Residual Monte Carlo with Discrete Scattering Angles in the 1-D Transport Equation

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2013 American Nuclear Society Winter Meeting

Washington, DC

November 10-14, 2013

Residual Monte Carlo

- Standard Monte Carlo is simply solving:

$$\mathbf{L}\psi = q$$

  where L is the transport operator and q is the source.

- Residual Monte Carlo is solving the following equations iteratively:

$$r^{(n)} = q - \mathbf{L}\psi^{(n-1)}$$

$$\mathbf{L}\epsilon^{(n)} = r^{(n)}$$

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

  where r is a residual error and ϵ is an error correction.

- Residual Monte Carlo does not make hard problems easy.
  - Good statistics are still needed in each iteration.
  - Iteration makes it possible to achieve higher precision.

Calculation of the Residual

- Residual calculation is the new piece required in a Monte Carlo code.

$$r^{(n)} = q - \mathbf{L}\psi^{(n-1)}$$

$$r = q - \mu\frac{\partial\psi(\mu, z)}{\partial z} - \sigma_t\psi(\mu, z) + \frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^1 \sigma_s(\mu_0)\psi(\mu', z)d\mu'd\phi'$$

To evaluate this we need to have Monte Carlo flux tallies on a basis that permits cell-wise evaluation of the residual:

$$r_{i,m} = q_{i,m} - \mu\frac{\partial\psi_{i,m}}{\partial z} - \sigma_{t,i}\psi_{i,m} + \sigma_{s0,i}\int_0^{2\pi}\int_{-1}^1 p(\mu_0)\psi_i(\mu')d\mu'd\phi'$$

$$\psi_{i,m} = \psi_{i,m}^a + \psi_{i,m}^z\frac{2}{h_i}(z - z_i) + \psi_{i,m}^\mu\frac{2}{h_m}(\mu - \mu_m)$$

$$\psi_i(\mu) = \sum_{m=1}^M \psi_{i,m}\left[H(\mu - \mu_{m-\frac{1}{2}}) - H(\mu - \mu_{m+\frac{1}{2}})\right]$$

The solution is a projection onto the finite-element trial space. This is more accurate than solving the discretized finite-element problem.

Total Cross Section, Source, and Spatial Gradient Terms

- The residual terms containing the total cross section and source are trivial to evaluate when the cross section, flux, and residual are on the same basis:

$$- \sigma_{t,i} \psi_{i,m} + q_{i,m}$$

- Spatial gradient is composed of the gradient of the flux within the cell and any discontinuity of flux at cell boundaries.

- For the positive μ direction with an adjacent upwind cell, the residual is:

$$\mu \frac{\partial \psi_{i,m}}{\partial z} = \mu_m \frac{2}{h_i} \psi_{i,m}^z + (\mu - \mu_m) \frac{2}{h_i} \psi_{i,m}^z$$

$$+ \mu \left[\psi_{i,m}(z, \mu) - \psi_{i-1,m}(z, \mu) \right] \delta^+(z - z_{i-1/2}), \qquad z \in [z_{i-1/2}, z_{i+1/2})$$

Scattering Source Term

- Scattering Source

$$S_i(\mu) = \int_0^{2\pi} \int_{-1}^{1} \frac{\delta(\mu_0 - \mu_*)}{2\pi} \psi_i(\mu') d\mu' d\phi'$$

- We map the flux and integration into the scattering frame:

$$S_i(\mu) = \int_0^{2\pi} \int_{-1}^{1} \frac{\delta(\mu_0 - \mu_*)}{2\pi} \psi_i(\mu_0, \phi_0) d\mu_0 d\phi_0.$$

using the following relationship between the directions:

$$\mu' = \mu\mu_0 + \sqrt{1 - \mu^2}\sqrt{1 - \mu_0^2}\cos(\phi_0 - \phi')$$

- The delta function scattering and one-dimensional fluxes lead to this simplified integration:

$$S_i(\mu) = \frac{1}{\pi} \int_0^{\pi} \psi_i(\mu\mu_* + \sqrt{1 - \mu^2}\sqrt{1 - \mu_*^2}\cos(\phi_0)) d\phi_0.$$

Scattering Source Term (cont.)

- In the scattering source integration we project the result onto our linear basis. We can precalculate a transfer matrix to represent the scattering transfer in angular phase-space:

$$S_{i,m,m'}^{x,a} = \frac{1}{\pi} \int_{z_{i-\frac{1}{2}}}^{z_{i+\frac{1}{2}}} \frac{1}{h_i} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \frac{1}{h_m} \int_{\phi_{j-\frac{1}{2}}}^{\phi_{j+\frac{1}{2}}} \Psi_{i,m'}^{x}(\phi_0, z, \mu) d\phi_0 d\mu dz$$

$$S_{i,m,m'}^{x,z} = \frac{1}{\pi} \int_{z_{i-\frac{1}{2}}}^{z_{i+\frac{1}{2}}} \frac{6}{h_i^2} (z - z_i) \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \frac{1}{h_m} \int_{\phi_{j-\frac{1}{2}}}^{\phi_{j+\frac{1}{2}}} \Psi_{i,m'}^{x}(\phi_0, z, \mu) d\phi_0 d\mu dz$$

$$S_{i,m,m'}^{x,\mu} = \frac{1}{\pi} \int_{z_{i-\frac{1}{2}}}^{z_{i+\frac{1}{2}}} \frac{1}{h_i} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \frac{6}{h_m^2} (\mu - \mu_m) \int_{\phi_{j-\frac{1}{2}}}^{\phi_{j+\frac{1}{2}}} \Psi_{i,m'}^{x}(\phi_0, z, \mu) d\phi_0 d\mu dz$$

$$\Psi_{i,m'}^{x}(\phi_0, z, \mu) = \left[\psi_{i,m}^{a}, \psi_{i,m}^{z} \frac{2}{h_i}(z - z_i), \psi_{i,m}^{\mu} \frac{2}{h_m}(\mu - \mu_m) \right]$$

- The scattering source becomes the following simple matrix operation:

$$s_{i,m}^{y} = \sum_{m'=1}^{M} \sum_{x=a,z,\mu} S_{i,m,m'}^{x,y} \psi_{i,m'}^{x}$$

Residual Source Sampling

- Having calculated the residual in each cell, we then need to sample from the residual as a source in the Monte Carlo calculation of the error correction:

$$\mathbf{L}\epsilon^{(n)} = r^{(n)}$$

- We analytically evaluate the source strength. (We have also used quadrature integration, which will be needed for higher dimension problems. We found that even low-order quadrature is adequate.)
- We use a discrete cdf to find the cell or cell boundary of a source particle.
- We use rejection sampling to find the phase-space location within a cell or on the cell boundary.
- We assign negative weight to particles for negative source strength locations.

Flux

Residual/Source

0
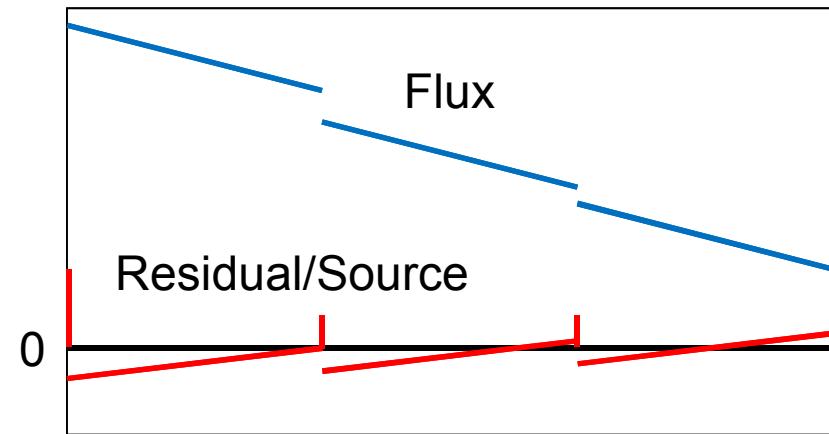
Test Problem with Solution in the Trial Space

- For a uniform flux solution, we use the method of manufactured solutions (and the residual calculation logic) to calculate the source: $q = \mathbf{L}\psi$

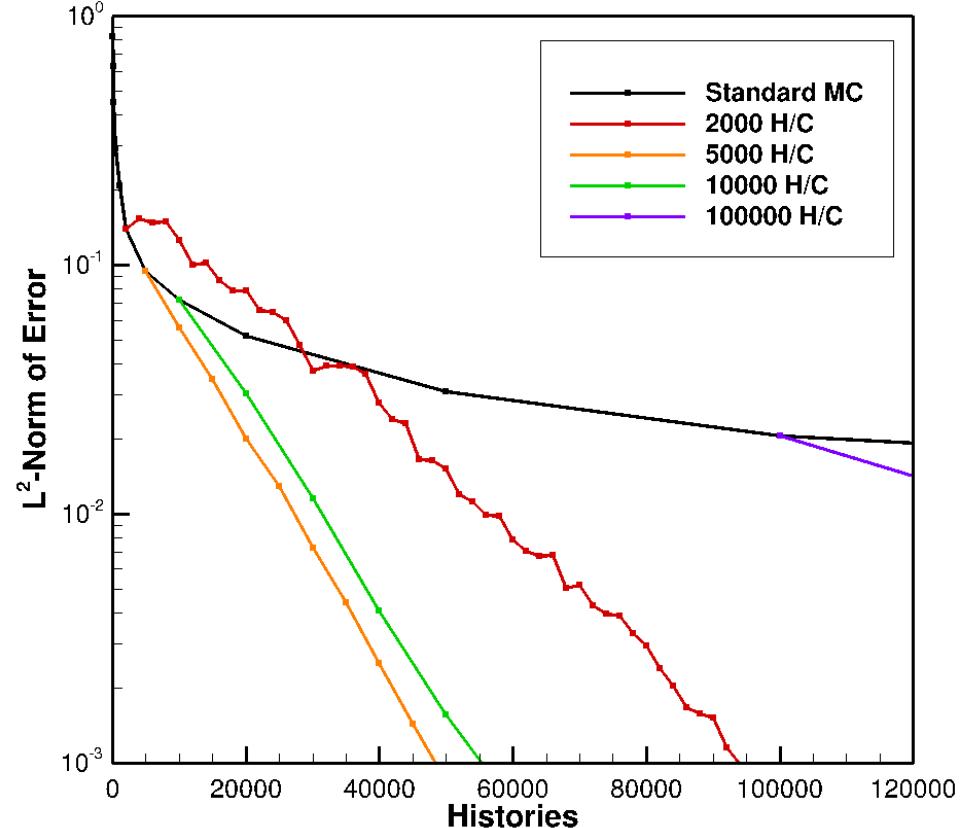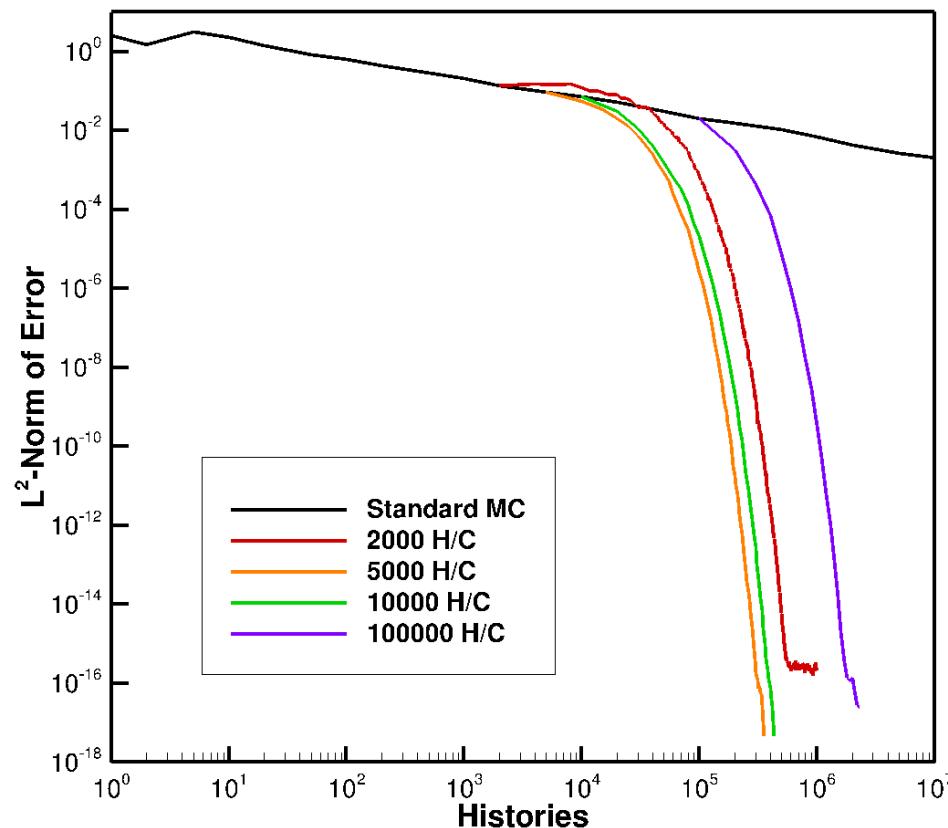- 100 cells in a uniform 10x10 grid in space and angle.

$$\sigma_t = 1, \ \sigma_{s0} = 0.9, \ \mu_* = 0.8, \ T = 3,$$
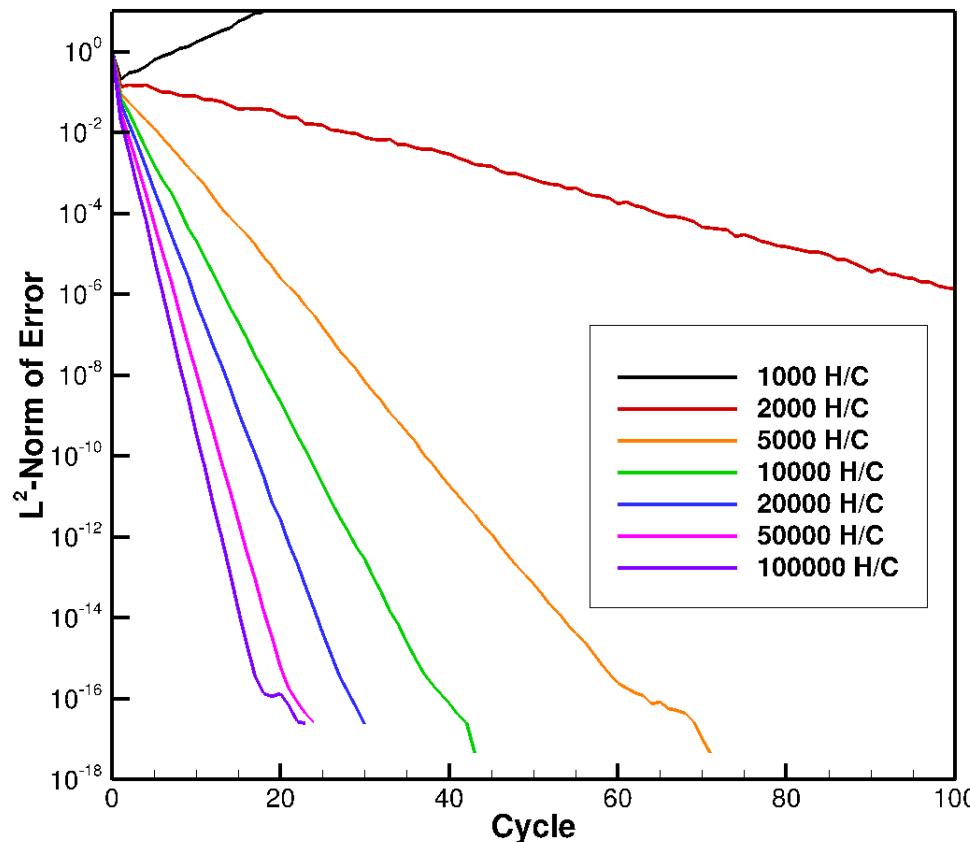
# Test Problem with Solution in the Trial Space (cont.)

- For a uniform flux solution, we use the method of manufactured solutions (and the residual calculation logic) to calculate the source: $q = \mathbf{L}\psi$
- 100 cells in a uniform 10x10 grid in space and angle.

$$\sigma_t = 1, \ \sigma_{s0} = 0.9, \ \mu_* = 0.8, \ T = 3,$$

Test Problem with Electron-Like Parameters

- Cross sections based on 1 MeV electrons:

$$\sigma_t = 77, \, \sigma_{s0} = 76.9, \, T = 0.1,$$

- The scattering distribution is 4 discrete scattering angles:

$$\mu_* = \{0.98, 0.56, -0.19, -0.82\}$$
$$p_* = \{0.9916, 0.0070, 0.0011, 0.0003\}$$

100 histories/cycle/cell

1600 histories/cycle/cell
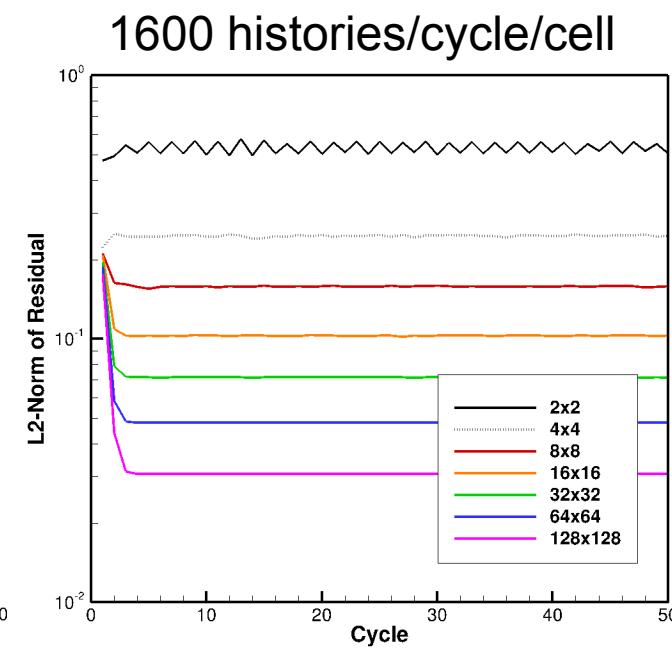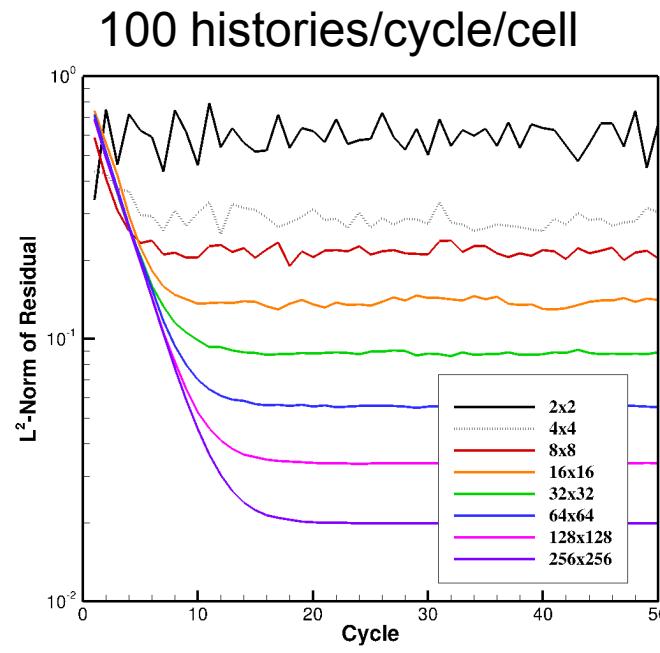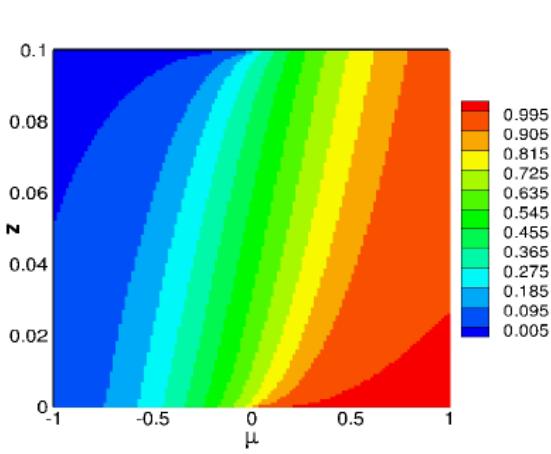
Convergence as a Function of Quadrature Order

- After careful debugging to achieve exponential convergence, we found that the convergence was not sensitive to the quadrature order used in integrating the scattering source term.
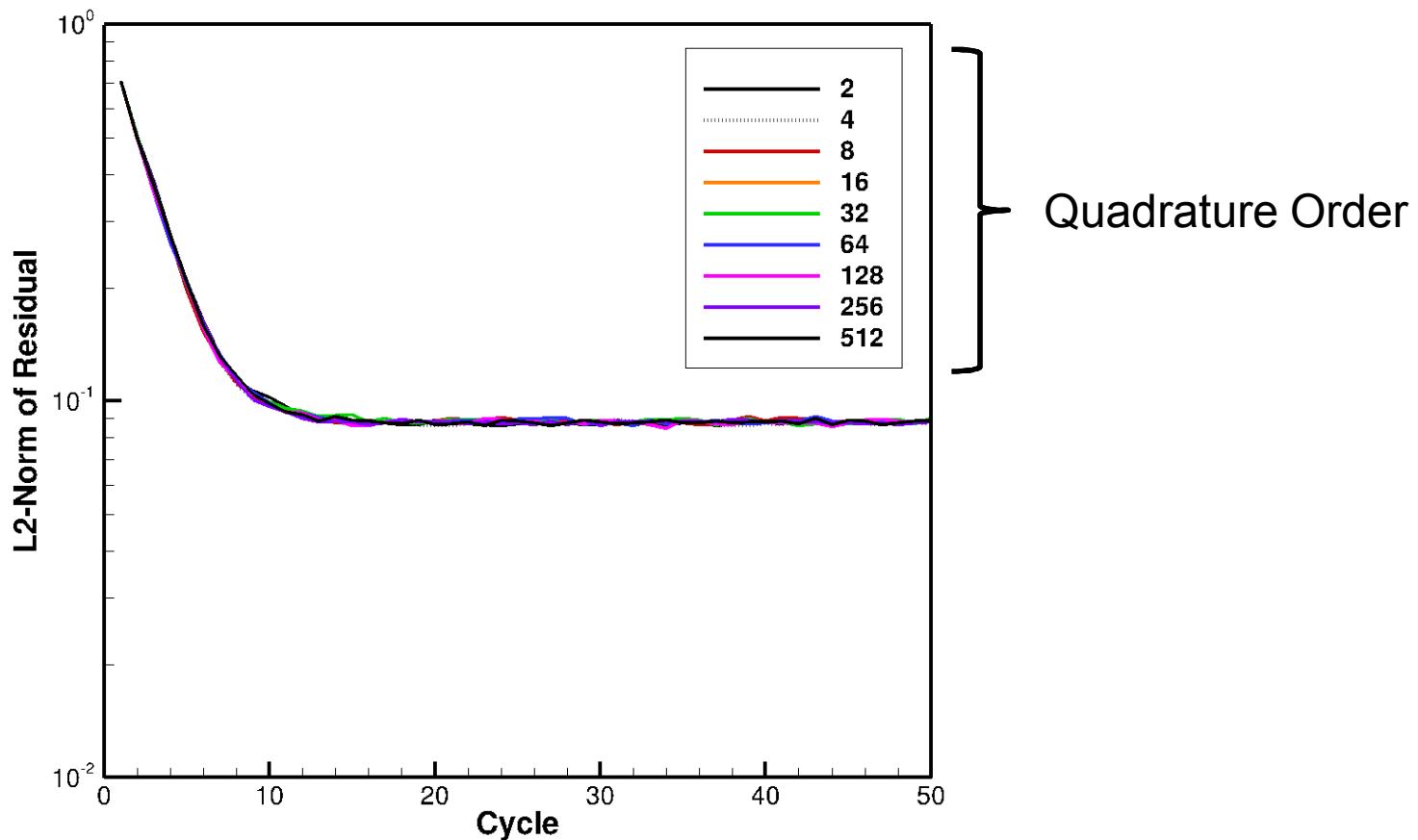
Conclusions and Future Work

- We have demonstrated the residual Monte Carlo method for the continuous 1-D transport equation with anisotropic scattering.

- This method can be extended to:
  - General anisotropic scattering kernels. This can be done by integrating the discrete scattering angle over the scattering kernel.
  - Multi-dimensional problems. Generalization of the tally and residual calculations appears to be straightforward. Integration of the scattering source over two angular dimensions is complicated but can follow the approach we have shown here.
  - Multigroup problems. This appears to be trivial.
  - Continuous energy. This would be a challenging undertaking, requiring the integration of the energy-scattering kernels.

- A production capability requires adaptive refinement of the trial space. [See Peterson, Morel, Ragusa (2013), but more research is needed.]

- Residual Monte Carlo could be an effective addition to the FW-CADIS approach, utilizing the forward deterministic calculation to initialize the Monte Carlo and the adjoint information to guide adaptive refinement.