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# THE IMPACT OF REFERENCE FRAME ORIENTATION ON DISCRETE ORDINATES SOLUTIONS IN THE PRESENCE OF RAY EFFECTS AND A RELATED MITIGATION TECHNIQUE

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## ABSTRACT

The discrete ordinates method is a popular and versatile technique for deterministically solving the radiative transport which governs the exchange of radiant energy within a fluid or gas mixture. It is the most common 'high fidelity' technique used to approximate the radiative contribution in combined-mode heat transfer applications. A major drawback of the discrete ordinates method is that the solution of the discretized equations may involve nonphysical oscillations due to the nature of the discretization in the angular space. These ray effects occur in a wide range of problems including those with steep temperature gradients either at the boundary or within the medium, discontinuities in the boundary emissivity due to the use of multiple materials or coatings, internal edges or corners in non-convex geometries, and many others. Mitigation of these ray effects either by increasing the number of ordinate directions or by filtering or smoothing the solution can yield significantly more accurate results and enhanced numerical stability for combined mode codes. When ray effects are present, the solution is seen to be highly dependent upon the relative orientation of the geometry and the global reference frame. This is an undesirable property. A novel ray effect mitigation technique is proposed. By averaging the computed solution for various orientations, the number of ordinate directions may be artificially increased in a trivially parallelizable way. This increases the frequency and decreases the amplitude of the ray effect oscillations. As the number of considered orientations increases a rotationally invariant solution is approached which is quite accurate. How accurate this solution is and how rapidly it is approached is problem dependent. Uncertainty in the smooth solution achieved after considering a relatively small number of orientations relative to the rotationally invariant solution may be quantified.

## INTRODUCTION

One of the most commonly used radiative transport solution techniques is the method of discrete ordinates [1, 2, 3]. It is so widely used largely because of the intuitive derivation of the equations and boundary conditions and the theoretical guarantee that it will converge to the correct solution as the number of ordinate directions goes to infinity. Unfortunately, this convergence is slow and the method may produce unrealistically oscillatory solutions known as 'ray effects.' These ray effects occur in a wide range of problems including those with steep temperature gradients either at the boundary or within the medium, discontinuities in the boundary emissivity due to the use of multiple materials or coatings, internal edges or corners in non-convex geometries, and many others. These ray effects are inherent to the solution of the discretized equations and may not be reduced by further spatial mesh refinement. In fact, spatial mesh refinement has been known to increase ray effects in some situations.

There have been a number of techniques proposed to help mitigate ray effects [4, 5, 6]. The most straightforward approach is to simply increase the number of ordinate directions. Unfortunately, this approach may involve prohibitive computational expense. Schemes which add ordinate directions adaptively [7, 8, 9] present one potential solution to this problem. A different approach involves filtering the solution to reduce or eliminate the spurious ray effect oscillations [10]. If the discrete ordinates method is to be modified more fundamentally, other discrete ordinate-like approaches which incorporate a continuous definition of the intensity in the angular space may be used [11, 12, 13, 14]. A separate, minimally intrusive approach is presented here which


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exploits the spatial dependence of the ray effect oscillations on the definition of the global reference frame.

## THE DISCRETE ORDINATES METHOD

The discrete ordinates method is a general term for a class of solution methods to the radiative transport equation that rely upon collocation in the angular variables. The transport equation is satisfied exactly along a set of discrete directions and a quadrature rule is used to approximate any integrals over the angular space such as those in the in-scattering term or in the definitions of the radiative flux and flux divergence. The choice of quadrature rule is left up to the user and may have a significant impact upon the quality of results obtained. There has been substantial research effort applied to the development and analysis of quadrature rules for integration over the unit sphere [15, 16, 17]. The solution of the radiative transport equation using the discrete ordinates method may be found by stepping through the domain [11, 18, 19, 20]. This is easily accomplished in structured meshes. However, in unstructured meshes, this solution technique may involve significant additional overhead. The discrete ordinates method has also been applied to unstructured meshes using stepping schemes and other more general solution techniques [21, 22, 23].

For a given angular quadrature, the integral in the in-scattering term may be approximated as a summation as shown in Equation 1.

$$\frac{\sigma_s}{4\pi}\int I\left(\vec{\tilde{\Omega}}\right)d\tilde{\Omega} \approx \frac{\sigma_s}{4\pi}\sum_i w_i I\left(\vec{\Omega}_i\right) \qquad (1)$$

The weights and nodes of the quadrature scheme are $w_i$ and $\vec{\Omega}_i$ respectively. The weights are normalized such that they sum to $4\pi$.

In this way, it is trivial to see that the transport equation may be written as a system of linear first order equations in the ordinate directions.

$$\vec{\Omega}_i \cdot \vec{\nabla} I_i + \sigma_T I_i = \kappa I_b + \frac{\sigma_s}{4\pi}\sum_j w_j I_j \qquad (2)$$

With diffuse walls, this equation is subject to the boundary condition

$$I_i = \varepsilon I_{bw} + \frac{1-\varepsilon}{\pi}\sum_{\vec{n}\cdot\vec{\Omega_j}<0} w_j I_j \left|\vec{n}\cdot\vec{\Omega_j}\right| \qquad (3)$$

Since the equation is first order, a boundary condition is only required on half the boundary for each directional intensity. The boundary condition above only applies if $\vec{n}\cdot\vec{\Omega_j} > 0$. That is, we only apply a condition on the intensity leaving an opaque surface.

The first-order discrete ordinates equation has stability problems when using the Galerkin finite element method. Equation 2 is a set of coupled convection-diffusion-reaction equations with zero diffusion coefficient. The method may be stabilized using the Streamline Upwind Petrov-Galerkin (SUPG) stabilization method; the test function $\tilde{I}_i$ is replaced with $\tilde{I}_i + \tau\vec{\Omega}_i \cdot \vec{\nabla}\tilde{I}_i$ where $\tau$ is a stabilization parameter. For our case (no diffusion) the stabilization parameter is determined to be approximately $h/2$ . A commonly used “optimal” value of $\tau$ is found to be

$$\tau = \frac{h}{2\left\|\vec{\Omega}\right\|}\left(\coth Pe - \frac{1}{Pe}\right) \qquad (4)$$

which reduces to $h/2$ since $\vec{\Omega}$ is a unit vector and $Pe \to \infty$.

Alternatively, the second-order discrete ordinates equations may be used. The second-order formulation has the advantage of being naturally diffusive and does not require additional stabilization. It also involves half as many unknowns as the first-order formulation. It has the comparative disadvantage of generating a less sparse matrix. Additionally, the second-order form has issues with void regions where the opacity approaches zero. While the first-order formulation allows for rapid solution by use of a stepping scheme, the second-order formulation is not well-suited to such acceleration techniques. The ray effect mitigation technique proposed here is agnostic as to the choice of first- or second-order formulation as well as to the choice of quadrature rule.

## PROPOSD RAY EFFECT MITIGATION TECHNIQUE

The key to the proposed ray effect mitigation technique is the recognition of a fundamental shortcoming of the discrete ordinates method. The solution is not invariant under arbitrary rotations of the reference frame. This property is inherent to the discrete ordinates method. Consider a test problem of a square duct with a single hot wall. The medium is purely absorbing. It neither scatters nor emits radiation. All four walls are black. An analytical series solution to this problem has been developed by Crosbie and Schrenker [30]. This technique was later expanded to inhomogeneous media with isotropic scattering [31] although those cases will not be considered here.

It is proposed that rotational invariance may be approached by averaging the solutions found using some number of arbitrarily rotated reference frames. It is observed that ray effect oscillations are virtually eliminated when averaging a relatively small number of these solutions. However, a very large number of solutions may be required to approach true rotational invariance. The set of discrete rotations may be chosen using either a deterministic system or random choice. Because an arbitrarily large number of potential rotations is

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desired and because the development of a deterministic system is a non-trivial task that is likely quadrature dependent, only stochastic rotations are considered here. Figure 1 compares 4 potential solutions to the above problem with an optical side length of unity and a scattering albedo of zero.

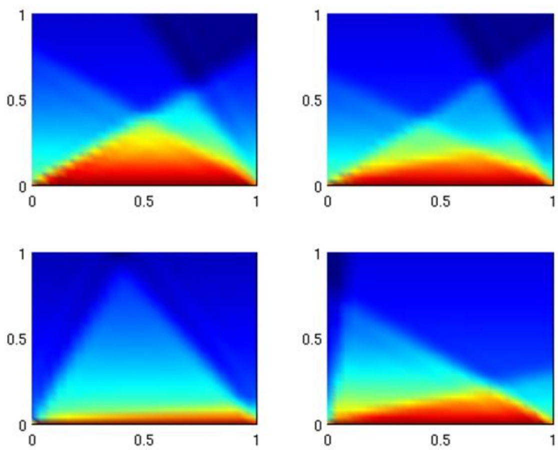


**Fig. 1**: $S_2$ energy density predictions for 4 different random rotations of the PN-TN quadrature in a square X-Y geometry. The medium is purely absorbing with an optical side length of unity.

As can be seen from Figure 1, the solution is highly dependent upon the choice of reference frame. Because the arbitrary rotations often cause the quadrature to become asymmetrical with respect to the geometry's symmetry plane asymmetrical solutions may result. In a simple geometry such as this, it is easy to align the reference frame to avoid these kinds of inconvenient and obvious failings. However, in a more complicated arbitrary geometry the errors may be less apparent.

For cases where the scattering albedo is zero and the walls are black like this one, the intensity in each direction is completely decoupled from the intensity in every other direction. As a result, the average solution will converge to the analytical solution as more and more rotations are considered. This is functionally equivalent to increasing the number of ordinate directions to an arbitrarily high number. However, for cases in which scattering or reflective boundaries are present, the ordinate directions are coupled together via the scattering source term. In these cases, the average does not converge to the analytical solution as the number of rotations considered approaches infinity. This is a result of each individual solution failing to accurately represent the scattering source term. From here on out, we will concern ourselves only with the above scenario but with a scattering albedo of unity rather than zero or some intermediary value.

We will compare four quadrature rule – rotation scheme combinations. The first two (LQN-3d and PNTN-3d) are the LQN and PN-TN quadrature rules under uniformly distributed random rotations about the origin. Commonly, for 2-D problems, the quadrature is aligned such that symmetry eliminates the need to evaluate half of the ordinate directions. This is not true under uniformly distributed random rotations and thus ordinates in all 8 octants must be used which essentially doubles the number of unknowns for a 2-D problem. For a fully 3-D problem all 8 octants must be used regardless and this disadvantage disappears. The third combination (PNTN-z) seeks to maintain this advantageous use of symmetry for 2-D problems. It is the PN-TN quadrature rule under uniformly distributed random rotations about the z-axis. The fourth and final combination is a stochastic quadrature (AR). The AR quadrature is defined by generating a specified number of uniformly distributed random unit vectors in the first octant. This set of vectors is the reflected into each other octant so as to enforce invariance under rotations of $90^0$ and allow the use of second-order solution methods. The resulting quadrature is then subjected to uniformly distributed random rotations about the origin.

The heat flux is measured along the (top) surface opposite the hot wall. The relative error is defined using the L2 norm of the difference between the predicted heat flux and the analytical solution provided by Crosbie and Schrenker [30].

$$\sqrt{\frac{\int\left(q''_{exact}-q''_{approx}\right)^2 dx}{\int\left(q''_{exact}\right)^2 dx}} \qquad (5)$$

## RESULTS

A large number of rotations must be considered before the rotationally invariant solution is approached. The number of rotations required is smaller for quadratures with more ordinates per octant. In contrast, only a small number of rotations must be considered before the heat flux prediction becomes smooth. Considering that apart from certain limiting cases the rotationally invariant solution is not equivalent to the exact solution, a sufficiently smooth solution may suffice. Further, the average solution approaches the rotationally invariant solution in a well understood way which allows for the quantification of the degree to which a given smooth solution has converged to the rotationally invariant solution.

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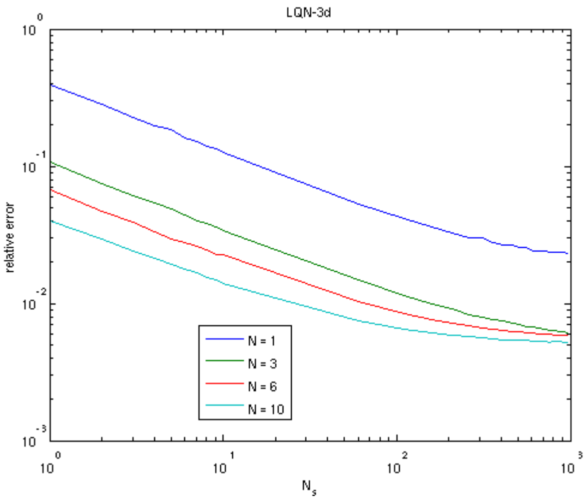


**Fig. 2**: Relative error in the average LQN-3d heat flux prediction as an increasing number of rotations is considered

Generally, as the number of ordinates per octant increases both the error and the number of samples required for convergence decreases. Figure 2 demonstrates this for the LQN-3d combination of quadrature rule and rotation scheme. It is seen that the expected value of the relative error converges relatively slowly and that it plateaus at a certain level which corresponds to the difference between the rotationally invariant solution and the true solution. The requirement that the solution approach rotational invariance is seen to be very difficult and computationally expensive to meet. Alternatively, if the solution is only required to be smooth (ie that the wavelength of the ray effect oscillations is small relative to the grid size or that the amplitude of the ray effect oscillations is sufficiently small relative to the solution magnitude) far fewer samples are required.

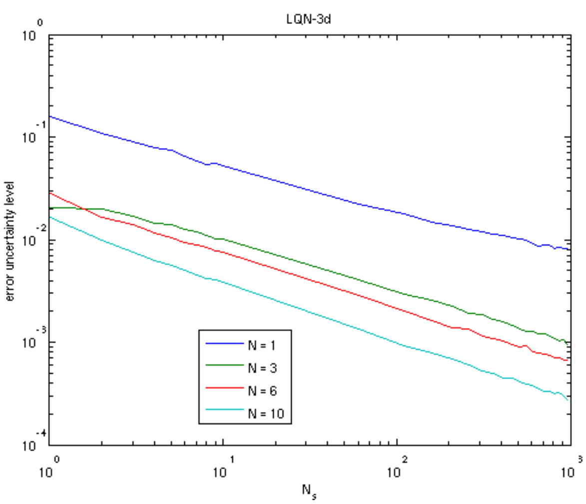


**Fig. 3**: Standard deviation of the relative error in the average LQN-3d heat flux prediction as a function of the number of rotations considered

Statistics upon these samples may then be generated to estimate the uncertainty in the average solution relative to the rotationally invariant solution. It is reiterated that the rotationally invariant solution is not equivalent to the analytical solution if scattering is present.

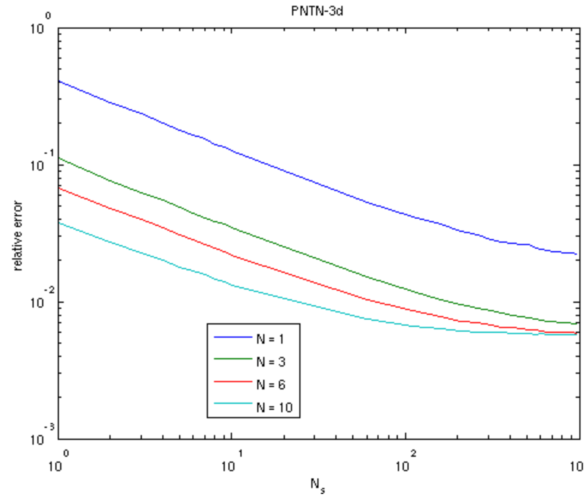


**Fig. 4**: Relative error in the average PNTN-3d heat flux prediction as an increasing number of rotations is considered

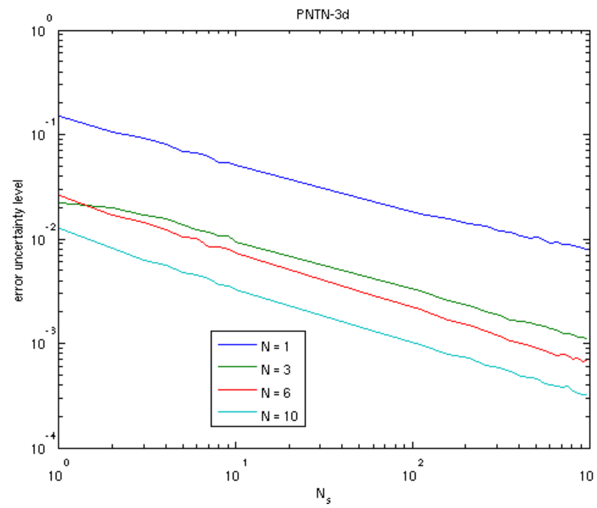


**Fig. 5**: Standard deviation of the relative error in the average PNTN-3d heat flux prediction as a function of the number of rotations considered

Similar behavior is observed for the PNTN-3d combination as for the LQN-3d combination. Both the error levels and the solution convergence rates are virtually indiscernible.


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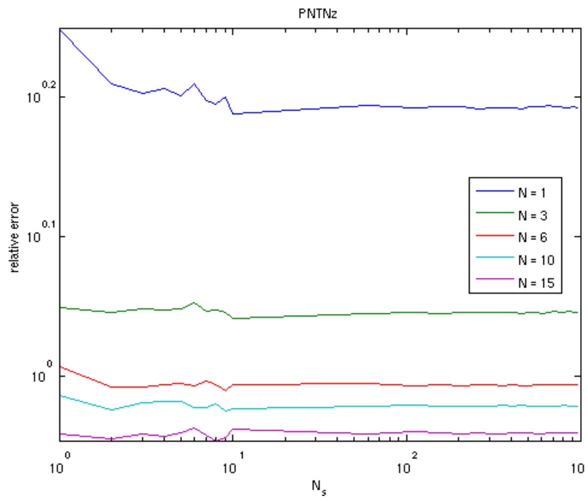


**Fig. 6**: Relative error in the average PNTN-z heat flux prediction as an increasing number of rotations is considered

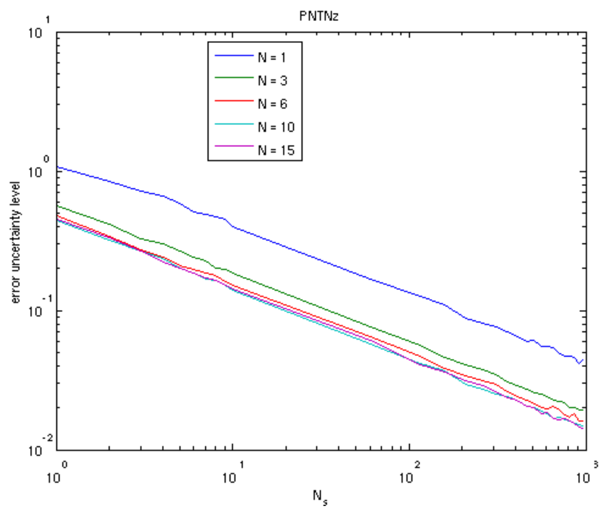


**Fig. 7**: Standard deviation of the relative error in the average PNTN-z heat flux prediction as a function of the number of rotations considered

The error using the PNTN-z combination of quadrature rule and rotation scheme is seen to be substantially higher than the combinations utilizing rotations about the origin. In this problem, the z-component of each ordinate enters the equations as a scaling coefficient for the attenuation rate in that direction. If only rotations about the z-axis are considered, only a small set of discrete values for this scaling coefficient are included. Although the rotations about the z-axis effectively increase the resolution in the circumferential angle sufficiently to mitigate the ray effects, the low resolution in the azimuthal angle still results in errors which dominate the solution.

The PNTN-z combination is only practical for 2-D geometries with appropriate symmetry. It could be considered a relatively inexpensive option for smoothing. However, the accuracy gains the other rotation schemes provide are significantly less pronounced.

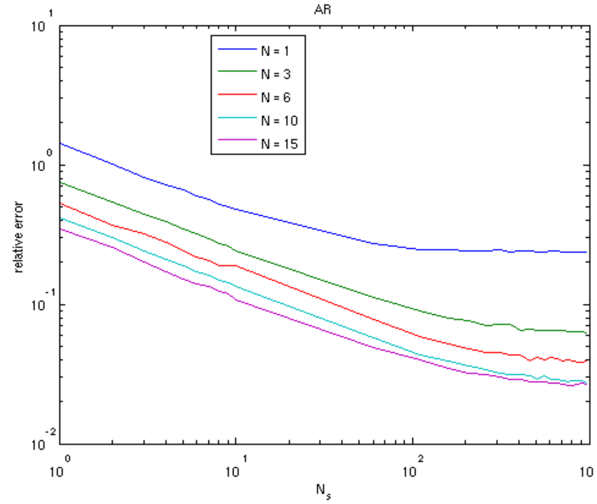


**Fig. 8**: Relative error in the average AR heat flux prediction as an increasing number of rotations is considered

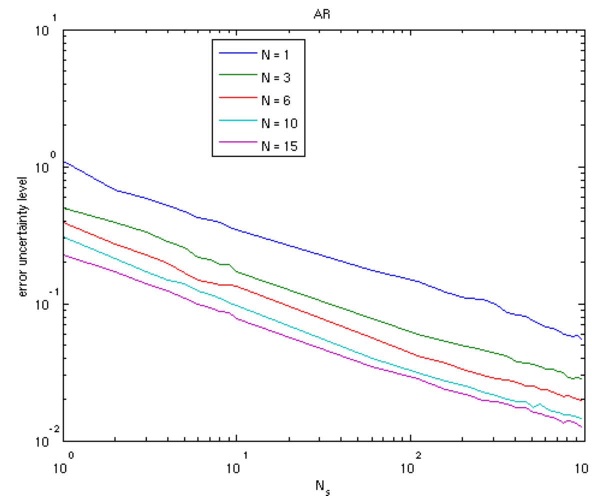


**Fig. 9**: Standard deviation of the relative error in the average AR heat flux prediction as a function of the number of rotations considered

The AR quadrature rule – rotation scheme allows for a larger number of intermediate numbers of ordinates per octant. The additional stochastic element and lack of enforced symmetry further increases the number of samples needed for convergence. It is seen to be generally inferior to the PNTN-3d and LQN-3d combinations. However, it remains superior to the PNTN-z combination.

The convergence toward the analytical solution as the number of ordinates per octant increases is quite slow. However, the number of samples required to approach rotational invariance decreases more rapidly with the number of ordinates per octant.


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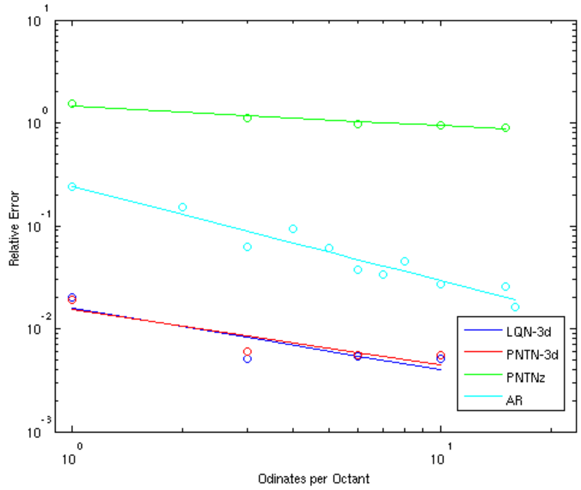

**Fig. 10**: Relative error in the average heat flux prediction as a function of the number of ordinates per octant

Figure 10 shows the relative error in the average solution as a function of the number of ordinates per octant used to generate each solution. Not all of the average solutions have sufficiently converged to the rotationally invariant solution which accounts for the scatter. The uncertainty in the results in Figure 10 is plotted in Figure 11.

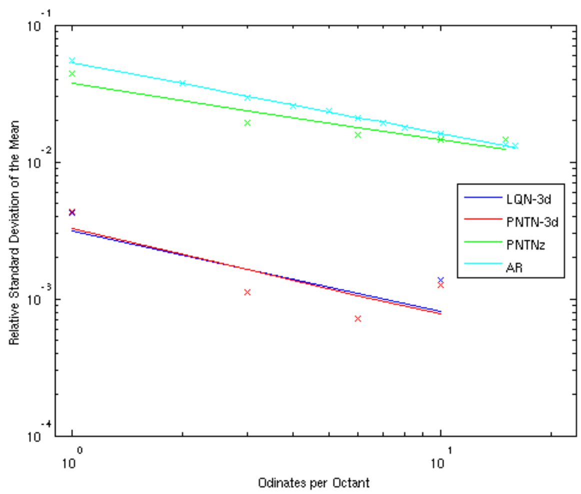

**Fig. 11**: Standard deviation of the mean of the samples as a function of the number of ordinates per octant

The difference between the PNTN-z combination and the AR combination is statistically significant. As is the difference between the AR combination and the other 2 combinations. The differences between the PNTN-3d and LQN-3d combinations are not statistically significant.

## CONCLUSIONS

The proposed ray effect mitigation technique allows for accurate solution to the radiative transport equation via the discrete ordinates method even in the presence of ray effect inducing discontinuities. The technique is trivially parallelizable since each solution is completely decoupled from all the others. For non-scattering media, the technique converges to the exact solution as the number of samples approaches infinity. The rotationally invariant solution which this technique approaches with increasing numbers of samples is not equivalent to the analytical solution for problems involving scattering media or non-black boundaries. However, it approaches the analytical solution as the number of ordinates per octant approaches infinity. Determining the rate of this convergence with any degree of accuracy would require significantly more samples than were considered here. Generating a smooth solution absent of ray effects requires considerably fewer samples than approximating the rotationally invariant solution. The degree to which a smooth solution resembles the rotationally invariant solution may be estimated by simple statistics.

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