# 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

# Outline


1. Overview
2. Low-Order Solver
3. High-Order Solver
4. HOLO Algorithm
5. Test Problems
6. Conclusions

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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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- Monte Carlo (MC) allows for high fidelity solutions, but is expensive
  - Typically power iteration with batch estimates of $k_{\text{eff}}$ and fission source
  - Could accelerate source with lower-rank solution (e.g., CMFD)

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

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

## Basic Idea

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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  - Useful for coupled physics and non-linear systems
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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 $k_{\mathrm{eff}}$ 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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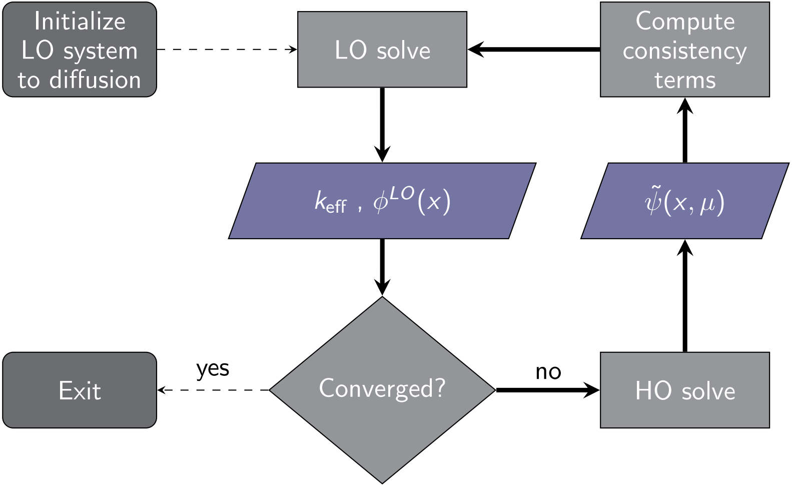
  - Can reduce statistical error globally $\propto e^{-\alpha N}$
  - Does not make difficult problems easier
- Requires a discretized form of the angular flux
  - Use projection onto space-angle FE mesh
  - Adaptive mesh refinement mitigates truncation error, allowing convergence to be maintained

# High-Order Low-Order Algorithm



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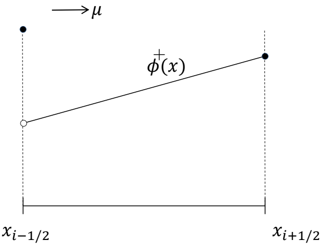
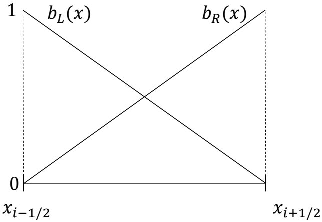
# LO Discretization & Space-Angle Moments

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



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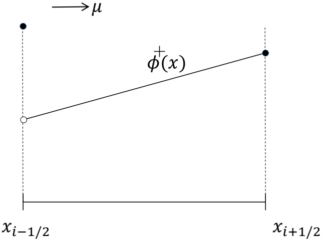


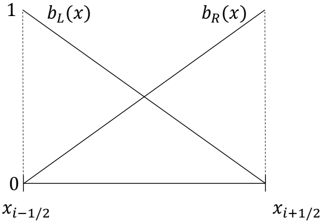


- *Examples* of moments:

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

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

# Forming LO Equations Over an Element

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

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

- 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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$$
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- Cell unknowns are moments: $\langle\phi\rangle^{+}_{L,i}$, $\langle\phi\rangle^{+}_{R,i}$, $\langle\phi\rangle^{-}_{L,i}$, $\langle\phi\rangle^{-}_{R,i}$
- To close system, need angular consistency terms and spatial closure
  - Estimate *average* $\mu$ terms from HO solution
  - Use the LD spatial closure, consistent with our HO solver

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# 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

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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 $\Delta k_{\text{eff}}^{(l)}$

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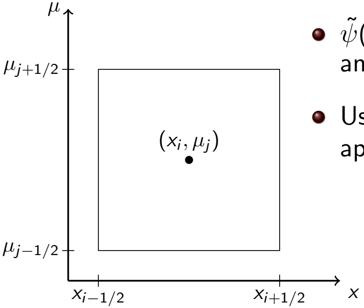
## Space-Angle LDFE Mesh




- $\tilde{\psi}(x,\mu)$ is linear over each cell, preserving $0^{\text{th}}$ and $1^{\text{st}}$ moment in $x$ and $\mu$
- 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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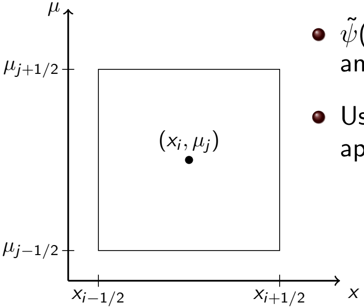


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- Use standard LD and upwinding to get face terms

# High Order System and ECMC Algorithm

- Pure absorber transport problem

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

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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

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- Initialize $\tilde{\psi}(x, \mu)$ to latest HO solution for first batch

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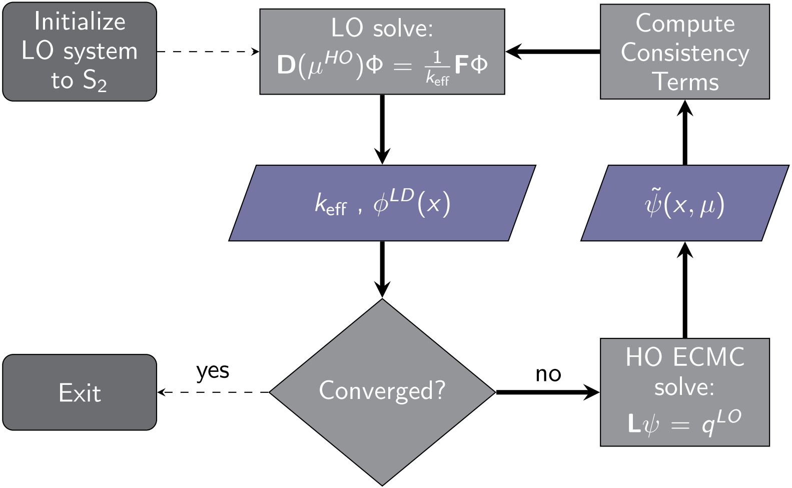
# High-Order Low-Order Algorithm



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# Critical slab benchmark

## Problem Parameters

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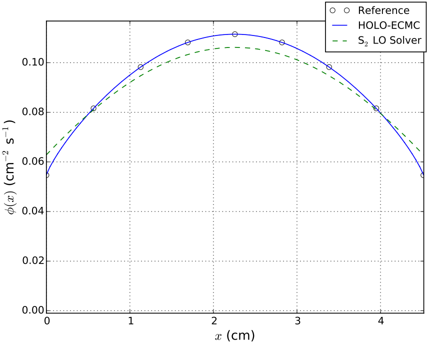


- $|\Delta\Phi|_{\text{rel}} < 10^{-4}$ in 4 outer iterations, using $\sim 2.4 \times 10^7$ histories
- For 10 independent simulations:

| | |
|---|---|
| $\overline{k_{\text{eff}}}$ | 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 |

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# Optically thick, near-critical slab

## Problem Parameters

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

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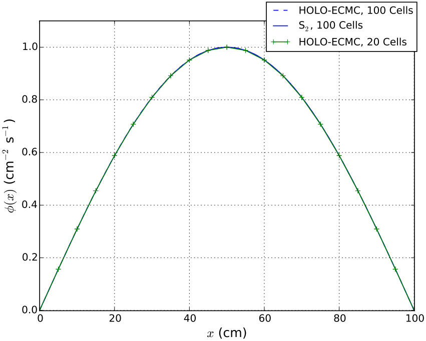


- LO fission source convergence:
  - PI: **389** iterations
  - NKA: **27** iterations
- 3 outer iterations, $4.4\times10^6$ total histories
- $k_{\text{eff}} = 0.99793$

# Comparison of statistical noise for standard and ECMC HO solvers

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

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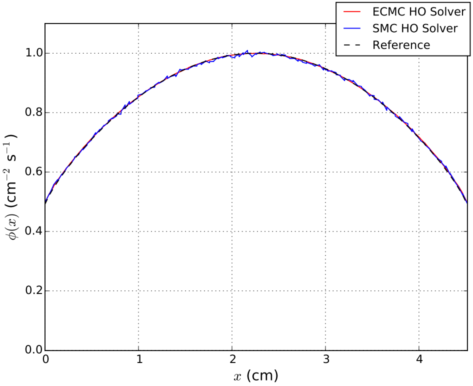

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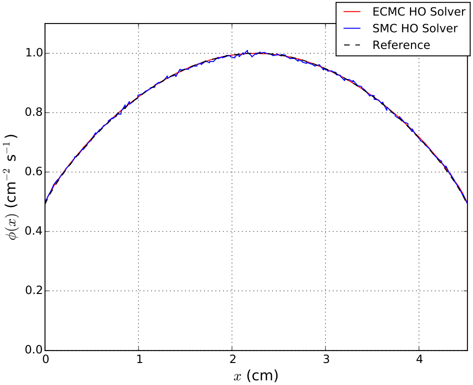


$$\frac{\|\sigma(\psi^{SMC})\|}{\|\tilde{\epsilon}^{ECMC}\| + \|\sigma(\epsilon^{ECMC})\|} = 16$$

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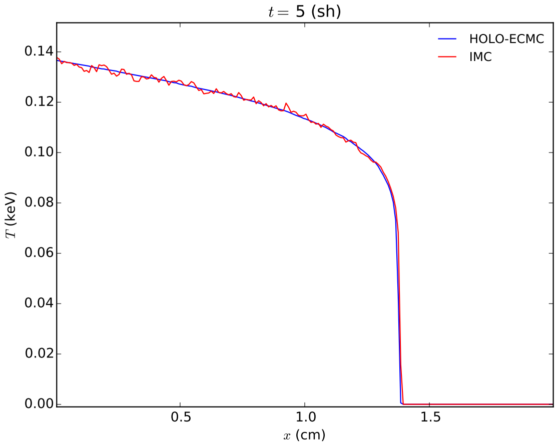
- Working on application to thermal radiative transfer problems

# 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 $\mu$ basis moments time $\psi$ 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 $\|\tilde{\epsilon}\|_2 < \text{tol} \times \|\psi\|_2$

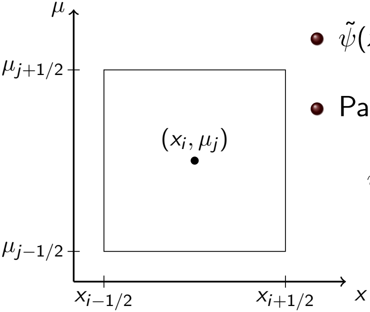
# HOLO Algorithm

## 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 $x$–$\mu$ 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




- $\tilde{\psi}(x,\mu) = \psi_{a,i} + \psi_{x,i}\frac{2}{h_x}(x - x_i) + \psi_{\mu,i}\frac{2}{h_\mu}(\mu - \mu_i)$
- 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