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FILTERED SPHERICAL HARMONICS METHODS FOR TRANSPORT PROBLEMS

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ABSTRACT

We present a new way of using spherical harmonics expansions to solve transport problems. Our approach uses filtered expansions to give positive solutions and reduce wave effects in the solutions. We present two specific filters: one based on maintaining positivity in a P_1 expansion, and the other that is a function of the total cross-section and the order of the expansion. We compare solutions using our filtered expansions to the standard spherical harmonics expansions, Monte Carlo, diffusion, discrete ordinates, and analytic transport solutions. These numerical results suggest that our filtered expansions give solutions that are comparable to other methods in terms of accuracy. Additionally, we point out how filtered spherical harmonics expansions could be improved.

Key Words: particle transport, spherical harmonics

1. INTRODUCTION

Spherical harmonics expansions are a common way of treating the angular variable in the first-order form of the neutral particle transport equation [1, 2]. These expansions can be shown to be an asymptotic limit of the transport equation [3]. To get numerical solutions, the expansion must be truncated at some order, however, when scattering from the material medium is small the truncated expansion can give nonphysical osciallations in the solution. These oscillations are the result of the spherical harmonics being the expansion that best approximates the transport solution in a least-squared sense [4]. These oscillations can cause the solution to become negative and make multiphysics simulations fail [5–7]. Moreover, it can be proven that for a given order of spherical harmonics expansion there exists a problem where the solution becomes negative [7].

The goal of this study is eliminate the oscillations in the solution to the spherical harmonics (P_N) equations and ensure that the solution is positive. We accomplish this by using filtered spherical harmonics expansions. These filters are based on finding the P_N expansion that minimizes the L^2 norm of the error subject to a cost function related to the second angular derivative of the expansion. Such a filter is analagous to an artificial viscosity used in the numerical solution of hyperbolic conservation laws. This gives a general form for a filter with the strength of the filter a free parameter. We give two prescriptions for choosing this filter strength. The first takes the P_1 expansion and using the filter guarantees that this expansion is positive in the angular flux, in a similar manner to a slope limiter. The other filter chooses the filter strength based on the order of the expansion and the size of the total macroscopic cross-section of the material. As the order of expansion or the cross-section becomes larger, the filter strength decreases. Though we give two recipes for a filter, we do not assert that these are optimal. In fact, we suggest ways to create better filters.

In the following section we present the theory of filtered spherical harmonics expansions. For much of this section we follow the derivations given by Boyd [4]. We then concoct two filters and discuss their properties in Sec. 3. Section 4 discusses the P_N equations and how we solve them numerically. Numerical results are presented in Sec. 5, followed by a conclusions section.

2. FILTERED SPHERICAL HARMONICS EXPANSIONS

The spherical harmonics expansion takes the angular flux, $\psi(\mathbf{x}, \hat{\Omega}, v, t)$, and expands the angular variable $\hat{\Omega} = (\mu, \varphi)$ in terms of spherical harmonics functions

$$\psi(\mathbf{x}, \hat{\Omega}, v, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^m(\hat{\Omega}) \psi_l^m(\mathbf{x}, v, t). \tag{1}$$

where the spherical harmonics functions are given by

$$Y_l^m = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\mu) e^{im\varphi}, \tag{2}$$

$P_l^m(\mu)$ are the associated Legendre functions. The expansion coefficients in Eq. (1) are given by

$$\psi_l^m(\mathbf{x}, v, t) = \int_{4\pi} \bar{Y}_l^m(\hat{\Omega}) \psi(\mathbf{x}, \hat{\Omega}, v, t)\, d\hat{\Omega}. \tag{3}$$

The expansion in Eq. (1) must be made finite so that numerical computation can be performed. The most common means of making Eq. (1) finite is to truncate the series above a certain value of $l = N$,

$$\psi_l^m = 0 \qquad l > N. \tag{4}$$

Though this truncation is straightforward, it causes the solution to transport problems to have oscillations. Indeed, Boyd, when discussing truncated spherical harmonics expansions for general problems exclaims [4], "Truncating a [spherical harmonics] series is a rather stupid idea." These oscillations can be explained by the fact that the spherical harmonics expansion is the minimizer of the functional

$$\mathcal{J} = \int_{4\pi} \left(\psi(\mathbf{x}, \hat{\Omega}, v, t) - \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^m(\hat{\Omega}) \psi_l^m(\mathbf{x}, v, t) \right)^2 d\hat{\Omega}. \tag{5}$$

This functional can allow large oscillations about the true solution because it minimizes the square of the error.

Following Boyd [4], one can change the functional that is minimized to

$$\mathcal{J} = \int_{4\pi} \left(\psi(\mathbf{x}, \hat{\Omega}, v, t) - \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^m(\hat{\Omega}) \tilde{\psi}_l^m(\mathbf{x}, v, t) \right)^2 d\hat{\Omega} + \alpha \int_{4\pi} \left(\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \nabla_{\hat{\Omega}}^{2k} Y_l^m(\hat{\Omega}) \tilde{\psi}_l^m(\mathbf{x}, v, t) \right)^2 d\hat{\Omega}. \tag{6}$$

In this new functional $\nabla_{\hat{\Omega}}$ is the gradient operator with respect to $\hat{\Omega}$ and $\alpha > 0$ is a parameter. This filter is, in a sense, adding artificial viscosity to the expansion: oscillations make this new term in the cost function large.

We will now find the new expansion coefficients, $\tilde{\psi}_l^m$. Noting that the spherical harmonics are eigenfuctions of the Laplacian operator on the sphere,

$$\nabla^2_{\hat{\Omega}} Y_l^m = -l(l+1)Y_l^m, \tag{7}$$

one can show that

$$\tilde{\psi}_l^m = \frac{\psi_l^m}{1 + \alpha l^{2k}(l+1)^{2k}}. \tag{8}$$

Therefore, the filtered expansion forces the expansion coefficients to decrease with increasing l. These filters are also conservative in that they do not change the magnitude of ψ_0^0 meaning that the scalar flux is unchanged. There still is the free parameter α that we must specify. In this study we suggest two ways of defining α, though we note that further research will probably uncover better filters.

3. TWO FILTERS

3.1. Strictly Positive P_1 Reconstruction

The first filter that we describe is based on the P_1 expansion of the angular flux. This expansion is

$$\psi = \frac{1}{2\sqrt{\pi}}\psi_0^0 + \frac{1}{2}\sqrt{\frac{3}{\pi}}\psi_1^0\mu + \sqrt{\frac{3}{2\pi}}\psi_1^1 e^{-i\varphi}\sqrt{1-\mu^2}, \tag{9}$$

where we have used the relation that $\psi_l^m = (-1)^m \psi_l^{-m}$ [8]. Notice that this reconstruction can be negative; when

$$|\psi_1^0| > \frac{\psi_0^0}{\sqrt{3}}, \tag{10}$$

or

$$|\psi_1^1| > \frac{\psi_0^0}{\sqrt{6}}, \tag{11}$$

then ψ will be less than zero for some combination of (μ, φ).

This possibility for a negative value suggests some kind of slope limiter. When ψ_1^m is too large we want to scale it back. The amount to scale it by is given in the modified reconstruction

$$\psi = \frac{1}{2\sqrt{\pi}}\psi_0^0 + \frac{1}{2}\theta_1\sqrt{\frac{3}{\pi}}\mu + \sqrt{\frac{3}{2\pi}}\theta_2\psi_1^1 e^{-i\varphi}\sqrt{1-\mu^2}, \tag{12}$$

with

$$\theta_1 = \min\left(\frac{\psi_0^0}{\sqrt{3}|\psi_1^0|}, 1\right), \tag{13}$$

and

$$\theta_2 = \min\left(\frac{\psi_0^0}{\sqrt{6}\,|\psi_1^1|}, 1\right). \tag{14}$$

This reconstruction guarantees that ψ is positive.

We can cast the limited reconstruction of Eq. (12) as a filter by defining α as

$$\alpha = \frac{1-\theta}{2^{2k}}, \tag{15}$$

where the unadorned θ is the minimum of θ_1 and θ_2. With this definition of α we then apply the filter as in Eq. (8).

One important property of this filter is that it only is applied where it is needed, i.e. in regions where the angular flux can be negative—when $\theta = 1$ the filter does nothing. Also, in the diffusion limit it should not have an effect. This can be seen by the fact that in the diffusion limit ψ_1^m is an order ϵ quantity whereas ψ_0^0 is order one, so that θ will be one.

There is a drawback to this filter in that it limits the P_N equations wavespeed to the P_1 wavespeed, $v/\sqrt{3}$ where v is the particle speed. This is a result of the hard limit we place on the size of ψ_1^m. For higher order P_N expansions, there are higher moments that can create a positive reconstruction with ψ_1^m outside the bounds of Eqs. (5) and (6). We believe that the reconstruction could be modified to ensure that the P_3 expansion is positive. This would require devising conditions where a cubic is positive and we have not been successful to date in deriving such a condition. Even higher P_N expansions could be modified to give a positive reconstruction, though we believe as the order increases deriving positivity constaints becomes increasingly more difficult (and tedious). Finally, we point out that the slow wavespeed could be remedied by employing a $P_{1/3}$ type correction that adjusts the P_1 wavespeed to be v [9].

3.2. Material Property Dependent Filter

The second filter we discuss does not explicitly guarantee a positive reconstruction of ψ, rather it imposes a filter in parts of the problem where the material interaction is weak. This filter writes α as

$$\alpha = \frac{\omega}{(N^2\sigma_t L + 1)^2}, \tag{16}$$

where N is the order of the P_N expansion, σ_t is the total macroscopic cross-section of the material, L is some characteristic length, and ω is a positive number.

This filter has the property that as the order of the expansion increases, the filter effects the solution less. Therefore, as $N \to \infty$ the solution does still converge to the transport solution. Moreover, this filter does not effect the diffusion limit: when σ_t is an $O(1/\epsilon)$ quantity, then $\alpha = 1 + O(\epsilon^2)$. Perhaps the biggest upside to this filter is that it is linear in ψ_l^m. Unlike the filter based on the P_1 reconstruction, this filter can be implemented in a straightforward manner.

At low expansion orders, for example P_1, this filter is strong is streaming regions. When $\sigma_t = 0$ for $N = 1$,

$$\tilde{\psi}_1^m = \frac{1}{1+4\omega}\psi_l^m, \tag{17}$$

regardless if the solution "needs" to be filtered or not. The other drawback to this filter is that it has a free parameter, ω. Though this parameter gives flexibility to increase or decrease the filter strength, it would be better to have a prescribed value that guarantees positivity.

4. THE SPHERICAL HARMONICS EQUATIONS

To show how we implement the filtered expansion, we begin with the equation for the time dependent transport of neutral particles,

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \hat{\Omega} \cdot \nabla \psi = S, \tag{18}$$

where $\psi(\mathbf{x}, \hat{\Omega}, v, t)$ is the angular flux, v is the particle speed, $\hat{\Omega}$ is the direction of flight variable, σ_t is the macroscopic interaction cross-section of the material, and S is a source function that takes into account the material-particle interaction, such as a scattering source. Also, we will be dealing with 2-D Cartesian geometry so that $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial z})$. We then expand $\hat{\Omega}$ in spherical harmonics functions as discussed above to get the system

$$\frac{1}{v}\frac{\partial \psi_l^m}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x}\left(-C_{l-1}^{m-1}\psi_{l-1}^{m-1} + D_{l+1}^{m-1}\psi_{l+1}^{m-1} + E_{l-1}^{m+1}\psi_{l-1}^{m+1} - F_{l+1}^{m+1}\psi_{l+1}^{m+1}\right)$$
$$+ \frac{\partial}{\partial z}\left(A_{l-1}^{m}\psi_{l-1}^{m} + B_{l+1}^{m}\psi_{l+1}^{m}\right) + \sigma_t \psi_l^m = S_l^m \qquad \text{for } l = 1 \ldots n,\ m = 1 \ldots l \tag{19a}$$

and

$$\frac{1}{v}\frac{\partial \psi_l^0}{\partial t} + \frac{\partial}{\partial x}\left(E_{l-1}^{1}\psi_{l-1}^{1} - F_{l+1}^{1}\psi_{l+1}^{1}\right) + \frac{\partial}{\partial z}\left(A_{l-1}^{0}\psi_{l-1}^{0} + B_{l+1}^{0}\psi_{l+1}^{0}\right) + \sigma_t \psi_l^0 = S_l^0 \quad \text{for } l = 0 \ldots n, \tag{19b}$$

where

$$A_l^m = \sqrt{\frac{(l-m+1)(l+m+1)}{(2l+3)(2l+1)}} \qquad B_l^m = \sqrt{\frac{(l-m)(l+m)}{(2l+1)(2l-1)}}$$
$$C_l^m = \sqrt{\frac{(l+m+1)(l+m+2)}{(2l+3)(2l+1)}} \qquad D_l^m = \sqrt{\frac{(l-m)(l+m-1)}{(2l+1)(2l-1)}}$$
$$E_l^m = \sqrt{\frac{(l-m+1)(l-m+2)}{(2l+3)(2l+1)}} \qquad F_l^m = \sqrt{\frac{(l+m)(l+m-1)}{(2l+1)(2l-1)}}.$$

For the P_N method the scalar flux, $\phi = \int_{4\pi} d\hat{\Omega}\,\psi$, is given by $\phi = 2\sqrt{\pi}\psi_0^0$, and the number of unknowns in the P_N equations is $\frac{1}{2}(n^2 + 3n) + 1$. The initial conditions for P_N are given by

$$\psi_l^m(\mathbf{x}) = \int_{4\pi} d\hat{\Omega}\, Y_l^{m*}(\hat{\Omega})\Psi(\mathbf{x}, \hat{\Omega}). \tag{20}$$

The boundary conditions we will use are ghost cell boundary conditions [5, 7] that are equivalent to the Mark boundary condition.

4.1. Numerical Method

To solve Eqs. (19) we will use a linear discontinuous Galerkin method for the spatial discretization and a semi-implicit time integration method [10]. This approach has been shown to be robust in the diffusion limit, and it gives a straightforward means to apply our filters.

We apply the filters after each time step by computing α in each spatial cell and then scaling ψ_l^m to get $\tilde{\psi}_l^m$ as in Eq. (8). This approach is simple in that it allows us to treat any nonlinearity in the filter explicitly. How to deal with nonlinear filters with implicit solvers is an open question that we leave to future work, though we note that the filter given in Sec. 3.2 is linear and could be used with an implicit solver. We use $\omega = 1/3$ for the material based filter.

4.2. Sources

Our subsequent numerical results will solve two types of problems: linear problems with isotropic scattering and nonlinear transport problems where the background material emits particles as a blackbody source.

4.2.1. Isotropic Scattering

For problems of linear transport with isotropic scattering and only one particle speed, the source function S becomes

$$S = \frac{\sigma_{\mathrm{s}}}{4\pi}\phi - \sigma_{\mathrm{t}}\psi, \tag{21}$$

where σ_{s} is the scattering macroscopic cross-section, and σ_{t} is the total macroscopic cross-section. This source makes

$$S_0^0 = -\sigma_{\mathrm{a}}\psi_0^0, \tag{22}$$

$$S_l^m = -\sigma_{\mathrm{t}}\psi_l^m, \qquad l > 0. \tag{23}$$

4.2.2. Radiative Transfer Problems

In problems of the radiative transfer of grey x-rays [2] the source term is given by

$$S = -\sigma_{\mathrm{a}}\left(\psi - \frac{acT^4}{4\pi}\right), \tag{24}$$

where $a = 0.01372\,\mathrm{GJ\ cm^{-3}\ keV^{-4}}$ is the radiation constant, $c = 2.998 \times 10^{10}$ cm/s is the speed of light, σ_{a} is the absorption macroscopic cross-section, and the temperature T is governed by

$$C_{\mathrm{v}}\frac{\partial T}{\partial t} = \sigma_{\mathrm{a}}\left(\phi - acT^4\right). \tag{25}$$

The moments of S are then

$$S_0^0 = -\sigma_{\mathrm{a}}\left(\psi_0^0 - \frac{acT^4}{2\sqrt{\pi}}\right), \tag{26}$$

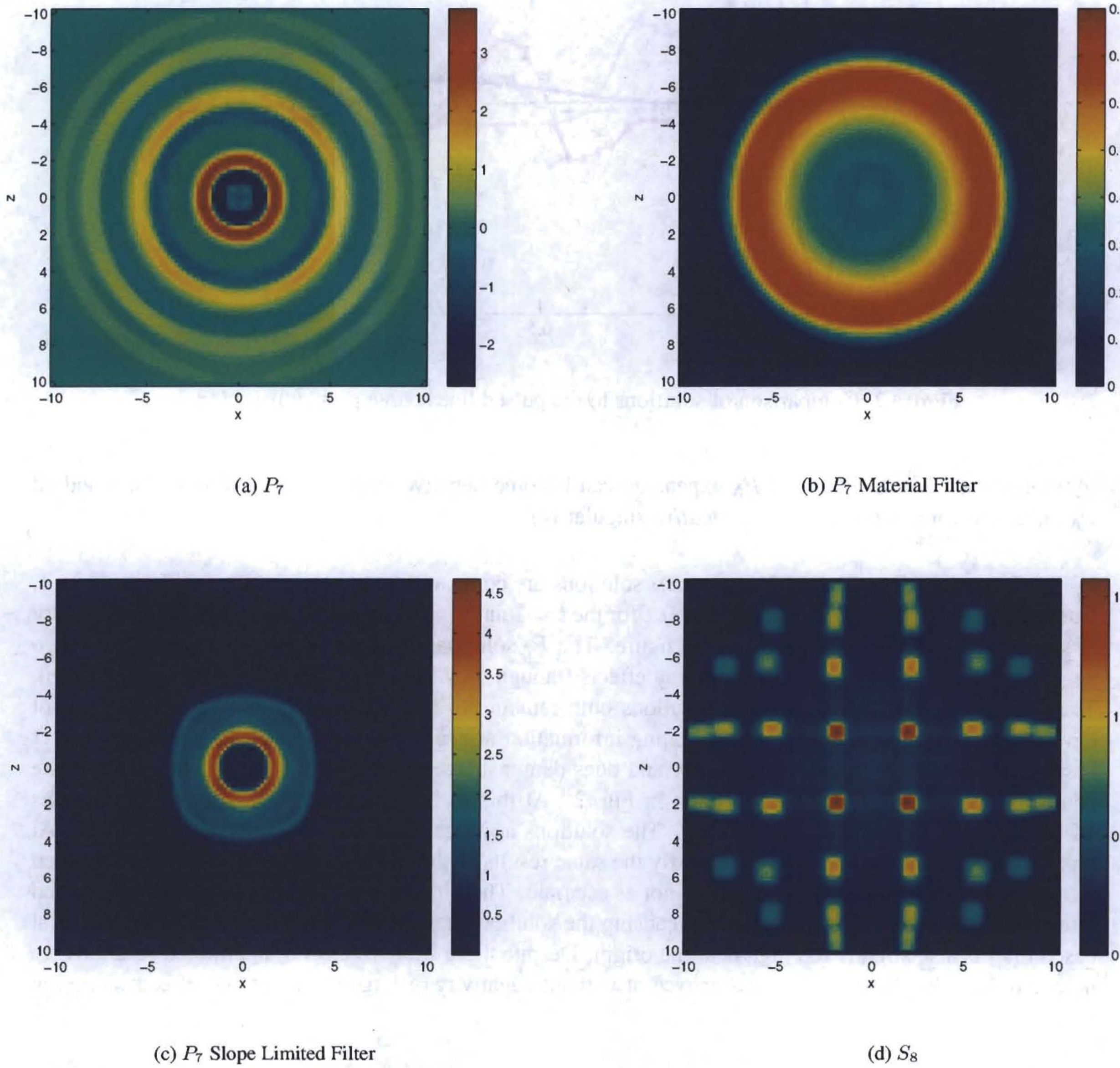
$$S_l^m = -\sigma_{\mathrm{a}}\psi_l^m, \qquad l > 0, \tag{27}$$

and Eq. (25) is in terms of ψ_0^0,

$$C_{\mathrm{v}}\frac{\partial T}{\partial t} = \sigma_{\mathrm{a}}\left(2\sqrt{\pi}\psi_0^0 - acT^4\right). \tag{28}$$

5. NUMERICAL RESULTS

The first problem we solve is a linear transport problem as described in Sec. 4.2.1. This problem has an infinite line source pulsed at the origin at time 0. The material has $\sigma_{\mathrm{t}} = \sigma_{\mathrm{s}} = 1$ and the particle speed is $v = 1$. There is an analytic transport solution to this problem given by Ganapol [11]. This is sort of a pathological problem due to the presence of a singularity in the solution at $x/t = 1$. Nevertheless, this



(a) P_7 (b) P_7 Material Filter

(c) P_7 Slope Limited Filter (d) S_8

Figure 1. Solutions to the pulsed line source problem at $t = 1$ using several methods.

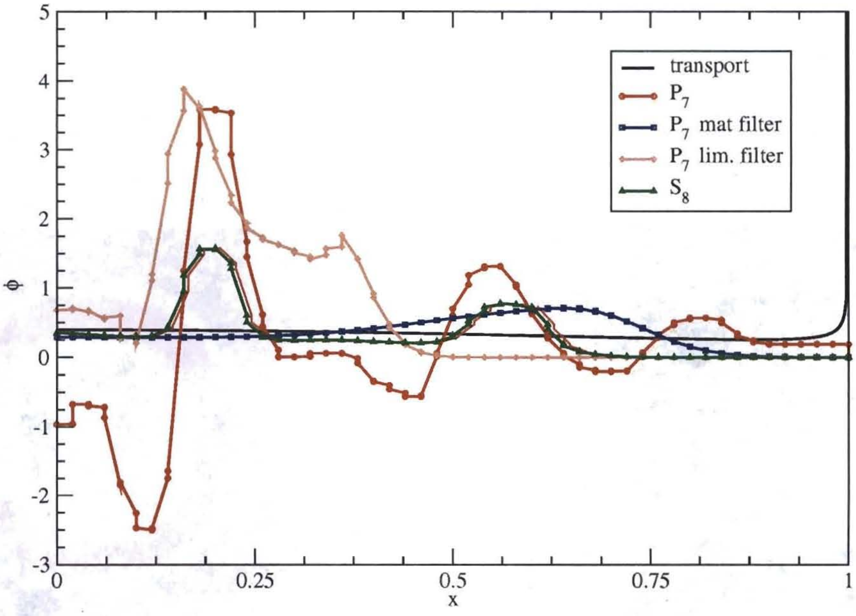


Figure 2. Comparison of solutions to the pulsed line source problem and $t = 1$.

solution shows that the standard P_N expansion can become negative (indeed the solution to the standard P_N equations for this problem has a *negative* singularity).

In Fig. 1 standard P_N, filtered P_N, and S_N solutions are compared on the line source problem at $t = 1$. Our numerical solutions used $\Delta x = 0.01$, 0.1 for the $t = 1$ and $t = 10$ solutions respectively. The difficulty in solving this problem is apparent in the figure. The P_7 solution has large amplitude waves that does go negative, and the S_8 solution has strong ray effects (though they look like "dot" effects on this problem). The two filtered spherical harmonics solutions both remain positive. The material based filter does not have waves in the solution and is propagating information at nearly the correct speed. The slope-limiter based filter moved information too slowly and does demonstrate wave-like behavior. These solutions are compared to Ganapol's transport solution in Fig. 2. At this early time none of the numerical solutions adequately capture the transport solution. The solutions at a later time, $t = 10$, are show in Fig. 3. At this time the P_7 and S_8 solutions give nearly the same results as the transport solution. The material based filter and the slope limiter based filter are not as accurate. The filter based the slope limiter has not moved information far enough into the problem, causing the solution near the origin to be too high. The material based filter is also slightly too high near the origin. Despite these shortcomings of the filtered solutions we note that the solution at $t = 10$ was arrived at without negativity or large wave (or ray) effects along the way.

The next problem that we solve is a radiative transfer problem first suggested in alternate form by Brunner [12]. This problem is a simplified hohlraum from an inertial confinement fusion experiment and is diagrammed in Fig. 4. A source of radiation is present on the left of the problem. This radiation flows into the problem and heats that block at the center.

The radiation field from this problem for different methods is shown in Fig.5. The radiation is measured by the radiation temperature, $T_{\text{rad}} = \sqrt[4]{\phi/ac}$. We compare the solution for our filtered spherical harmonics

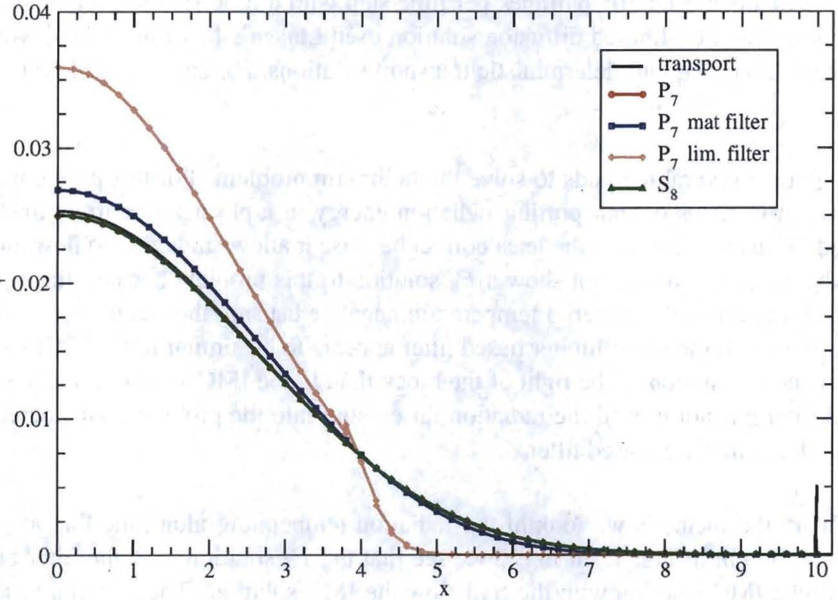


Figure 3. Comparison of solutions to the pulsed line source problem and $t = 10$.

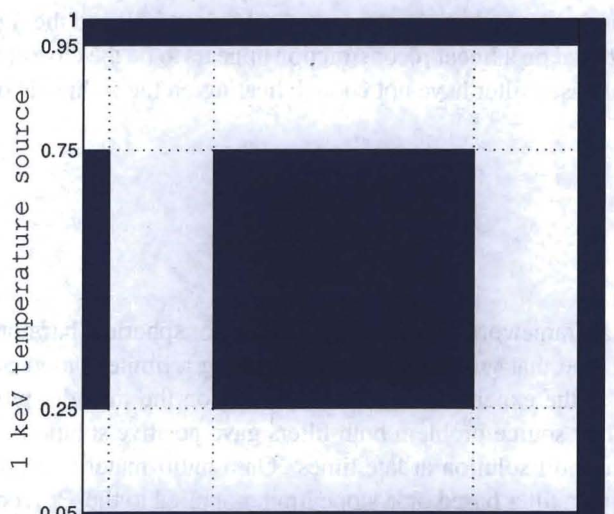


Figure 4. Layout for the 2-D hohlraum problem. The blue regions have $\sigma_a = 100T^{-3}$ cm^{-1} for T in keV. The white regions have $\sigma_a = 0$. Also, $C_v = 0.3$ GJ/cm^3-keV.

approximations to implicit Monte Carlo (IMC) [13], flux-limited diffusion, and S_8 calculations. The implicit Monte Carlo calculations used 10^6 particles per time step with a time step size of 10^{-2} ns and 200 mesh cells per direction. The flux-limited diffusion solution used Larsen's flux limiter [14] with $n = 2$ and 200 mesh cells in each direction. Our deterministic transport solutions, P_N and S_N used 100 cells per direction.

In Fig. 5 we compare several methods to solve the holhraum problem. For this problem the IMC solution is the most correct in terms of transporting radiation energy in a physically correct manner. Conversely, the flux-limited diffusion solution is the least correct because it allows radiation to flow around the block in the center of the problem. We do not show a P_7 solution to this problem because the P_7 radiation energy became negative and drove the material temperature negative causing the calculation to fail. The solution to the P_7 equations with the slope limiter based filter appears to be similar to the IMC solution except that there is slightly more radiation to the right of the block than in the IMC solution. The P_7 solution with the material based filter has not moved the radiation far enough into the problem. This defect is mitigated by going to P_{11} with the material based filter.

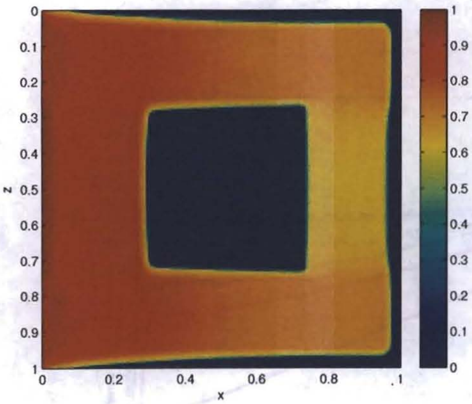
To better compare the methods we look at the radiation temperature along the line at $y = 0.125$ cm in Fig. 6 and $x = 0.85$ cm in Fig. 7. In Fig. 6 we see that the P_7 solution with the filter based on the slope limiter is above the IMC solution with the S_8 below the IMC solution. The material based filter solutions dip below the IMC solution; the P_7 version of this filter is far below the IMC solution near the right edge of the problem, and the P_{11} solution is closer to IMC but still below S_8. These comparisons hold on the right of the block as shown in Fig. 7 where the slope limiter based filter solutions is higher than IMC, with the material based filter solutions are below IMC.

The material temperatures from different methods are compared in Fig. 8. In this figure we can see ray effects present in the S_8 solution in the hot spots present on the right wall and the right side of the block. The P_7 solution using the filter based on a linear reconstruction appears to be the closest to the IMC solution. The solutions using the material based filter have not enough heating on the right side of the problem compared to IMC.

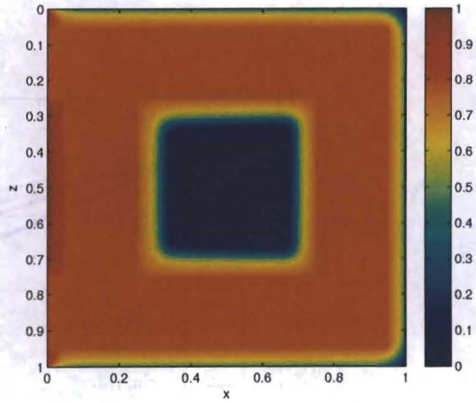
6. CONCLUSION

We have presented a general framework for developing filters for spherical harmonics approximations. We also developed two filters: one that guaranteed positivity using a limiter based on the P_1 expansion, and one that enforced a decay in the expansion coefficients based on the material properties and the order of expansion. On the pulsed line source problem both filters gave positive solutions, however, both solutions also did not capture the transport solution at late times. On a multi-material problem of thermal radiative transfer the P_7 solution using a filter based on a slope limiter applied to the P_1 reconstruction was nearly as accurate as the S_8. This is significant because the filtered solution did not have negativite energies or ray effects. On the same problem the material based filter was not as accurate as S_8 even when P_{11} was used.

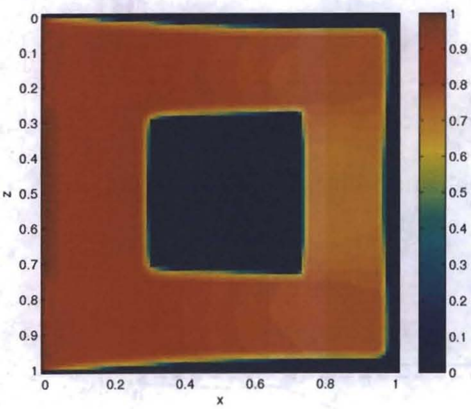
We would like to again emphasize that the filters presented in this study are not likely the best filters for transport. Nevertheless, we believe that filters are a way to remove the drawbacks of the spherical harmonics equations. Possible directions for future work include a filter based on a positive P_3 reconstruction, though this is certainly not the only way forward.



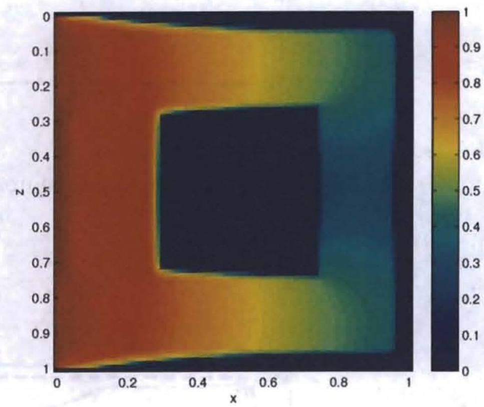
(a) Implicit Monte Carlo



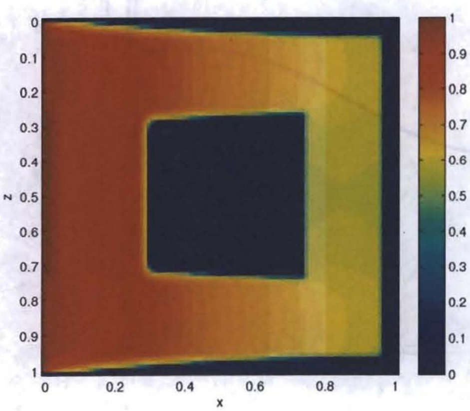
(b) Flux-limited Diffusion



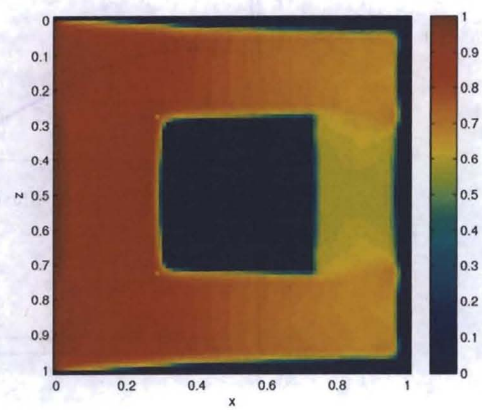
(c) P_7 Slope Limited Filter



(d) P_7 Material Filter



(e) P_{11} Material Filter



(f) S_8

Figure 5. Radiation temperature solutions the hohlraum problem at $t = 1$ ns.

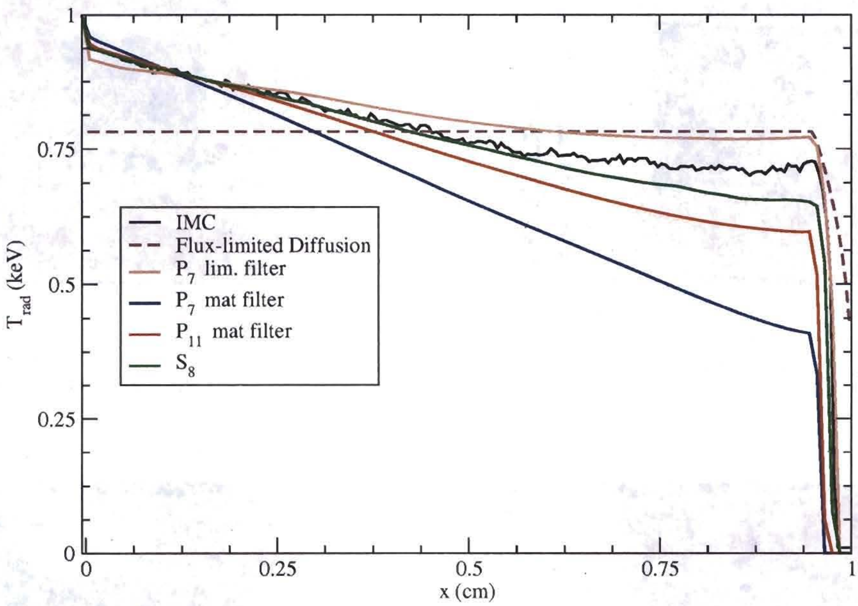


Figure 6. Radiation temperatures for the hohlraum problem at $y = 0.125$ cm.

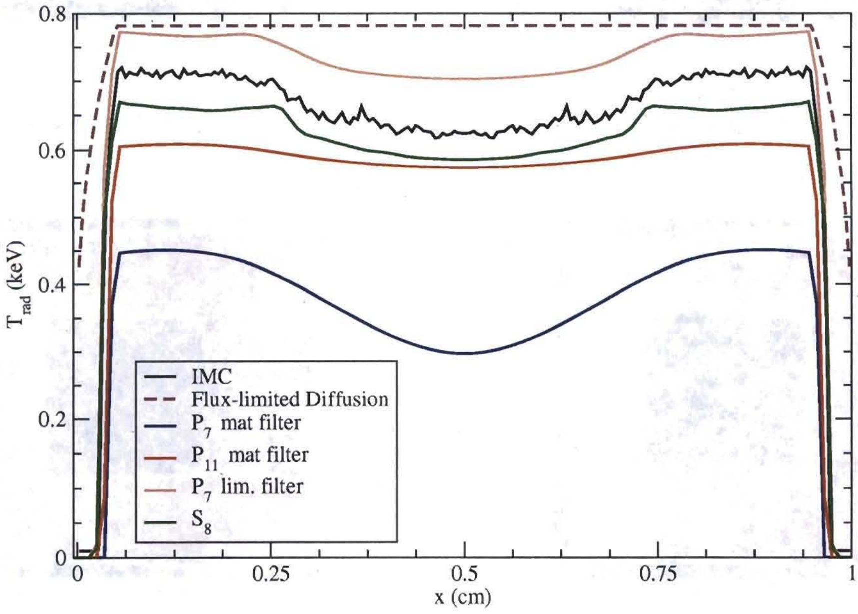
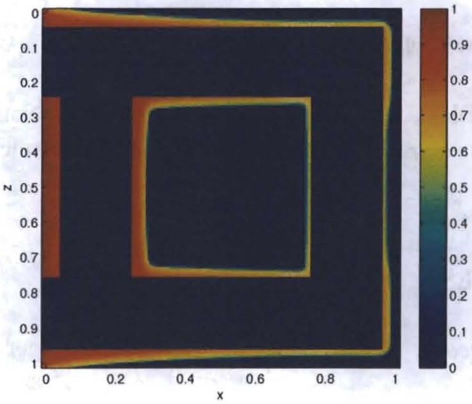
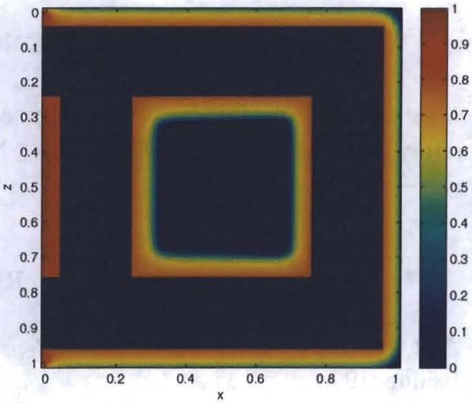


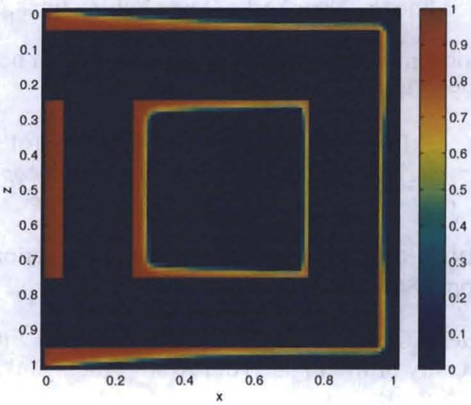
Figure 7. Radiation temperatures for the hohlraum problem at $x = 0.85$ cm.



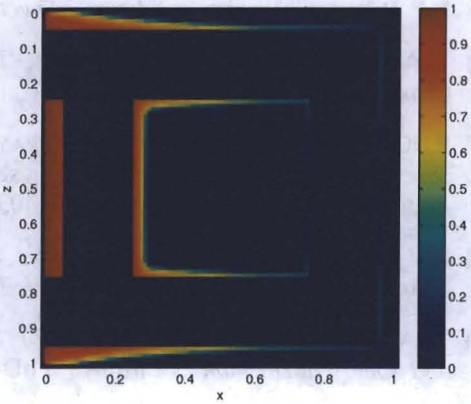
(a) Implicit Monte Carlo



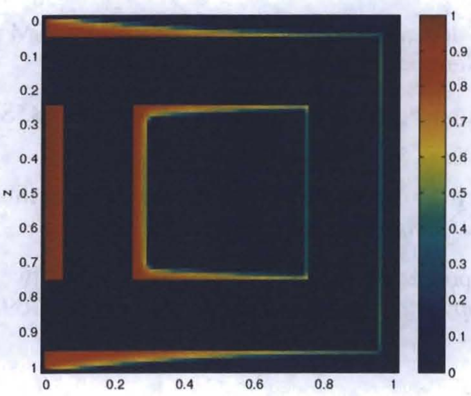
(b) Flux-limited Diffusion



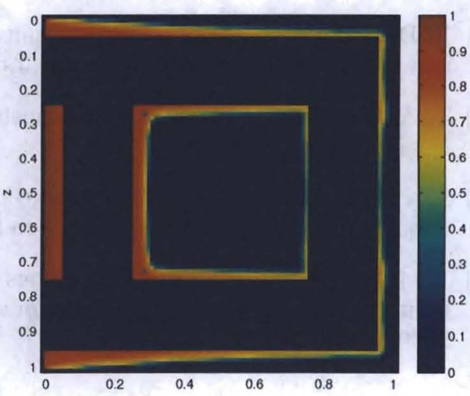
(c) P_7 Slope Limited Filter



(d) P_7 Material Filter



(e) P_{11} Material Filter



(f) S_8

Figure 8. Material temperature solutions the hohlraum problem at $t = 1$ ns.

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