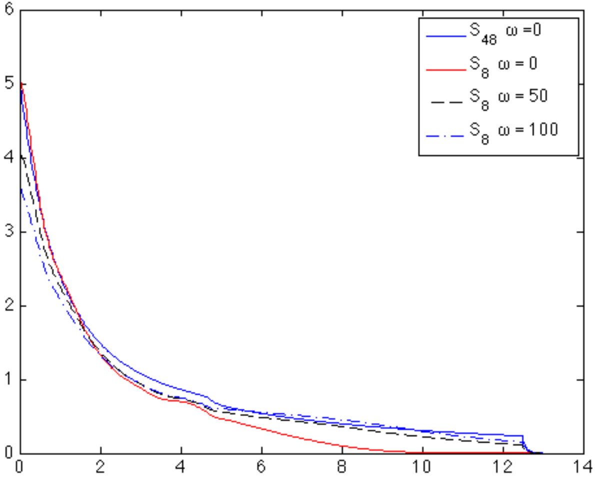


Convergence for filtered and unfiltered solutions.

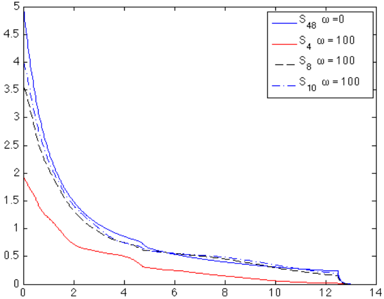


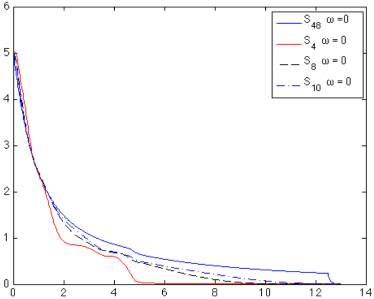


Solutions for several values of ω with S_8 at $y = 11$.



Convergence for filtered and unfiltered solutions.





Summary of Results

- Results from P_n suggest that filtered expansions are effect for improving solutions.
- Using an analogous approach for S_n seems to reduce ray effects, though not eliminate them altogether.
- We haven't determined how to pick ω yet.
  - Our experiments seem to indicate that there is an affect of the mesh size on the effectiveness of the filter.
  - Smaller Δx means that the filter does less.
- There is still work to be done in the theory and efficient solution for these methods, but I believe there is some promise here.