SAND2004-2643P

Implementation of Ray-Effect Mitigation Techniques for 3D Radiation Transport

Frederick Gleicher

University of New Mexico

Manager: Len Lorence (15341)

Technical Advisor: Wesley Fan

Sandia National Laboratories

Sandia is a multiprogramming laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

LOCKHEED MARTIN

Sandia National Laboratories

Radiation Transport

- Sandia has strong interest in modeling radiation transport through materials.
- Coupled photon-electron transport to model radiation effects on weapon and system components.
- Other applications include modeling of fusion reactions and thermal radiation transfer in fires.
- Boltzmann transport equation can be used to model radiation transport.

Radiation Transport

- The Boltzmann transport equation is an expression of the particle balance in space r, energy E and direction Ω. This form is time independent.

Streaming Collision

$$\hat{\Omega}\cdot\nabla\Psi(\vec{r},E,\hat{\Omega})+\sigma(\vec{r},E)\Psi(\vec{r},E,\hat{\Omega})=$$

$$\int_0^\infty dE'\int d\Omega'\,\sigma_s(\vec{r},E'\rightarrow E,\hat{\Omega}'\cdot\hat{\Omega})\Psi(\vec{r},E',\hat{\Omega}')+q(\vec{r},\hat{\Omega},E)$$

Scattering External Source

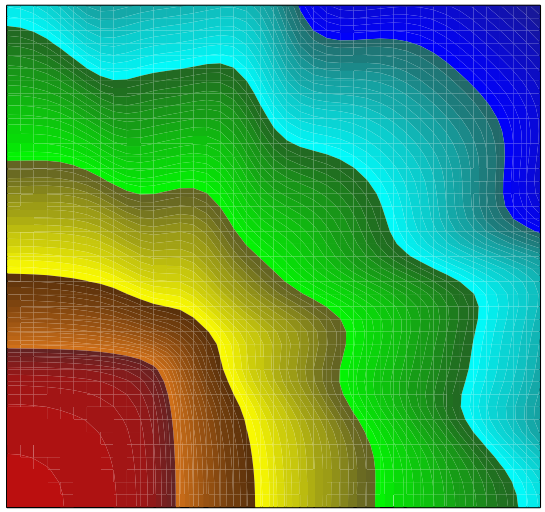
Angular Treatment

- **Discrete Ordinates (S_n method)**
- The angular flux Ψ can be expanded in interpolation polynomials and evaluated along discrete directions.
- Discrete Ordinates results in a lower triangular matrix which is easy to invert.
- Discrete Ordinates are easily implemented.
- However, ray effects result from the Discrete Ordinates method.

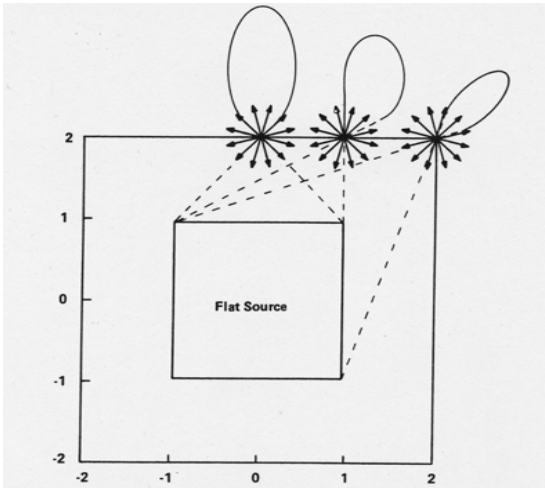
Ray Effects

- Ray effects are distortions in the scalar flux for problems with isolated sources and low scattering ratios.

- Ray Effects are inherent to the nature of discrete ordinates. The effect arises because the solution is allowed to propagate along an ordinate rather than a continuum of directions.



Corner source in box with constant σ_a and without ray effect mitigation



From *Computational Methods Of Neutron Transport*
By Lewis & Miller

Ray Effect Mitigation

- Ray Effects were first identified from anomalous calculational results by Gelbard in 1965 in a two dimensional Boltzmann transport equation.
- First Ray Effect mitigation technique implemented by K.D. Lathrop in 1968.
- Reed and Jung have formulated the latest in fictitious source for Ray Effect mitigation in 1976. The fictitious source method makes the S_n equations look like an equivalent spherical harmonic equation by adding on a source that is the next in the spherical harmonic series.
- Ray effect mitigation techniques have only been implemented in 2D. The purpose of this work is to extend this technique in 3D.

Modified Discrete Ordinates Equation

- For discrete ordinates the transport equation becomes

$$[A]\frac{\partial}{\partial x}\vec{\Psi} + [B]\frac{\partial}{\partial y}\vec{\Psi} + [C]\frac{\partial}{\partial z}\vec{\Psi} + ([\sigma_t] + [\sigma_s])\vec{\Psi} = \overline{S}_n$$

- For regular Discrete Ordinates the matrices [A], [B], and [C] are diagonal
- For the fictitious source the matrices [A], [B] and [C] are full

Reed Mitigation Source

- Algebraically the fictitious source is complex
- Reed Fictitious Source

$$
\begin{aligned}
S_{fic}(r,\Omega_n) = & \sum_{m=0}^{N} Y_{Nm}^{c}(\Omega_n)\left[\alpha_{N-1,m+1}^{c(2)}\frac{\partial}{\partial x}\phi_{N-1,m+1}^{c}(r) + \alpha_{N-1,m-1}^{c(4)}\frac{\partial}{\partial x}\phi_{N-1,m-1}^{c}(r)\right] \\
& + \sum_{m=0}^{N} Y_{Nm}^{c}(\Omega_n)\left[\beta_{N-1,m+1}^{c(2)}\frac{\partial}{\partial y}\phi_{N-1,m+1}^{s}(r) + \beta_{N-1,m-1}^{c(4)}\frac{\partial}{\partial y}\phi_{N-1,m-1}^{s}(r)\right] \\
& + \sum_{m=0}^{N} Y_{Nm}^{s}(\Omega_n)\left[\alpha_{N-1,m+1}^{s(2)}\frac{\partial}{\partial x}\phi_{N-1,m+1}^{s}(r) + \alpha_{N-1,m+1}^{s(4)}\frac{\partial}{\partial x}\phi_{N-1,m-1}^{s}(r)\right] \\
& + \sum_{m=0}^{N} Y_{Nm}^{c}(\Omega_n)\left[\beta_{N-1,m+1}^{s(2)}\frac{\partial}{\partial y}\phi_{N-1,m+1}^{c}(r) + \beta_{N-1,m-1}^{s(4)}\frac{\partial}{\partial y}\phi_{N-1,m-1}^{c}(r)\right] \\
& + \sum_{m=0}^{N}\left[Y_{Nm}^{c}(\Omega_n)\gamma_{N-1,m}^{c(2)}\frac{\partial}{\partial z}\phi_{N-1,m}^{c}(r) + Y_{Nm}^{s}(\Omega_n)\gamma_{N-1,m}^{s(2)}\frac{\partial}{\partial z}\phi_{N-1,m}^{c}(r)\right]
\end{aligned}
$$

- For Reed-Jung source there are additional terms.

CEPTRE Finite Element Code

- The Fictitious source was implemented in an existing discrete ordinance code
- CEPTRE – Coupled Electron Photon Transport Radiation Effects Code
  - Multigroup Energy discretization
  - Discrete Ordinates with arbitrary order anisotropic scattering
  - Continuous linear or quadratic finite-element approximation
  - Simultaneous space-direction solution by conjugate gradient method
- CEPTRE main purpose is to do radiation effects with an emphasis in electron-photon coupled interactions.

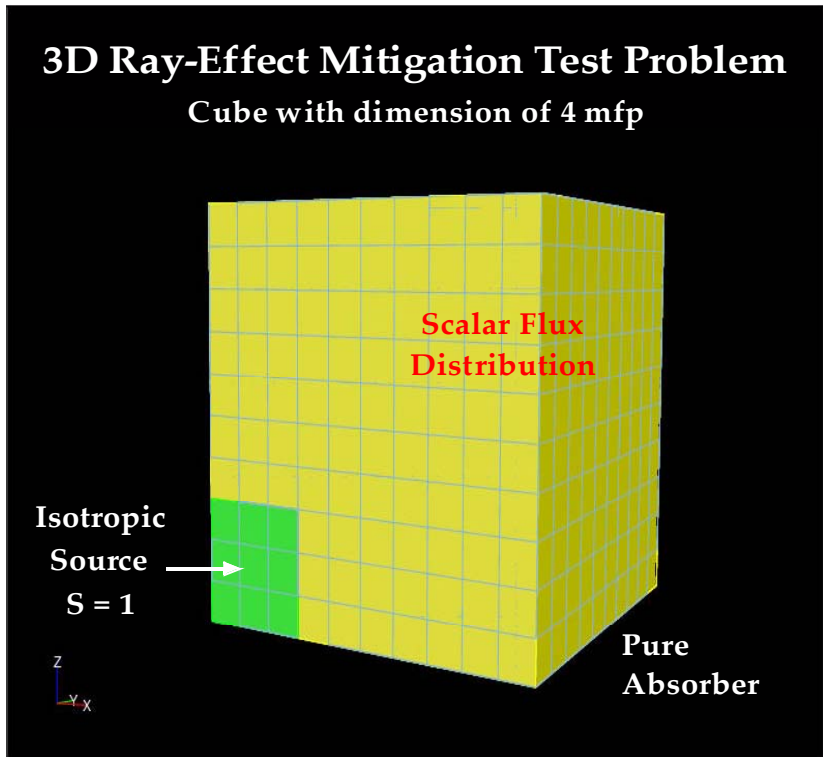
Test Problem

- **Exact Solution Available**

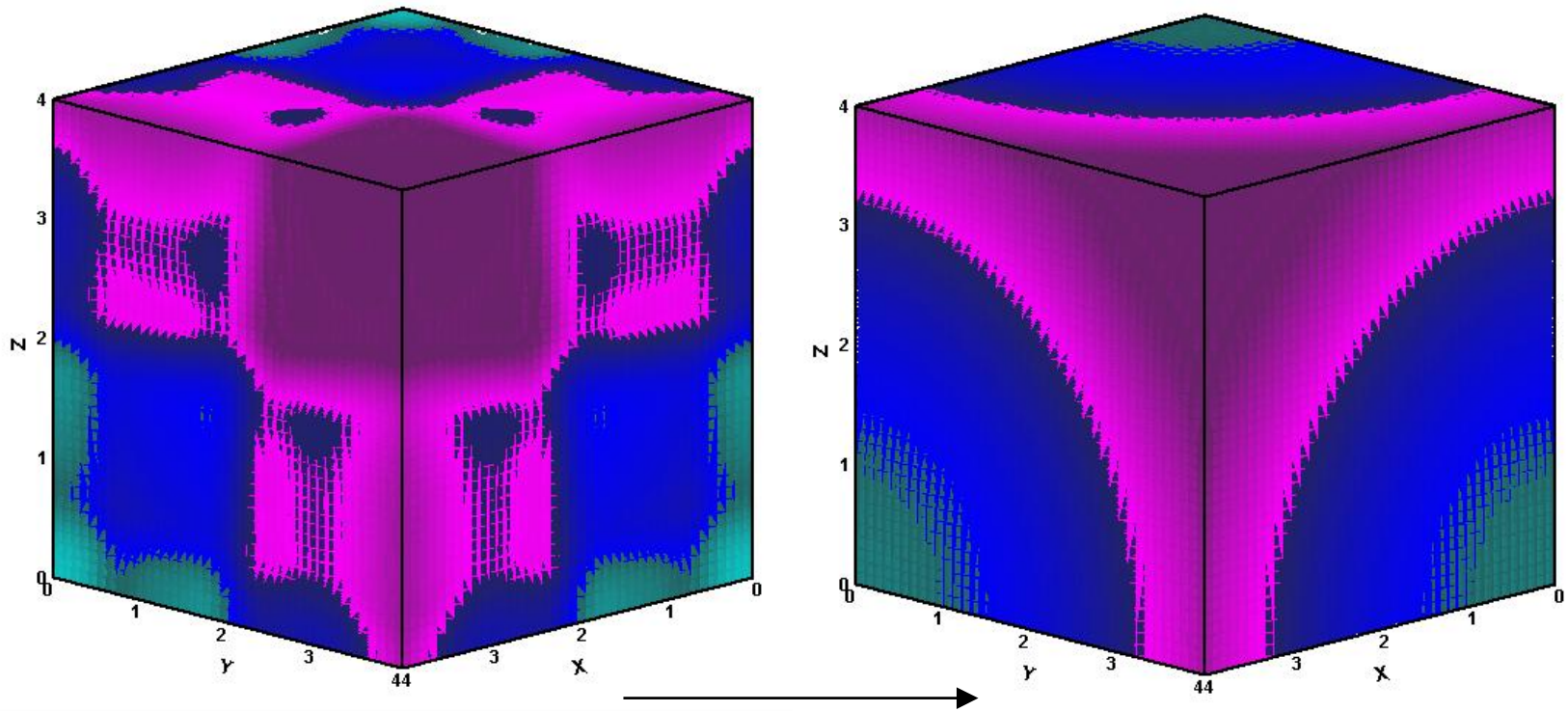
$$\Psi(\vec{r},\vec{\Omega}) = \Psi(\vec{r} - s_b\vec{\Omega},\vec{\Omega})\exp(-\sigma_a s_b)$$

$$+\int_0^{s_b} Q(\vec{r} - s\vec{\Omega},\vec{\Omega})\exp(-\sigma_a s)ds$$

- **64000 Hex Elements and S_8 Quadrature (total 80 Directions)**
- **5.12 Million Unknowns**

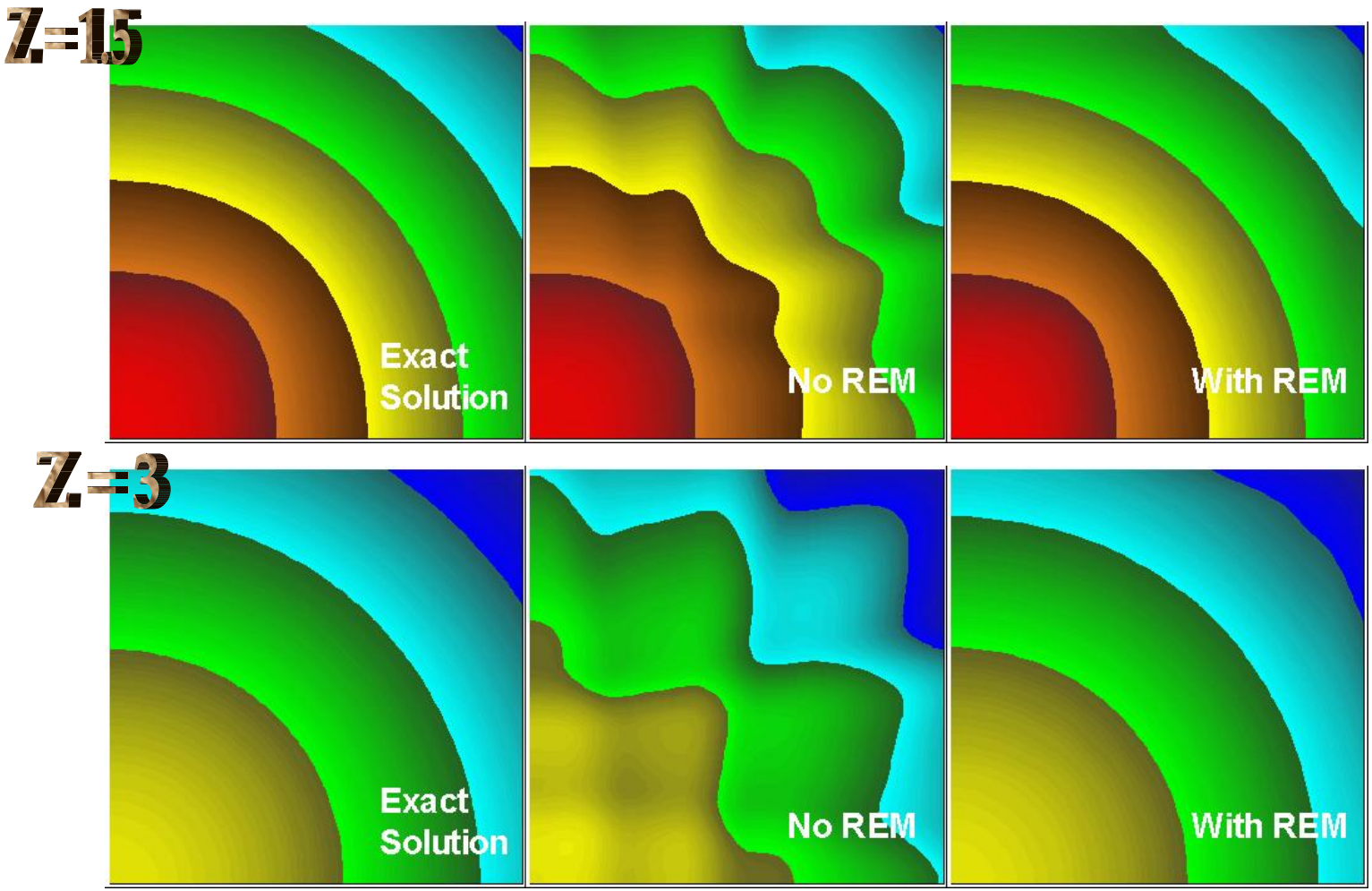


Scalar Flux Distribution on Exterior Surface



Ray-Effect Mitigation Produces Smooth and Accurate Profile

Comparison of Scalar Flux Distribution



Conclusions

- Two different mitigation techniques for 3D discrete ordinates approximation have been successfully formulated.
- The CEPTRE code is in the process of being debugged and evaluated.
- Further investigations on the interface and boundary conditions are needed .