Hybrid Deterministic/Monte Carlo Solutions to the Neutron Transport k-Eigenvalue Problem with a Comparison to Pure Monte Carlo Solutions

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Multigroup Equations

We'll consider solving the multigroup formulation of the k-eigenvalue problem, which result from discretizing in energy,

$$\hat{\Omega} \cdot \nabla \psi_g(\hat{\Omega}, \vec{r}) + \Sigma_{t,g} \psi_g(\hat{\Omega}, \vec{r}) = \frac{1}{4\pi} \sum_{g'=1}^{G} \Sigma_s^{g' \to g} \phi_{g'}(\vec{r})$$
$$+ \frac{\chi_g}{4\pi k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \phi_{g'}(\vec{r}). \tag{1}$$

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k-Eigenvalue Problem

Compute dominant eigenvalue for

$$\mathcal{L}\Psi = \frac{1}{4\pi}\left(\mathcal{S} + \frac{1}{k_{eff}}\mathcal{F}\right)\Phi.$$

- Traditional methods are based on the power method.
- Plagued by slow convergence when dominance ratio, ρ,

$$\rho = \max_i \frac{|k_i|}{|k_{eff}|}$$

  is close to 1.
- Must converge scattering and fission source terms.

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Accelerating PI

- PI converges slowly when
  1. Scattering ratio is near 1
  2. Dominance ratio is near 1
- We'll use Nonlinear Diffusion Acceleration to move a large portion of the work to a "low-order" system of reduced dimension.
- This allows us to
  1. Solve the k-eigenvalue problem for a sequence of LO problems.
  2. Accelerate eigenvalue convergence using Newton's method.

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Moment Based Acceleration

Consider the neutron transport equation

$$\hat{\Omega} \cdot \nabla \psi_g(\hat{\Omega}, \vec{r}) + \Sigma_{t,g} \psi_g(\hat{\Omega}, \vec{r}) = \frac{1}{4\pi} \sum_{g'=1}^{G} \Sigma_s^{g' \to g} \phi_{g'}(\vec{r}) + \frac{\chi_g}{4\pi k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g} \phi_{g'}(\vec{r}).$$

and its zeroth angular moment

$$\nabla \cdot \vec{J_g} + \Sigma_{t,g} \phi_g = \sum_{g'=1}^{G} \Sigma_s^{g' \to g} \phi_{g'} + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g} \phi_{g'}. \qquad (2)$$

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Nonlinear Diffusion Acceleration[1]

Consider Fick's law augmented with a correction term, $\hat{D}$,

$$\vec{J_g} = -\frac{1}{3\Sigma_{t,g}}\nabla\phi_g + \hat{D}_g^{HO}\phi_g. \tag{3}$$

Substituting Equation 3 into 2 yields the NDA low-order (LO) equation,

$$\nabla\cdot\left(-\frac{1}{3\Sigma_{t,g}}\nabla\phi_g + \hat{D}_g^{HO}\phi_g\right) + \Sigma_{t,g}\phi_g = \sum_{g'=1}^{G}\Sigma_s^{g'\to g}\phi_{g'} + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g}\phi_{g'}. \tag{4}$$

- Upon convergence, the NDA LO solution agrees with the HO solution (transport equation solution).

[1] See *Application of the Jacobian-Free Newton-Krylov Method to Nonlinear Acceleration of Transport Source Iteration in Slab Geometry* by Knoll, Park and Smith CASL-U-2013-0309-000

NDA-based Eigenvalue Methods[2]

1. Input some approximation to the scalar flux, Φ^m, and eigenvalue k_{eff}^m.
2. Compute
$$\psi^{m+1} = \frac{1}{4\pi}\mathcal{L}^{-1}\left(\mathcal{S} + \frac{1}{k_{eff}^m}\mathcal{F}\right)\Phi^m$$
$$\Phi^{HO} = \int d\hat{\Omega}\ \psi^{m+1}, \quad J^{HO} = \int d\hat{\Omega}\ \hat{\Omega}\cdot\psi^{m+1}$$
3. Compute $\hat{D}_g$ for each group.
4. Solve
$$(\mathcal{D} - \mathcal{S})\,\Phi^{m+1} = \frac{1}{k_{eff}^{m+1}}\mathcal{F}\Phi^{m+1}$$
where $\mathcal{D}$ is given by
$$\mathcal{D}_g = \nabla\cdot\left[-\frac{1}{3\Sigma_{t,g}}\nabla + \hat{D}_g\right] + \Sigma_{t,g}.$$

[2] See *Nonlinear Acceleration of Transport Criticality Problems* by Park, Knoll, Newman.

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Solving the LO Eigenvalue Problem

Rewrite LO eigenvalue problem as:

$$F(\Phi) = (\mathcal{D} - \mathcal{S})\,\Phi - \frac{1}{k_{eff}}\mathcal{F}\Phi$$

$$k_{eff} = \sum_{g'} \int dV \nu \Sigma_{f,g'} \phi_{g'}$$

Solve $F(\Phi) = 0$ with preconditioned Newton-Krylov method.

This yields NDA-NCA - Nonlinear Diffusion Acceleration with Nonlinear Criticality Acceleration.

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Motivation for Hybrid Methods

While deterministic algorithms can be designed to converge in very few iterations, there are some drawbacks:

- Discretization error takes several forms
  1. Multi-group cross-sections must be carefully computed in order to not introduce errors.
  2. Spatial discretization leads to truncation error which may demand significant mesh refinement.
  3. S_n approximation may yield "ray effects" or biasing along discrete angles in our quadrature set.
- Less potential for parallelism.
  1. S_n transport sweeps can be parallelized to some degree, but this becomes challenging.
  2. Monte Carlo methods are often highly parallelizable.

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Hybrid Methods

We'd like to build hybrid deterministic/stochastic methods.

Combine the advantages of both deterministic and stochastic methods:

- Accelerate convergence of expensive Monte Carlo simulations.
- No angular discretization error.
- Spatial discretization error can be adjusted to be far smaller than MC error.
- Potential for continuous treatment of energy in HO problem.
- Angular flux avoided entirely.
- Less expensive particle histories.

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Monte Carlo "Transport Sweep"

In each of the algorithms discussed, we need to be able to apply $\mathcal{L}^{-1}$ to a source vector.

We can do this with Monte Carlo:

1. Build source term $S = \left(\mathcal{S} + \frac{1}{k}\mathcal{F}\right)\Phi^{(n)}$.
2. Sample source term, S, for initial particle locations and/or particle weights.
3. Sample direction of travel and distance from known PDFs for each particle.
4. Tally new scalar flux, $\Phi^{(n+1)}$, and new current, $\vec{J}^{(n+1)}$.

We'll call this action a *Monte Carlo Transport Sweep* and represent this action as $\Phi^{(n+1)} = G^{MC}(\Phi^{(n)})$.

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NDA-NCA(MC)

The first step in NDA-NCA is to compute a new approximation to $\hat{D}$ and build a LO eigenvalue problem.

To approximate $\hat{D}$ we

1. Execute a transport sweep to compute Ψ^{HO}, given $\Phi^{(n)}$.
2. Compute 0th and 1st moments of Ψ^{HO}, Φ^{HO} and J^{HO}, respectively.
3. Compute $\hat{D}_g = \hat{D}_g(\phi_g^{HO}, J_g^{HO})$ for each group.

We can do this with Monte Carlo instead.

1. Build source term given $\Phi^{(n)}$.
2. Simulate particle flights and directly tally Φ^{HO}, J^{HO}.
3. Compute $\hat{D}_g = \hat{D}_g(\phi_g^{HO}, J_g^{HO})$ for each group.

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NDA-NCA(MC)

The next step is to solve the LO eigenvalue problem

$$(\mathcal{D} - \mathcal{S})\,\Phi^{m+1} = \frac{1}{k_{eff}^{m+1}}\mathcal{F}\Phi^{m+1}.$$

Important notes:

1. This problem is no harder to solve when the deterministic transport sweep has been replaced by a Monte Carlo transport sweep!
   - While $\mathcal{D}$ contains a potentially noisy $\hat{D}$ term, $\hat{D}$ is **constant** throughout the LO eigenvalue solve!
2. There is no MC simulation in the LO eigenvalue solve.

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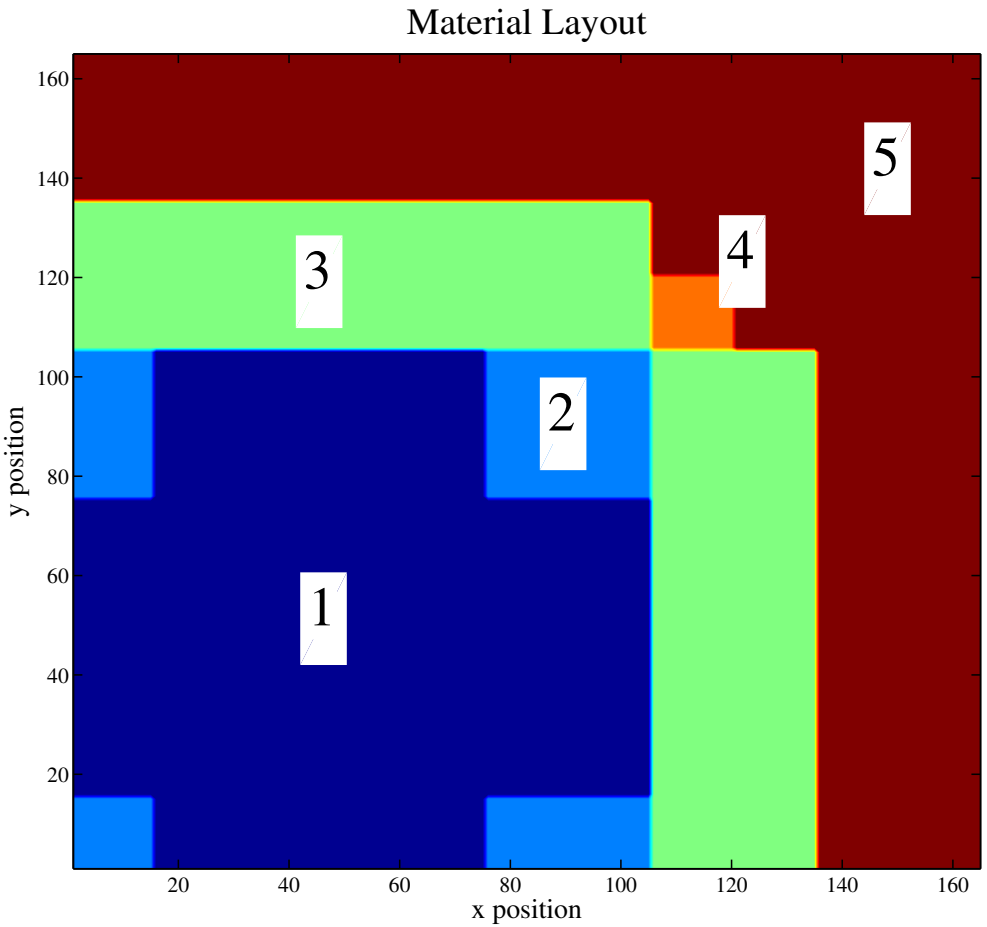
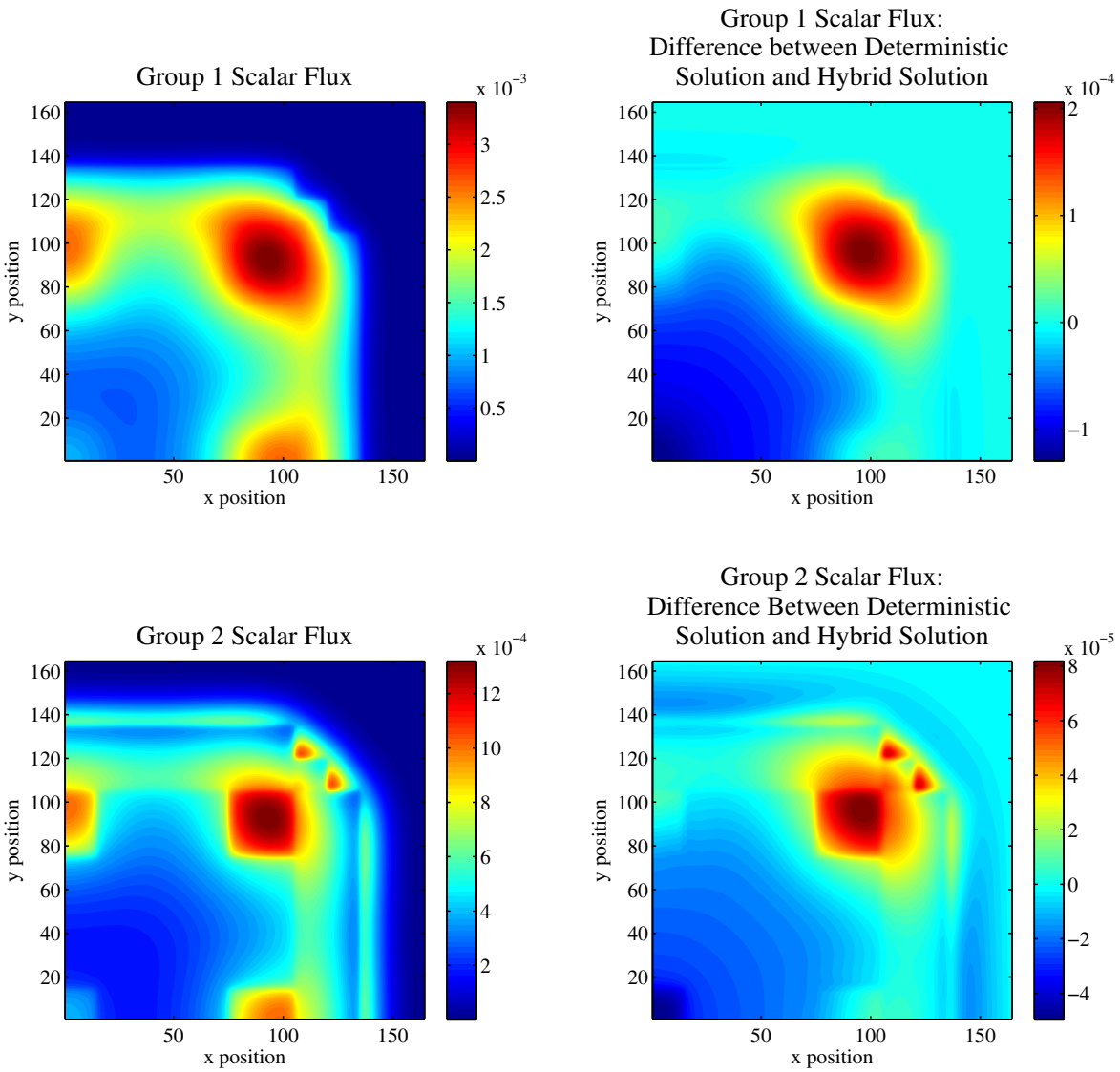
2-D Test: LRA-BWR Problem[3]



[3] See *Argonne Code Center: Benchmark Problem Book*, ANL-7416, suppl. 2, Argonne National Laboratory (1977)

2-D Test: LRA-BWR Problem



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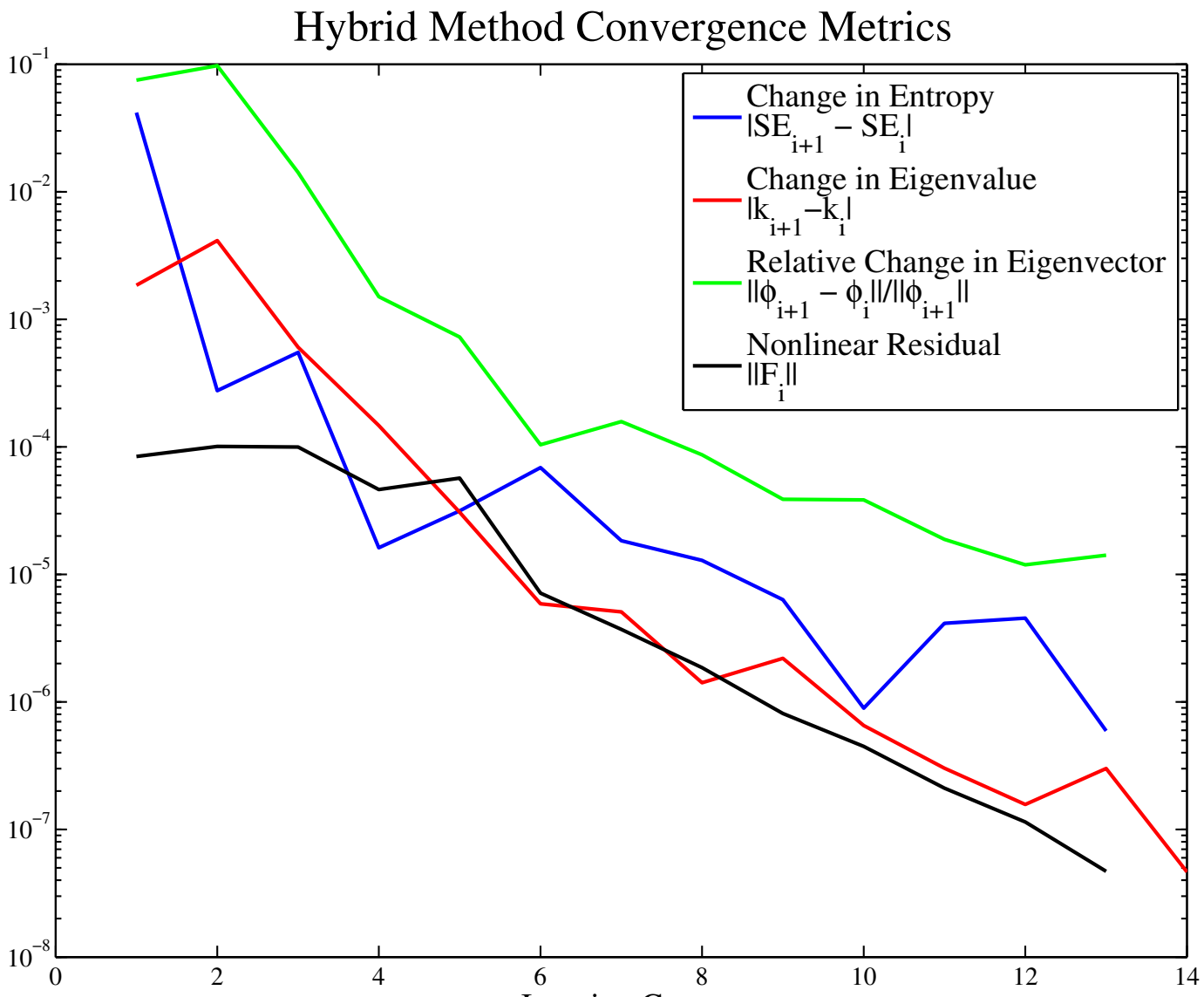
2-D Test: LRA-BWR Convergence



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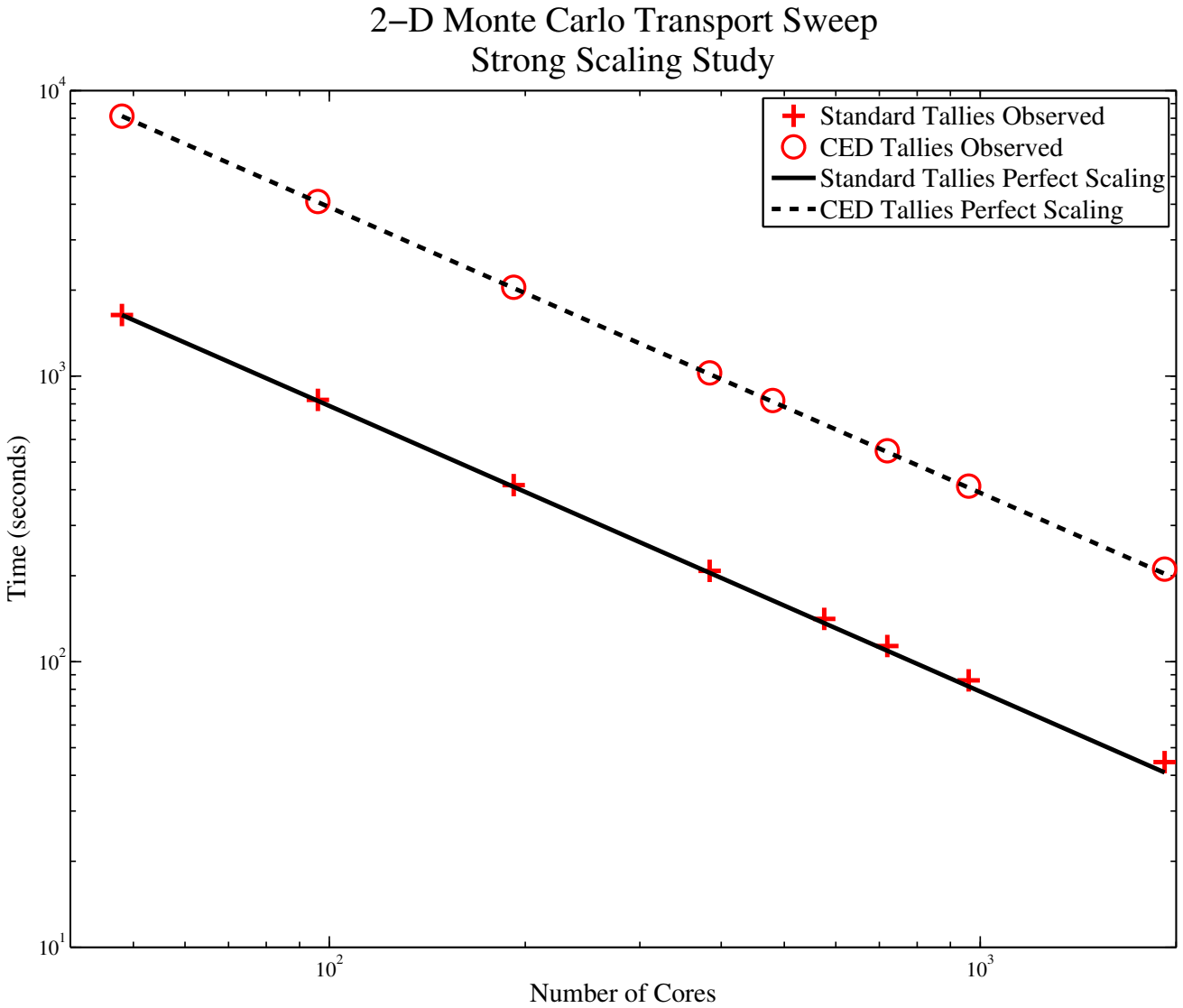
2-D Test: Scalability



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2-D Test: LRA-BWR Problem

- Solution error (compared to converged hybrid solution) less than 1 pcm was obtained using a total of roughly 6.4×10^{10} particles.
- The low-order problem appears to insert some degree of discretization error.
- On a given spatial mesh, the hybrid algorithm provides more accurate solutions than a purely deterministic implementation.[4]

[4] see *Hybrid Deterministic/Monte Carlo Methods for Solving the Neutron Transport Equation and k-Eigenvalue Problem*, by Willert (Ph.D. Thesis)

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Classic Monte Carlo

As a comparison, we'll solve the same problem using a classic Monte Carlo solution:

1. Approximate fission source
2. Sample fission source for particle locations
3. Simulate particle histories - steaming, scattering, absorption, fission
4. Store fission sites for next batch

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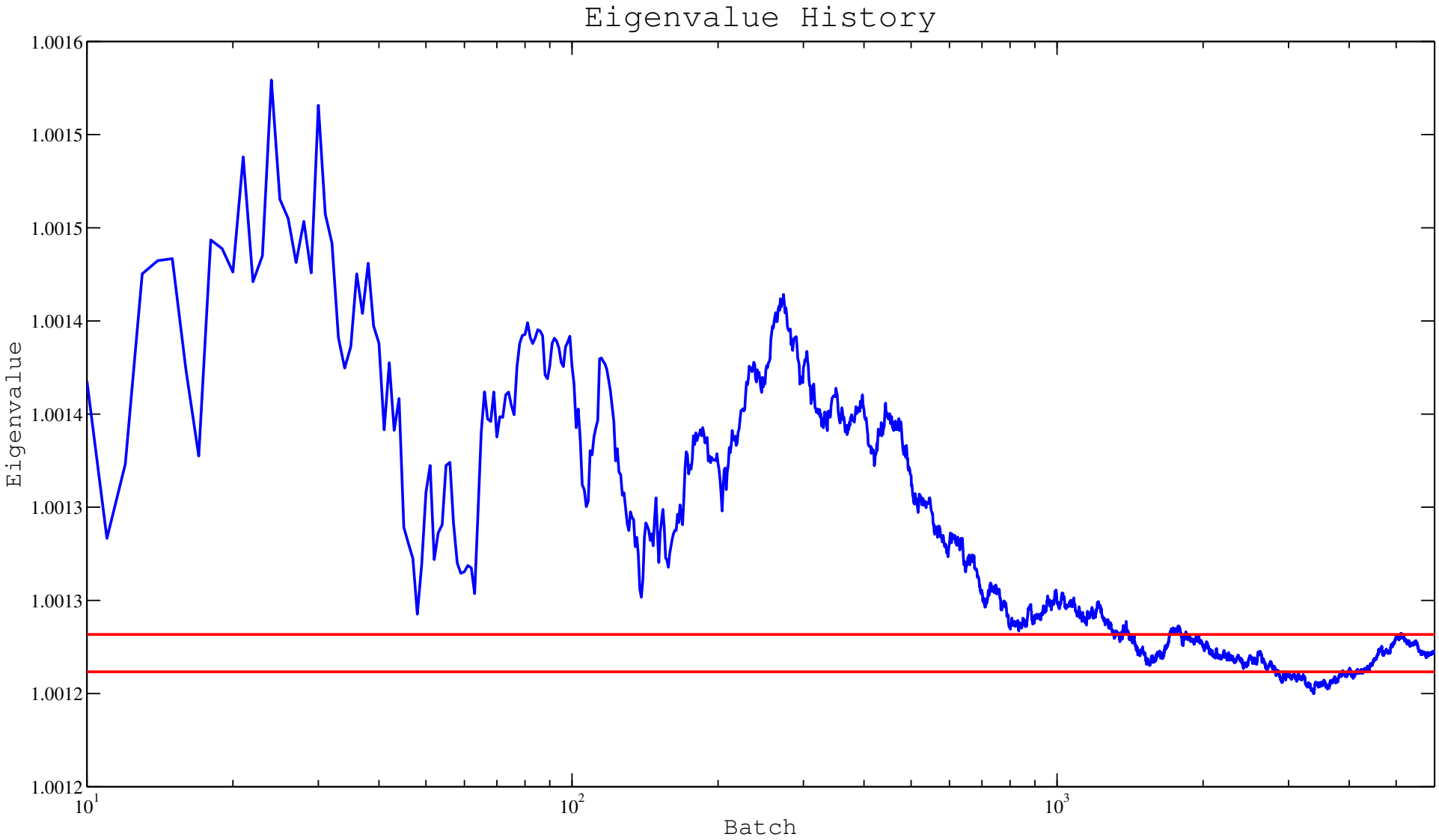
Classic Monte Carlo - Eigenvalue Convergence



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Remarks

1. For both hybrid methods and purely stochastic methods, convergence can be difficult to measure.
   - NDA-NCA(MC) computes 5 digits of the eigenvalue after 6.4×10^{10} particle flights.
   - MC computes 5 digits (maybe) of the eigenvalue after 1.5×10^{11} particle flights.
2. Each MC particle undergoes roughly 25 interactions before leaving the domain, being absorbed or undergoing a fission event. NDA-NCA(MC) particles undergo exactly 1 interaction.

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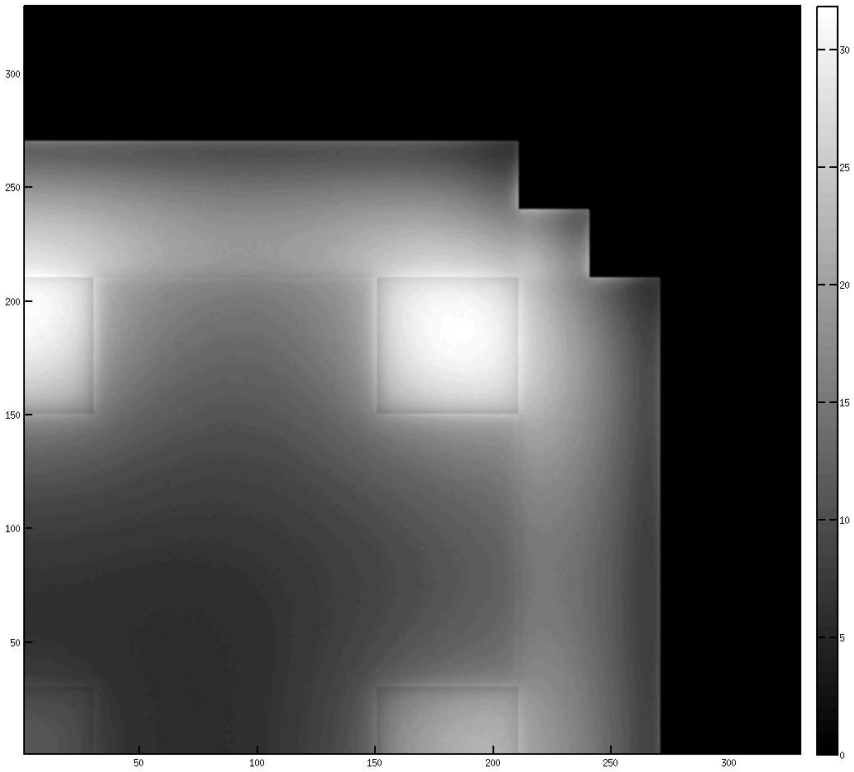
Method Comparison



- MC particles are only born in fissionable regions.
- NDA-NCA(MC) particles must resolve flux and current everywhere in the domain.
- Only 65% of cells contain fissionable material.

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NDA-NCA(MC) Considerations

1. NDA-NCA(MC) particles do less work than standard MC particles, but they must be distributed *everywhere* in the domain.
2. How can we alleviate this issue? Potential solutions:
   - Geometric hybrid - use deterministic solutions outside fissionable region.
   - Source biasing - concentrate particles in fissionable region. However, we still need good statistics in reflector region.
3. NDA-NCA(MC) would allow for a *residual Monte Carlo* formulation:
   - Given some approximation ψ_0 to the true solution, solve

$$\mathcal{L}(\delta\psi) = \frac{1}{4\pi}\left(\mathcal{S} + \frac{1}{k}\mathcal{F}\right)\phi - \mathcal{L}\psi_0$$

   with Monte Carlo, and recover $\psi = \psi_0 + \delta\psi$.

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Summary

- We have built a hybrid algorithm, NDA-NCA(MC) for computing the dominant eigenvalue, k_{eff}.
- We have demonstrated that for a high dominance ratio 2-D test problem, the expense of the two algorithms is comparable, with a slight edge going to NDA-NCA(MC).

Current/future work:

- Modify the NDA-NCA(MC) algorithm to use particle histories more efficiently.
- Low-order spatial truncation error has been studied in 1-D. We should attempt to study/quantify this error in multiple dimensions.

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