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Residual Monte Carlo With Discrete Scattering Angles

SEERI Student Research Presentations

Don Bruss, Texas A&M University and
Sandia National Laboratories
Brian Franke, Sandia National Laboratories
01341 Radiation Effects Theory Department

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Outline

- **The Problem**
- **Monte Carlo Methods**
- **Finite Element Methods**
- **Residual Monte Carlo**
- **Details:**
  - Anisotropic scattering
  - Construction of a scattering matrix
- **Test Problems and Results**
- **Conclusions and Future Work**

Radiation Transport

- We wish to solve the steady state, monoenergetic, slab geometry (1-D) radiation transport equation,

$$\mu\frac{\partial}{\partial z}\psi + \sigma_t\psi = \frac{\sigma_s}{2}\phi + q.$$

- Of course, this isn't as easy as it looks, even with our simplifications!

$$\mu\frac{\partial}{\partial z}\psi\left(z,\mu\right) + \sigma_t(z)\psi\left(z,\mu\right) = \frac{1}{2}\int_{-1}^{1}\sigma_s(z,\mu'\rightarrow\mu)\psi\left(z,\mu'\right)d\mu' + q(z,\mu).$$

- We'll express this in operator form for simplicity

$$\mathbf{L}\psi = \mathbf{S}\psi + q.$$

- A tremendous amount of work goes into solving this equation.
  - A full model of a nuclear reactor is an exascale-sized project!
  - Time dependent, energy dependent, 3-D geometry, anisotropic scattering, very fine spatial resolution.
  - Radiation coupled to other physics.

Monte Carlo Methods

- The idea: simulate discrete particles moving through the problem randomly.
- If enough particles are modeled, the answer will represent the actual physical solution to the problem.
- Base simulated particles on actual physics.
  - Birth particles at their origin.
  - Randomly decide how far the particles travel.
  - Simulate collision to determine particle’s fate.
  - If particle survives collision, pick a new direction.

$$I = I_0 \exp(-\sigma_t \Delta z),$$

$$\Delta z = -\frac{1}{\sigma_t} \ln\left(\frac{I}{I_0}\right).$$

- The Monte Carlo method is very powerful.
- Advantages:
  - Can handle extremely complicated geometry.
  - Physical solution (as true as the physics put into the problem and the material properties).
  - Extremely parallelizable.
- Disadvantages:
  - Slowly converging.
  - Converges proportional to the square root of the number of particles simulated.
- Numerous variance reduction strategies are available to accelerate convergence or improve accuracy.

Monte Carlo example

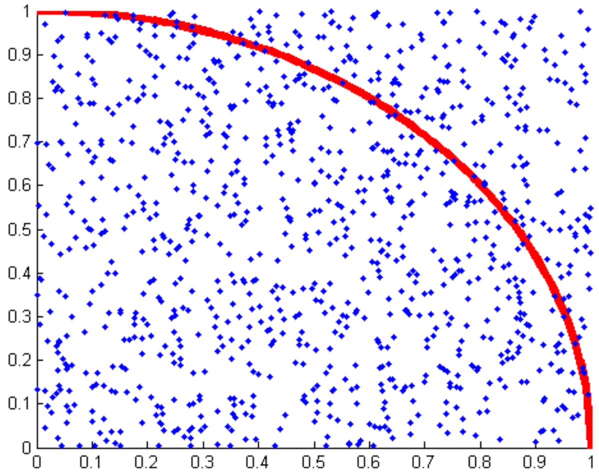
- Estimate π with monte carlo.
- Pick a pair of random numbers corresponding to *(x,y)* coordinates in the unit square.
- Score a point if the coordinates are inside the unit circle.
- Estimate π by the area ratio,

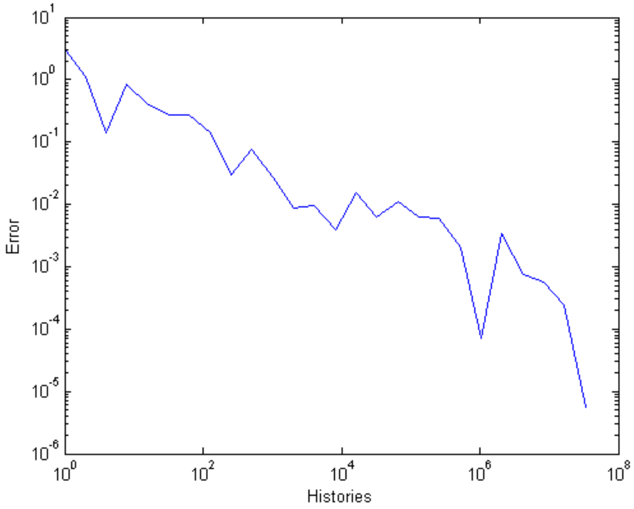
$$\frac{A_{circle}}{A_{square}} = \frac{\pi r^2}{(2r)^2}$$

$$\pi \approx 4 * \frac{points\ in\ circle}{total\ points}$$

- Error converges proportional to the square root of the number of histories!

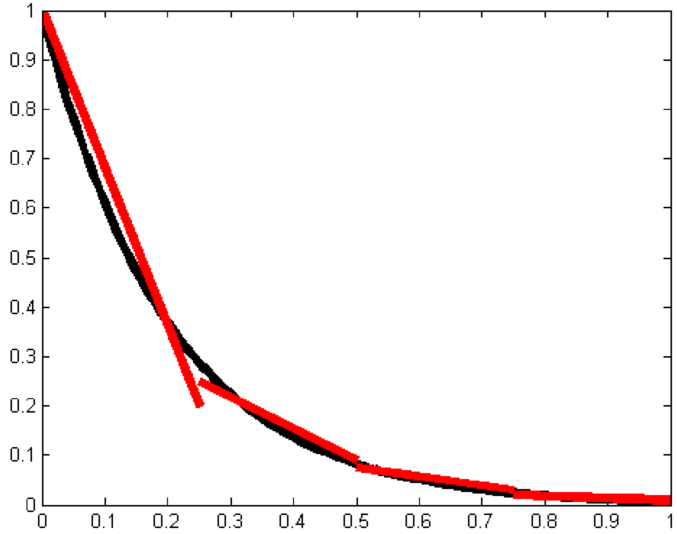
$$\epsilon \propto \frac{1}{\sqrt{n}}$$





Finite Element Methods

- The idea: Divide problem into many small cells, and then solve the problem in each cell.
- Solution within each cell can have many forms.
- One of the most common forms is linear discontinuous finite elements.
- Solve for linear solution for angular flux in each cell across the problem.
- Upwind angular flux into next cell along direction of travel.
- Advantages:
  - Can be very fast to solve.
  - Lots of math support for convergence, convergence rate.
  - “Easy” to refine mesh to increase accuracy.
- Disadvantages:
  - Complicated (but not impossible) to parallelize.
  - Challenge increases as geometry complexity increases.
  - Can yield non-physical solutions.



Residual Monte Carlo Method

- Residual Monte Carlo is not a new idea.
  - Originally the work of Halton, 1962.
  - Residual was calculated by projecting Monte Carlo solution onto polynomial trial space.
  - High order polynomials can be very oscillatory.

- Renewed interest in the late 2000s.
  - Finite element trial space replaces polynomial trial space.
  - Recent success by Morel, Peterson, and Tooley.

- State of the art:
  - 1-D problems with neutral particles.
  - Finite element in space and angle.
  - Adaptively refined finite element mesh.
  - Isotropic scattering.

- Goal:
  - Improve understanding of theory,
  - Demonstrate capabilities in a variety of problems,
  - Move towards implementation in a production code!

Residual Monte Carlo Method

- Use MC method to solve for the error after each batch; iteratively decrease the error.
- This yields exponential convergence.
  - It is possible to reduce the error to the best representation on the finite element trial space.
  - Trial space can be refined.
  - In theory, arbitrarily small convergence tolerance can be achieved in a reasonable time frame.

- Residual Monte Carlo does not make a hard problem easy!
  - Still need good statistics in each batch.
  - Problems that are solvable by MC methods can now be solved to almost arbitrary precision levels.
- Residual Monte Carlo yields a projection of the true solution onto the finite element trial space.
  - In general, this is more accurate than the solving the finite element problem.

Algorithm:

1) Perform one MC iteration.

$$(\mathbf{L}+\mathbf{S})\,\psi^{(n)} = q.$$

2) Calculate the residual on the finite element basis functions.

$$r^{(n)} = q - (\mathbf{L}+\mathbf{S})\,\psi^{(n)}.$$

3) Solve the problem with MC using the residual as the source term.

$$(\mathbf{L}+\mathbf{S})\,\epsilon^{(n)} = r^{(n)}.$$

4) Update the angular flux with the solution of the Monte Carlo problem.

$$\psi^{(n+1)} = \psi^{(n)} + \epsilon^{(n)}.$$

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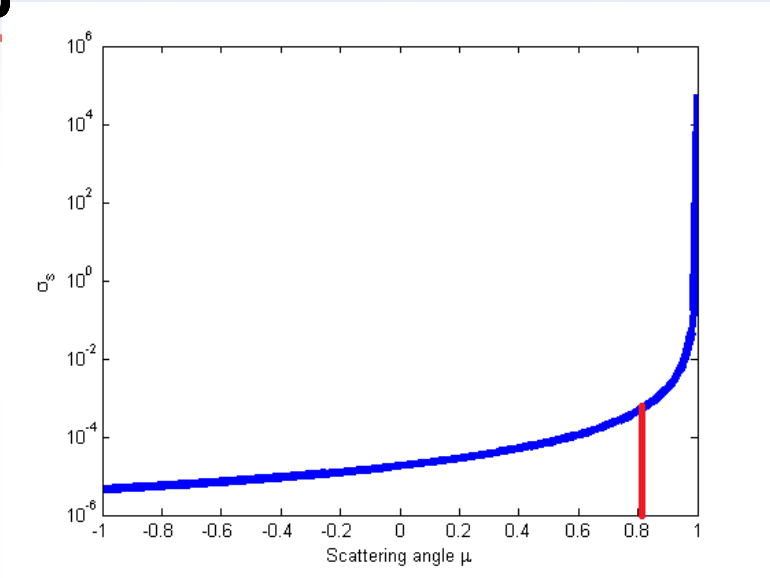
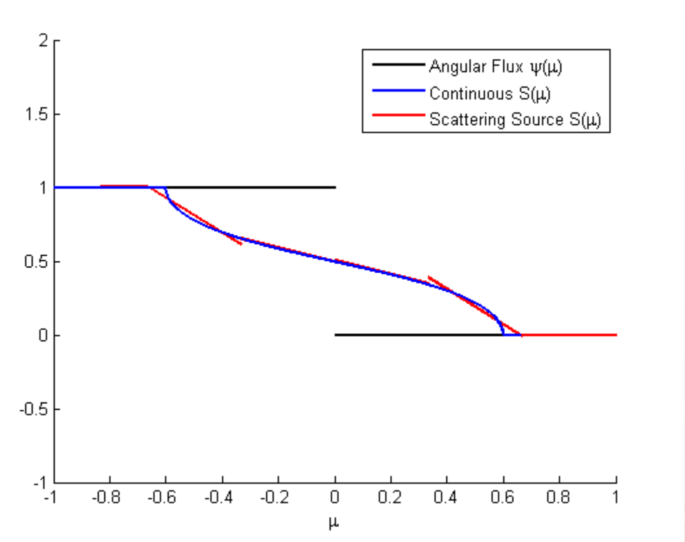
Anisotropic Scattering

- Scattering is not always isotropic.
  - Isotropic: neutron absorption, excitation of target nuclei, emission of neutron.
  - Anisotropic: electron interactions, high energy particles (forward peaked).
- Cross section described as a function of scattering angle.
  - Screened Rutherford distribution
  - Parameter η a material property

    (typical value ~9E-6)
- One method to handle anisotropic scattering is to choose discrete angles to preserve moments of the scattering source.
  - Example from one of our test problems:

    $\mu \approx 0.81$, $\sigma_s \approx 4.99\text{E-}4\ \sigma_{s,0}$
- For each discrete scattering angle:
  - Scattering source from each angular section of Ψ is computed.
  - Scattering source summed over sections of Ψ.
  - Scattering source fit to finite element basis functions.





Scattering Matrix

- Finite element angular flux is represented

$$\psi_{i,m} = \psi^A_{i,m} + \frac{2}{h_i}(z - z_i)\psi^Z_{i,m} + \frac{2}{h_m}(\mu - \mu_m)\psi^\mu_{i,m}.$$

- The scattering source is expressed

$$S_{i,m}(\mu) = \frac{1}{\pi}\int_0^\pi \psi_{i,m}\left(\mu\mu_* + \sqrt{1-\mu^2}\sqrt{1-\mu_*^2}\cos\left(\phi_0\right)\right) d\phi_0.$$

  - We evaluate this analytically.

- The average, z-slope, and μ-slope of the scattering source are needed:

$$S^A_{i,m} = \int_{z_{i-1/2}}^{z_{i+1/2}} \frac{1}{h_i} \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \frac{1}{h_m} S_i dz d\mu.$$

$$S^Z_{i,m} = \int_{z_{i-1/2}}^{z_{i+1/2}} \frac{6}{h_i^2}\left(z - z_i\right) \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \frac{1}{h_m} S_i dz d\mu.$$

$$S^\mu_{i,m} = \int_{z_{i-1/2}}^{z_{i+1/2}} \frac{1}{h_i} \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \frac{6}{h_m^2}\left(\mu - \mu_m\right) S_i dz d\mu.$$

Scattering Matrix

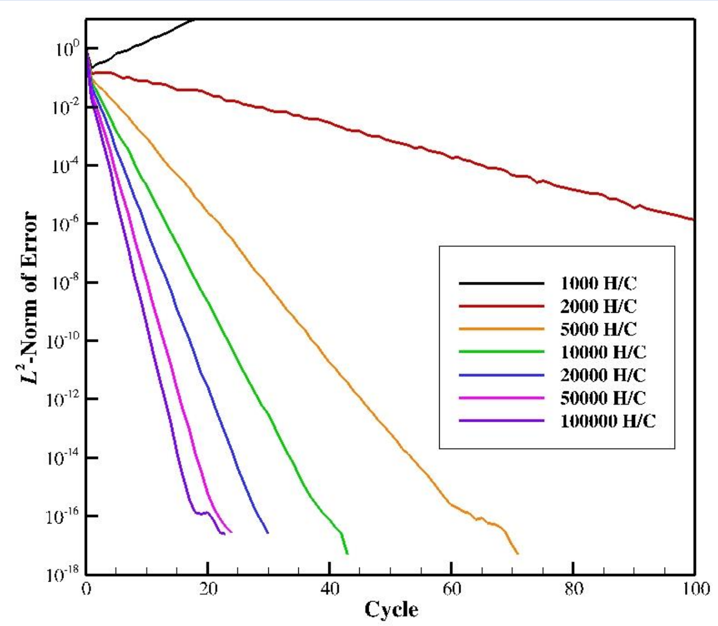
- The scattering matrix is computed before the MC calculations begin.
- 2-D integrals performed with Gauss Quadrature
  - Iteration until matrix elements converge.
  - Solution seems to be insensitive to tolerance in the matrix construction.
- Scattering matrix is *(k x k x 3 x 3)*, *k* angular sections of *Ψ.*

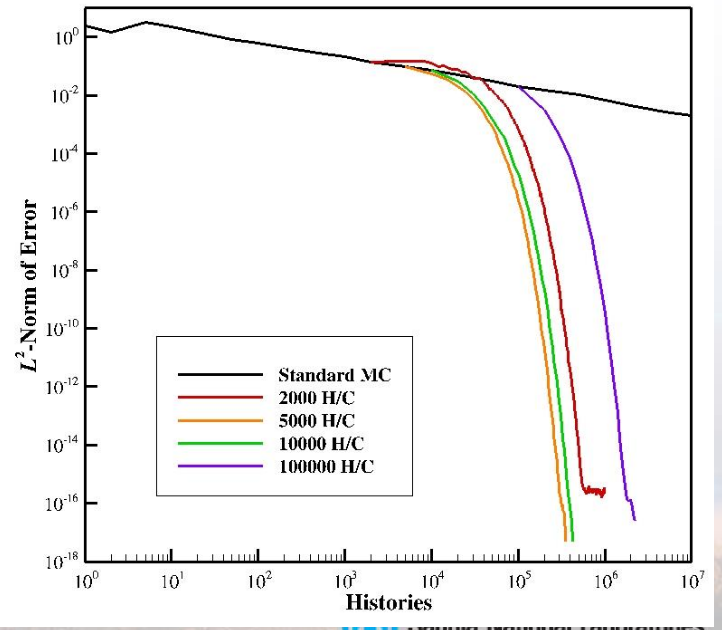
$$S_i = \sigma_{s,0} \sum_{j=1}^{k} [M_{3x3}] \begin{bmatrix} \psi_j^A \\ \psi_j^Z \\ \psi_j^\mu \end{bmatrix}$$

- $\boldsymbol{M_{3x3}}$ contains analytic integration over *Φ*, quadrature integration over space and angle, and terms to compute average, spatial slope, and angular slope.
- Quadrature order increased until maximum change in matrix elements reaches some tolerance.
  - Problems seem insensitive to this tolerance.
  - Tolerance of 1E-2 used in these results.

Results: Exact Problem

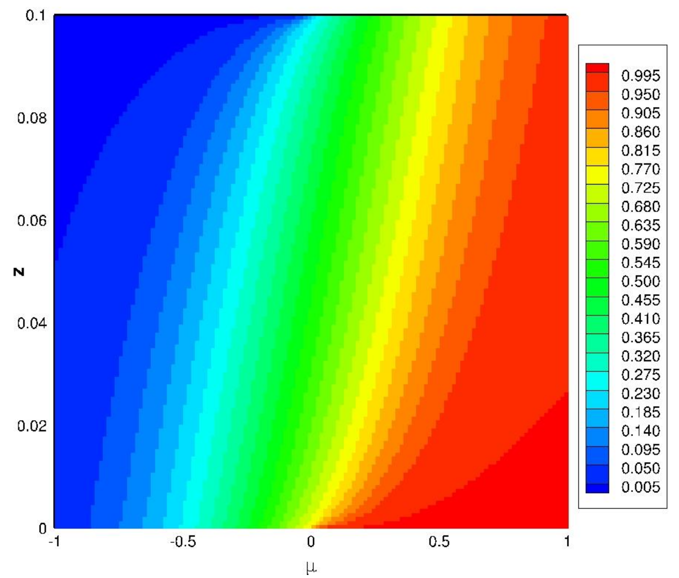
- Scattering source and solution exactly represented by the finite element basis functions.
- Problem should converge to machine roundoff.
- Problem specifics
  - 100 cells (10 angular, 10 spatial)
  - $\sigma_t = 1.0$, $\sigma_{s,0} = 0.9$
  - $\mu = 0.8$
  - $L = 3.0$
- Number of histories per cycle varied between 1E3 and 1E6
- Optimal number of histories per cycle is difficult to estimate *a priori*.

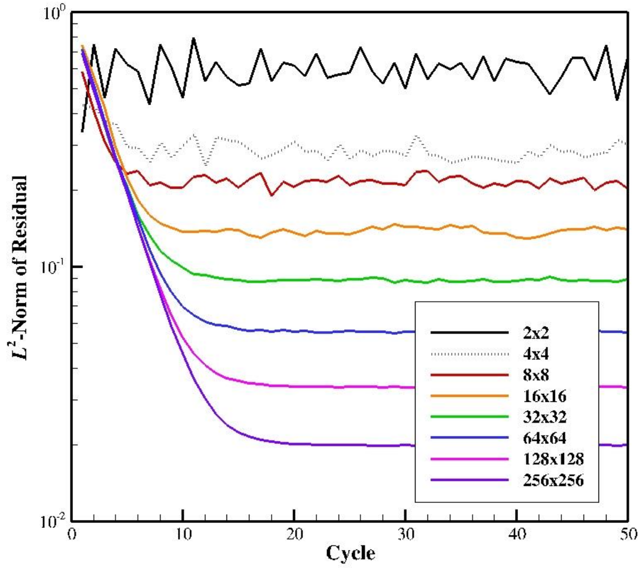




Results: Harder Problem

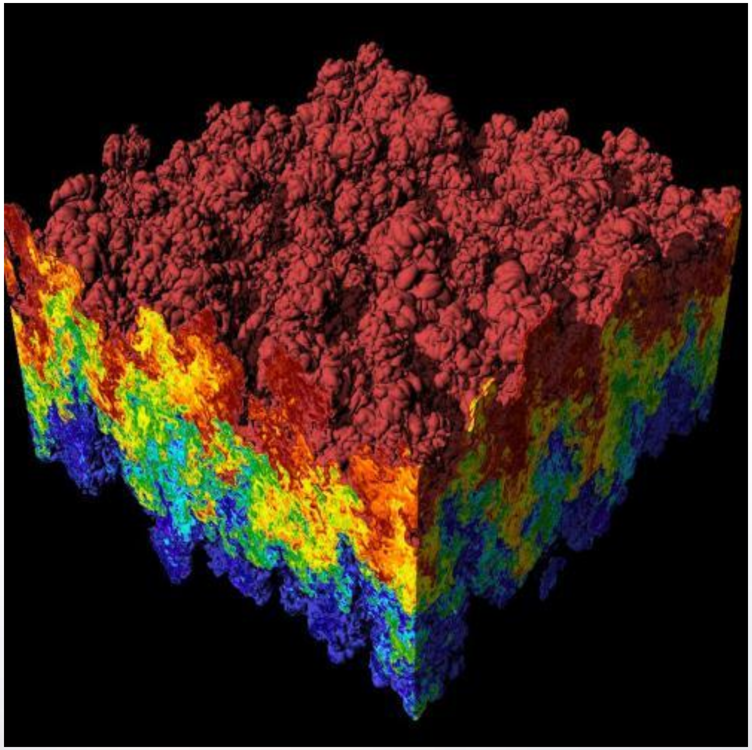
- Problem roughly equivalent to electrons incident on water.
- Four discrete angles
  - $\mu = 0.98, 0.56, -0.19, -0.82$
  - Weights 0.9916, 0.0070, 0.0011, 0.0003
  - Unit isotropic flux at $z = 0$
- $\sigma_t = 77.0$, $\sigma_{s,0} = 76.9$
- L = 10
- $N \times N$ grid in space and angle.
- 100 histories per cell per cycle.
- L2 norm of residual plotted versus cycle for various grid.





Conclusions

- Residual Monte Carlo method demonstrated for anisotropic scattering.
- With minor extension, we can claim that the residual Monte Carlo method is applicable for electron transport.
- There is currently much interest in residual Monte Carlo methods.
  - Successful demonstration of the method to new physics increases understanding of the method.
  - Future work will be encouraged by these successful results.
  - We suspect that it is only a matter of time before residual Monte Carlo is implemented in a production code.
- Ability to drive error in transport physics to arbitrarily small values is key in some multiphysics applications.



Raleigh-Taylor instabilities, courtesy of Lawrence Livermore National Laboratories, https://wci.llnl.gov/codes/visit/gallery_02.html

Future Work

- We are still working on being able to process general anisotropic scattering kernels.
- We can currently accept initial guesses for the solution to accelerate convergence, but have not had time to investigate this in much depth.
- As the finite element mesh is refined, the residual will decrease. We are investigating how this changes the residual Monte Carlo solution and how that solution compares to the straight Monte Carlo solution.

- Extension to multigroup appears to be straightforward- minor generalization of what we have now.

- Continuous slowing down would allow us to model electrons.
- Adaptive mesh refinement is very important, but so far not applied in this work.

- Extension to 2-D and 3-D a natural extension of this work.
- Implement in a production code?

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