A High-Order Low-Order Algorithm with Exponentially-Convergent Monte Carlo for Thermal Radiative Transfer

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

Outline

Overview

High temperature heat transfer is an interaction between matter and a radiation field. The radiation field heats the material and moves energy through photon streaming and scatter. The material conducts energy and emits radiation proportional to T^4. Coupled radiation and material heat conduction is important in:

- NIF shots
- Glass cooling
- Astrophysics

The thermal radiative transfer equations

- 1D, frequency-integrated (grey) equations

$$\frac{1}{c}\frac{\partial I}{\partial t}+\mu\frac{\partial I}{\partial x}+\sigma_t I=\frac{\sigma_s}{2}\phi+\frac{1}{2}\sigma_a acT^4 \tag{1}$$

$$C_v\frac{\partial T}{\partial t}=\sigma_a\phi-\sigma_a acT^4. \tag{2}$$

$$\phi(x)=\int_{-1}^{1} I(x,\mu)\mathrm{d}\mu \tag{3}$$

- Cross sections (σ) can be a strong function of T
- Tightly coupled and contain non-linear Planckian emission source $\sigma_a acT^4$

The implicit Monte Carlo method

- These equations are typically solved with MC via the Implicit Monte Carlo (IMC) method
- In IMC, the material energy equation is linearized over a time step and eliminated from the system
- Results in an effective source and scattering cross section for a linear transport problem
- Drawbacks
  - Effective scattering cross section can be very large
  - System is not truly implicit, because of linearization

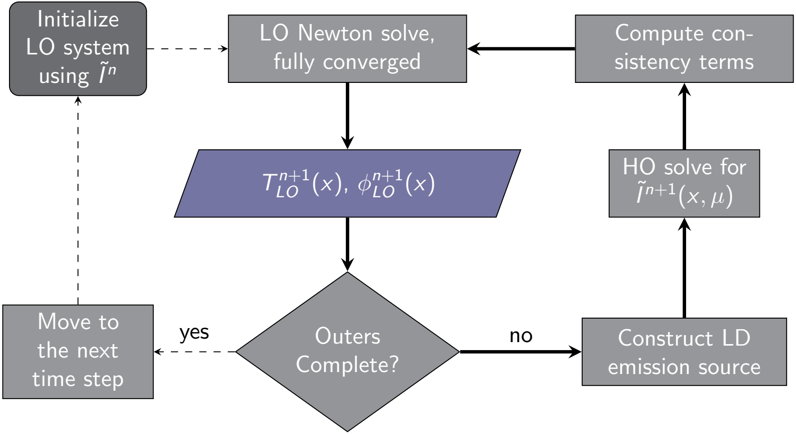
A High-Order Low-Order Solution

Basic Idea

Build a low-order (LO) system that can be efficiently solved, with high-order (HO) correction from simpler MC simulations

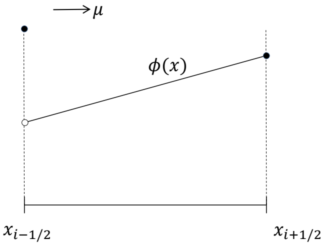
- Useful when global solution of particle density needed
- The LO solution preserves the HO solution, upon convergence (giving consistency)
- The LO solver resolves non-linear temperature dependence
  - Produces a linear-discontinuous (LD) finite element representation of sources
  - Lower dimensional problem in anglular variable
- The HO system is a fixed-source, pure-absorber transport problem
  - ECMC allows for the statistical noise to be reduced globally, giving accurate consistency terms

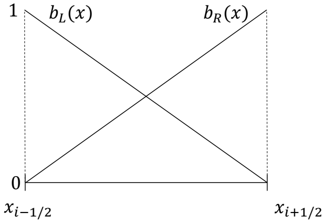
High-Order Low-Order Algorithm



LO Discretization & Space-Angle Moments

- Linear Discontinuous (LD) finite elements in space and half range angular integrals





Spatial moments

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

Angular half-ranges

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

LO System

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

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

- Cell unknowns: $\langle\phi\rangle^+_{L,i}$, $\langle\phi\rangle^+_{R,i}$, $\langle\phi\rangle^-_{L,i}$, $\langle\phi\rangle^-_{R,i}$
- Need angular consistency terms and spatial closure (LD)

Computing LO Consistency terms from HO Solution

- For $\mu > 0$, L moment

$$\langle \mu \rangle^{+}_{L,i} \simeq \frac{\frac{2}{h_i} \int\limits_{0}^{1} \int\limits_{x_{i-1/2}}^{x_{i+1/2}} \mu \, b_{L,i}(x) \tilde{\psi}^{HO}(x,\mu) \mathrm{d}\mu \mathrm{d}x}{\frac{2}{h_i} \int\limits_{0}^{1} \int\limits_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) \tilde{\psi}^{HO}(x,\mu) \mathrm{d}\mu \mathrm{d}x} \tag{4}$$

- ECMC gives LDFE $\tilde{\psi}^{HO}(x,\mu)$ for computing terms directly
- To get S_2, set $\langle \mu \rangle^{\pm} = \pm \frac{1}{\sqrt{3}}$

Solving LO System with Power Iteration

- Global System: $$\mathbf{D}\Phi = \frac{1}{k_{\text{eff}}}\mathbf{F}\Phi$$

Algorithm

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

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

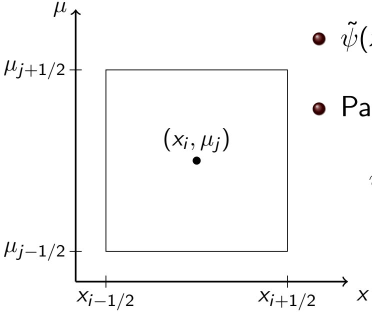
$$k_{\text{eff}}^{(l+1)} = k_{\text{eff}}^{(l)}\frac{\int \nu\Sigma_f \phi^{(l+1)} \mathrm{d}x}{\int \nu\Sigma_f \phi^{(l)} \mathrm{d}x}.$$

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

Exponentially Convergent Monte Carlo

- An iterative form of residual Monte Carlo
- Requires a functional form of the angular flux in space and angle
  - Use finite element representation
- Can reduce statistical error globally $\propto e^{-\alpha N}$
  - Does not make difficult problems easier
- Adaptive mesh refinement allows the error to continue to be reduced
  - Increase N per batch by factor of new cells added

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.

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

- Particles are allowed to 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

High Order System and ECMC Algorithm

- Pure absorber transport problem

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

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

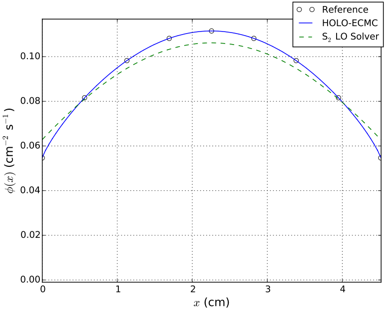
ECMC Algorithm

- Residual Equation: $\mathbf{L}\tilde{\epsilon}^{(m)} = \tilde{r}^{(m)} = q^{LO} - \mathbf{L}\tilde{\psi}^{(m)}$
- Compute $\tilde{\epsilon}^{(m)} = \mathbf{L}^{-1}\tilde{r}^{(m)}$ with MC, projecting the solution
- Update: $\tilde{\psi}^{(m)} = \tilde{\psi}^{(m-1)} + \tilde{\epsilon}^{(m)}$
  - If $\tilde{\epsilon}$ is reduced each batch, exponential convergence achieved
  - h-refine when $\epsilon(x,\mu)$ not represented sufficiently
  - Must sufficiently reduce noise in ϵ tallies, each batch
- Repeat until $\|\tilde{\epsilon}\|_2 < \text{tol} \times \|\psi\|_2$

Critical slab benchmark

Problem Parameters

- $k_\infty = 2.29$, $\Sigma_t = 0.326$ cm^{-1}
- $2.4{\times}10^5$ histories per batch, 100 x & 20 μ cells
- Adaptive HO convergence

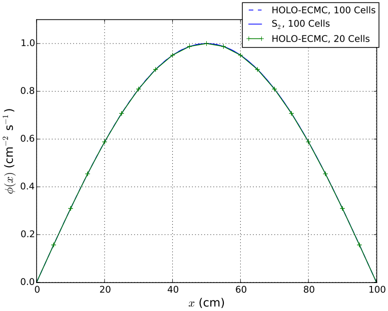


- $|\Delta\Phi| < 10^{-4}$ in 4 outer iterations, using $\sim 2.4 \times 10^7$ histories
- For 10 independent simulations:
  - $\overline{k_{\text{eff}}} = 0.999998$, $\sigma(k_{\text{eff}}) = 4.1 \times 10^{-6}$, max dev. $= 1.1 \times 10^{-5}$
  - $\overline{\sigma_{\text{rel}}(\phi_i)} = 1.4 \times 10^{-05}$

Optically thick, near-critical slab

Problem Parameters

- $k_\infty = 1$, $\Sigma_t = 30.0\ \text{cm}^{-1}$, $\Sigma_s = 29.5\ \text{cm}^{-1}$, DR$\simeq$**0.999**
- Relative Tolerance of 1.0E-05 for all solvers

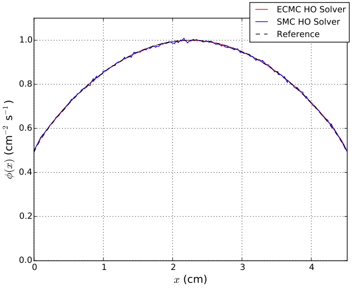


- Fission source convergence:
  - Power iteration not converged after 10,000 iterations
  - NKA converged in 246 iterations
- 1 outer iteration, 4.8×10^6 total histories
- $k_{\text{eff}} = 0.99997$

Comparison of statistical noise for standard and ECMC HO solvers

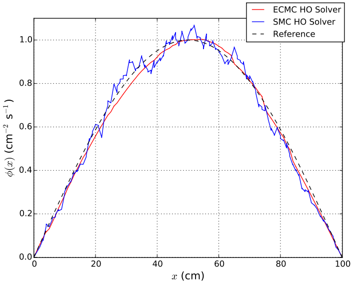
- One HO solve, with a fixed number of histories N. Comparison of ECMC with 5 batches or standard MC (SMC)

Critical Slab



$N = 1.5 \times 10^5$

Diffuse Slab, $k_\infty = 1$



$N = 10^6$

Current & Future Development

- Can Solve for k_{eff} and fission source with HOLO method
  - Pure absorber histories are cheaper than standard MC simulations
  - ECMC efficiently reduces noise globally
  - LO solver handles scattering, fission, and
- Stratified source sampling more efficient at reducing statistical variance than a constant number of particles per cell
- Need to use the estimated statistical error in tallies for $\tilde{\epsilon}(x, \mu)$

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, solve $\epsilon^{(m)} = \mathbf{L}^{-1}\tilde{r}^{(m)}$
   - 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

Exponential Convergence Plot