A High-Order Low-Order Algorithm with Exponentially-Convergent Monte Carlo for k-Eigenvalue Problems

Simon R. Bolding & Jim E. Morel

21 November 2014

CLASS seminar

NEUP Nuclear Energy University Programs
U.S. Department of Energy

TEXAS A&M ENGINEERING

Outline

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Eigenvalue Problem

- Slab geometry, one-speed transport equation

$$\mu\frac{\partial\psi}{\partial x} + \Sigma_t\psi(x,\mu) = \frac{1}{4\pi}\left(\Sigma_s + \frac{\nu\Sigma_f}{k_{\text{eff}}}\right)\phi(x)$$

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Alternatively, we use a low-order solution to determine k_{eff} and $\phi(x)$, corrected by MC solutions

A High-Order Low-Order Solution to a Transport Problem

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Build a low-order (LO) system that can be efficiently solved, such that it preserves a high-order (HO) solution from MC simulations

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- **LO system** is lower-dimensional, "S_2-like" equations
  - Handles scattering and fission source iterations
  - Useful for coupled physics and non-linear systems
  - Produces FE representation of sources for HO system
- **HO system** is a fixed-source, pure absorber transport problem
  - MC does not directly determine k_{eff} or fission source, only used to evaluate consistency terms
  - We will solve the HO system with ECMC

Overview of Exponentially Convergent Monte Carlo

- Iterative form of Residual Monte Carlo
  - Each batch tallies the error in current estimate of solution, which is a transport problem with a reduced source
  - Can reduce statistical error globally $\propto e^{-\alpha N}$
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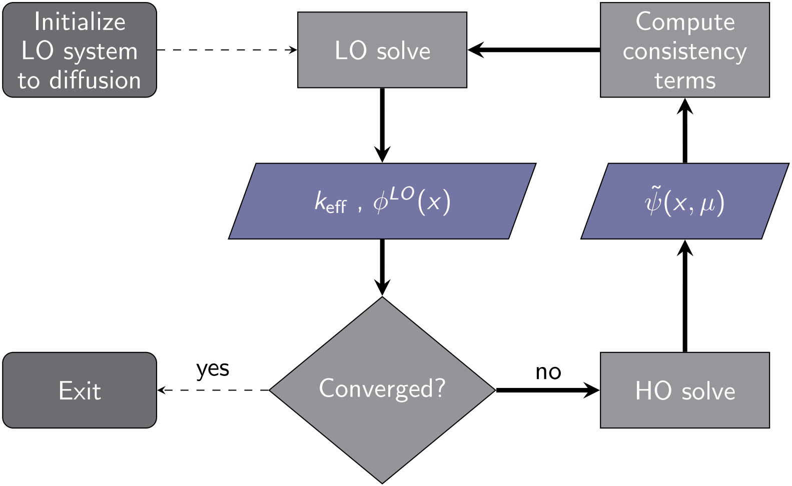
  - Can reduce statistical error globally $\propto e^{-\alpha N}$
  - Does not make difficult problems easier
- Requires a discretized form of the angular flux
  - Use projection onto space-angle FE mesh
  - Adaptive mesh refinement mitigates truncation error, allowing convergence to be maintained

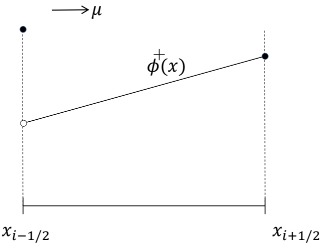
High-Order Low-Order Algorithm

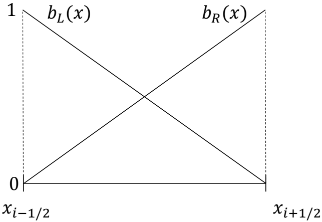


Outline

LO Discretization & Space-Angle Moments

- Linear discontinuous (LD) FE in space and half range angular averages





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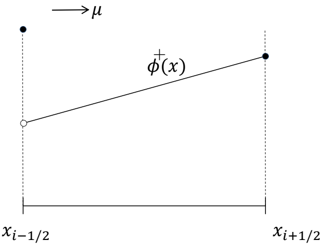

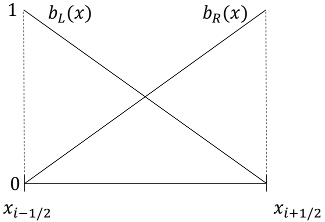

- *Examples* of moments:

Spatial: left basis

$$\langle \cdot \rangle_{L,i} = \frac{2}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)(\cdot)\mathrm{d}x$$

Angular: positive flow

$$\phi^+(x) = 2\pi \int_0^1 \psi(x,\mu)\mathrm{d}\mu$$

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Forming LO Equations Over an Element

- Taking moments of TE yields 4 equations, per cell i, e.g.

$$
\begin{aligned}
&-2\mu^{+}_{i-1/2}\phi^{+}_{i-1/2} + \langle\mu\rangle^{+}_{L,i}\langle\phi\rangle^{+}_{L,i} + \langle\mu\rangle^{+}_{R,i}\langle\phi\rangle^{+}_{R,i} + \Sigma_t h_i \langle\phi\rangle^{+}_{L,i} \\
&\qquad - \frac{\Sigma_s h_i}{4\pi}\left(\langle\phi\rangle^{+}_{L,i} + \langle\phi\rangle^{-}_{L,i}\right) = \frac{1}{k_{\text{eff}}}\frac{\nu\Sigma_f h_i}{4\pi}\left(\langle\phi\rangle^{+}_{L,i} + \langle\phi\rangle^{-}_{L,i}\right)
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$$

- Cell unknowns are moments: $\langle\phi\rangle^{+}_{L,i}$, $\langle\phi\rangle^{+}_{R,i}$, $\langle\phi\rangle^{-}_{L,i}$, $\langle\phi\rangle^{-}_{R,i}$

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- To close system, need angular consistency terms and spatial closure
  - Estimate *average* μ terms from HO solution
  - Use the LD spatial closure, consistent with our HO solver

Computing LO Consistency terms from HO Solution

- For $\mu > 0$, L moment

$$\langle\mu\rangle_{L,i}^{+} \simeq \frac{\int\limits_{0}^{1}\int\limits_{x_{i-1/2}}^{x_{i+1/2}} \mu\, b_{L,i}(x)\tilde{\psi}^{HO}(x,\mu)\mathrm{d}x\mathrm{d}\mu}{\int\limits_{0}^{1}\int\limits_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)\tilde{\psi}^{HO}(x,\mu)\mathrm{d}x\mathrm{d}\mu}$$

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- ECMC gives LDFE representation of $\tilde{\psi}^{HO}(x,\mu)$
  - Evaluate consistency terms directly
  - For initial solve, use S_2: $\langle \mu \rangle^{\pm} = \pm \frac{1}{\sqrt{3}}$

Solving LO System with Power Iteration

- Global System: $$\mathbf{D}(\mu^{HO})\Phi = \frac{1}{k_{\text{eff}}}\mathbf{F}\Phi$$

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Algorithm

1. Guess $\Phi^{(0)}$ and $k_{\text{eff}}^{(0)}$

$$\Phi^{(l+1)} = \frac{1}{k_{\text{eff}}^{(l)}}\mathbf{D}^{-1}\mathbf{F}\Phi^{(l)}$$

$$k_{\text{eff}}^{(l+1)} = k_{\text{eff}}^{(l)}\frac{\int \nu\Sigma_f\phi^{(l+1)}dx}{\int \nu\Sigma_f\phi^{(l)}dx}.$$

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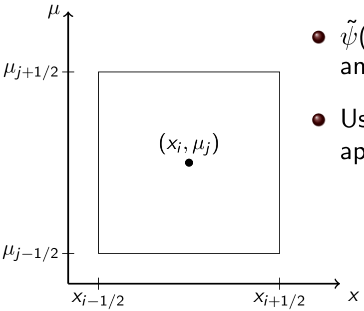
2. Accelerate $\Phi^{(l+1)}$ and $k_{\text{eff}}^{(l+1)}$ after each power iteration with Nonlinear Krylov Acceleration (NKA)
3. Converge $\Delta\Phi^{(l)}$ and $\Delta k_{\text{eff}}^{(l)}$

Outline

Space-Angle LDFE Mesh



- $\tilde{\psi}(x, \mu)$ is linear over each cell, preserving 0^{th} and 1^{st} moment in x and μ
- Use path-length estimators of flux to approximate moments e.g.

$$\langle \psi \rangle_{\mu,ij} = \frac{6}{h_\mu^2 h_x} \iint_{\mathcal{D}} (\mu - \mu_i)\psi(x, \mu) \mathrm{d}x \mathrm{d}\mu$$

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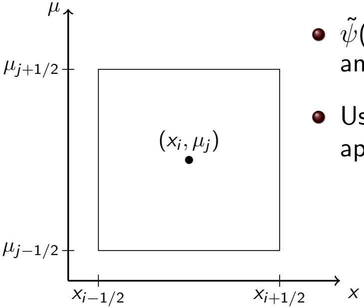

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- Use standard LD and upwinding to get face terms

High Order System and ECMC Algorithm

- Pure absorber transport problem

$$\left[\mu\frac{\partial}{\partial x}+\Sigma_t\right]\psi(x,\mu)=\boxed{\frac{1}{4\pi}\left(\Sigma_s+\frac{\nu\Sigma_f}{k_{\text{eff}}^{LO}}\right)\phi^{LO}(x)}$$

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

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- Update: $\tilde{\psi}^{(m+1)} = \tilde{\psi}^{(m)} + \tilde{\epsilon}^{(m)}$
  - If $\tilde{\epsilon}$ is reduced each batch, exponential convergence achieved
  - h-refine when $\epsilon(x,\mu)$ not represented sufficiently
- Repeat until $\|\tilde{\epsilon}\|_2 < \text{tol} \times \|\psi\|_2$

Other MC Details

Improving Statistics and Efficiency

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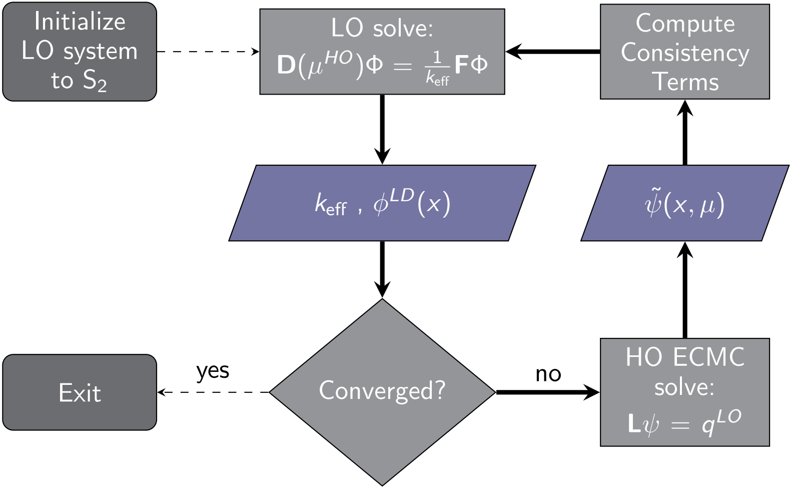
High-Order Low-Order Algorithm



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Critical slab benchmark

Problem Parameters

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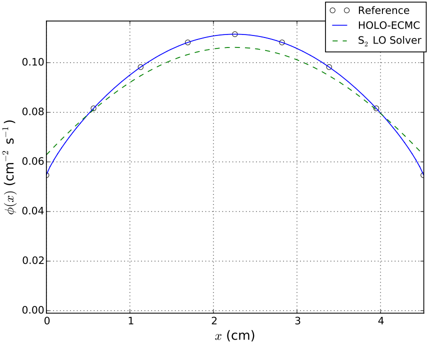

- $|\Delta\Phi|_{\text{rel}} < 10^{-4}$ in 4 outer iterations, using $\sim 2.4 \times 10^7$ histories
- For 10 independent simulations:

$\overline{k_{\text{eff}}}$	0.999998
$\sigma(k_{\text{eff}})$	0.4 pcm
$\Delta k_{\text{eff}}^{\max}$	1.1 pcm
$\overline{\sigma_{\text{rel}}(\phi_i)}$	1.4 pcm

Optically thick, near-critical slab

Problem Parameters

- $k_\infty = 1$, $\Sigma_t = 5.0$ cm^{-1}, $\Sigma_s = 4.5$ cm^{-1}, DR$\simeq$**0.984**
- Relative Tolerance of 1.0E-05 for HO and LO solvers, 1.0E-04 outer

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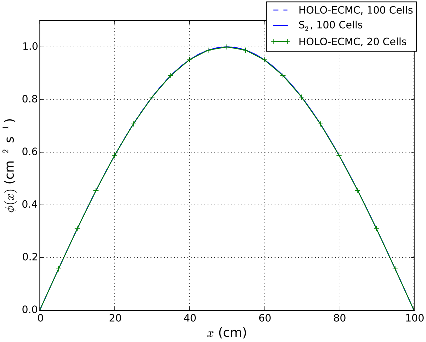

- LO fission source convergence:
  - PI: **389** iterations
  - NKA: **27** iterations
- 3 outer iterations, 4.4×10^6 total histories
- $k_{\text{eff}} = 0.99793$

Comparison of statistical noise for standard and ECMC HO solvers

One HOLO solve, with a fixed 1.5×10^5 histories. Comparison of ECMC with 5 batches and standard MC (SMC)

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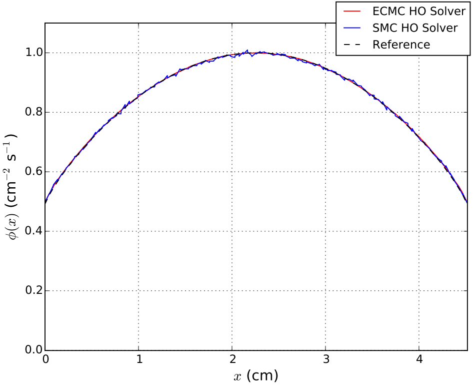

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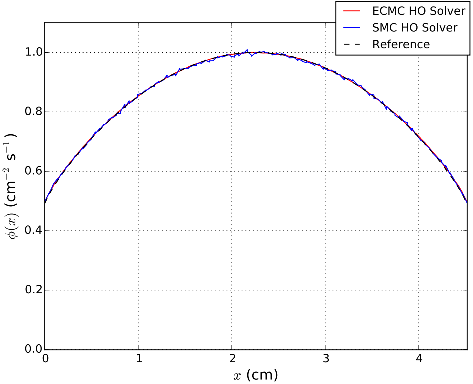

$$\frac{\|\sigma(\psi^{SMC})\|}{\|\tilde{\epsilon}^{ECMC}\| + \|\sigma(\epsilon^{ECMC})\|} = 16$$

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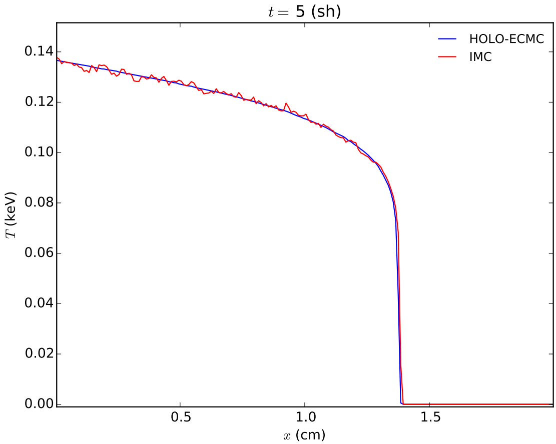
- Working on application to thermal radiative transfer problems

Marshak Wave Problem, Radiation Temperature Profile



- IMC: 100,000 particles per time step
- HOLO-ECMC: 15,000 particles per time step

Questions?

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ECMC procedure

Algorithm

1. $\tilde{\psi}^{(0)} = \tilde{\psi}$ or from last batch this time step
2. Using Monte Carlo, $\epsilon^{(m)} = \mathbf{L}^{-1}\tilde{r}^{(m)}$
   - Use volumetric tallies, weighted with x and μ basis moments time ψ to construct LD $\tilde{\epsilon}^{(m)}(x, \mu)$ over the current space-angle mesh
3. $\tilde{\psi}^{(j+1)} = \tilde{\psi}^{(m)} + \tilde{\epsilon}^{(m)}$
4. **IF** error stagnation:
   - Refine mesh based on relative jump error in $\tilde{\psi}(x, \mu)$
5. Repeat 2-4 until $\|\tilde{\epsilon}\|_2 < \text{tol} \times \|\psi\|_2$

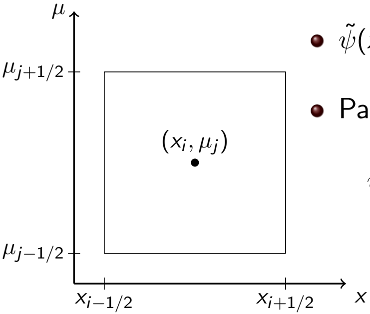
HOLO Algorithm

Algorithm

1. Initialize $\langle\mu\rangle^{\pm}$ parameters to S_2
2. Solve LO system using power iteration
3. Build q^{LD} for HO solver, and set $\tilde{\psi}$ to latest HO estimate on coarsest x–μ mesh
4. Solve $\tilde{\psi}(x,\mu) = \mathbf{L}^{-1} q^{LO}$ using ECMC
5. Compute new $\langle\mu\rangle^{\pm}$ parameters using $\tilde{\psi}^{HO}$ over LO mesh
6. Repeat 2-5 until $\underline{\Phi}^{LO}$ is converged

- Use adaptive convergence criteria

Space-Angle Mesh and MC Implementation Details



- $\tilde{\psi}(x,\mu) = \psi_{a,i} + \psi_{x,i}\dfrac{2}{h_x}(x - x_i) + \psi_{\mu,i}\dfrac{2}{h_\mu}(\mu - \mu_i)$
- Path-length estimators of moments, e.g.

$$\psi_{x,i} = \frac{6}{h_x^2 h_\mu} \iint_{\mathcal{D}} (x_{c,j} - x_i)\psi(x, mu)\mathrm{d}x\mathrm{d}\mu$$

- Particles only stream $w(s) = w_0 e^{-\Sigma_t s}$
- LDFE and upwinding eliminates surface tallies
- Cell-wise, global representation allows for stratified sampling
  - $N_{i,j} \propto |r_i(x,\mu)|$
  - Force $N_i \geq N_{\min}$ and adjust particle weights

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- Requires a discretized form of the angular flux
  - Use finite element representation
  - Adaptive mesh refinement allows the error to continue to be reduced