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

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Nuclear Energy University Programs

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Outline

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Overview

- We are interested in modeling thermal radiation transport in the high-energy density physics regime
  - Temperatures on order of 10^6 K or more
  - Significant energy and momentum may be exchanged with material
- Radiative transfer simulations important in modeling:
  - Material under extreme conditions
  - Inertial confinement fusion
  - Supernovae and other astrophysical phenomena.

The Grey TRT Equations

- The 1D, grey equations

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial x} + \sigma_t I(x,\mu) = \frac{1}{2}\sigma_a ac T^4(x),$$
$$C_v\frac{\partial T}{\partial t} = \sigma_a\left(\phi(x) - acT^4\right)$$
$$\phi(x) = \int_{-1}^{1} I(x,\mu)\mathrm{d}\mu.$$

- Fundamental unknowns are the radiation intensity $I(x,\mu)$ and material temperature $T(x)$
- Absorption cross section (σ_a) can be a strong function of T
- Equations are nonlinear and may be tightly coupled

The Implicit Monte Carlo Method

- Equations often solved with Monte Carlo (MC) via the Implicit Monte Carlo (IMC) method
- The material energy equation is linearized over a time step and eliminated from the system
  - Results in linear transport equation with a discrete emission and scattering terms
  - Continuous integration of time derivative
- Drawbacks
  - Effective scattering cross section can be very large
  - Nonlinearities not converged
  - Reconstruction of linear source shape in cell
    - Local acceleration methods based on diffusion approximation

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An alternative High-Order Low-Order approach

Basic Idea

Solve a fully non-linear, low-order (LO) system that can be efficiently solved, with high-order (HO) correction from efficent MC simulations

- The LO system is formed from space-angle moments of the TRT equations, formed over a fixed finite-element (FE) spatial mesh
- The LO solver resolves non-linear temperature dependence with Newton's method
  - Lower dimensionality in μ
  - Produces a linear-discontinuous (LD) FE representation of scattering and emission source
- The HO system is a fixed-source, pure-absorber transport problem
  - No effective scattering events
  - Solved with ECMC for efficient reduction of statisical noise

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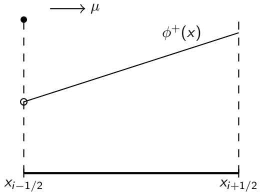
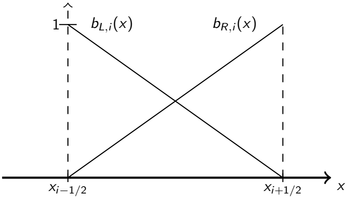
LO Discretization & Space-Angle Moments

- The LO system is "S_2-like" equations (similar to [Wolters 2013]), with a backward Euler discretization in time
- Linear discontinuous (LD) FE in space for ϕ, T, and $T^4(x)$





- Half-range integrals over $+$ and $-$ μ
- *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

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

Forming the LO System

1. Applying moments to the TRT equations yields 4 radiation equations, and 2 material energy equations, per cell

2. The resulting radiation equations are manipulated to produce weighted averages, which we refer to as consistency terms, e.g.,

$$\{\mu\}_{L,i}^{+} := \frac{\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu \, b_{L,i}(x) I^{n+1}(x,\mu) \, \mathrm{d}\mu \mathrm{d}x}{\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) I^{n+1}(x,\mu) \, \mathrm{d}\mu \mathrm{d}x}$$

3. Use HO $\tilde{I}^{n+1}(x,\mu)$ and the LD spatial closure to close the system

- Cell unknowns: $\langle\phi\rangle_{L,i}^{n+1,+}$, $\langle\phi\rangle_{R,i}^{n+1,+}$, $\langle\phi\rangle_{L,i}^{n+1,-}$, $\langle\phi\rangle_{R,i}^{n+1,-}$, $T_{L,i}$, $T_{R,i}$
- Non-linear, fully discrete system, solved with approximate Newton's method

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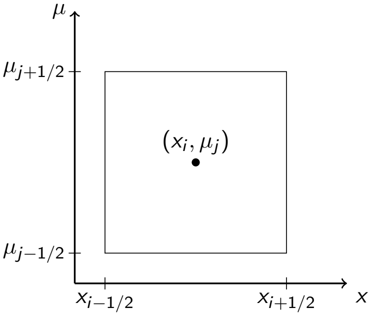
Overview of Exponentially Convergent Monte Carlo

- Each batch tallies the error in current estimate of solution, which is a transport problem with a reduced source
  - Can reduce statistical error globally $\propto e^{-\alpha N}$
  - In TRT problems, old angular intensity provides a *very good* guess of new solution, significantly reducing the required number of histories
- Requires a discretized form of the angular intensity $\tilde{I}(x,\mu)$
  - Use projection of the solution onto a space-angle FE mesh
  - LD FE $\tilde{I}^{HO}(x,\mu)$ allows for direct computation of consistency terms



High Order System and ECMC Algorithm

- Pure absorber transport problem because we have LD representation of T^4 from LO solution

$$\left[\mu\frac{\partial}{\partial x} + \left(\sigma_t + \frac{1}{c\Delta t}\right)\right] I^{n+1}(x,\mu) = \boxed{\frac{I^n}{c\Delta t} + \frac{1}{2}\sigma_a ac T_{LO}^{n+1,4}}$$

$$\mathbf{L} I^{n+1} = q_{LO}$$

FOR a fixed number of batches:

- Residual Equation: $\mathbf{L}\tilde{\epsilon}^{(m)} = \tilde{r}^{(m)} = q - \mathbf{L}\tilde{I}^{n+1,(m)}$
- Compute $\tilde{\epsilon}^{(m)} = \mathbf{L}^{-1}\tilde{r}^{(m)}$ with MC, projecting the solution
- Update: $\tilde{I}^{n+1,(m)} = \tilde{I}^{n+1,(m-1)} + \tilde{\epsilon}^{(m)}$
  - If $\tilde{\epsilon}$ is reduced each batch, exponential convergence achieved
  - Must sufficiently reduce noise in ϵ tallies, each batch
  - Issues when solution cannot be represented within a cell

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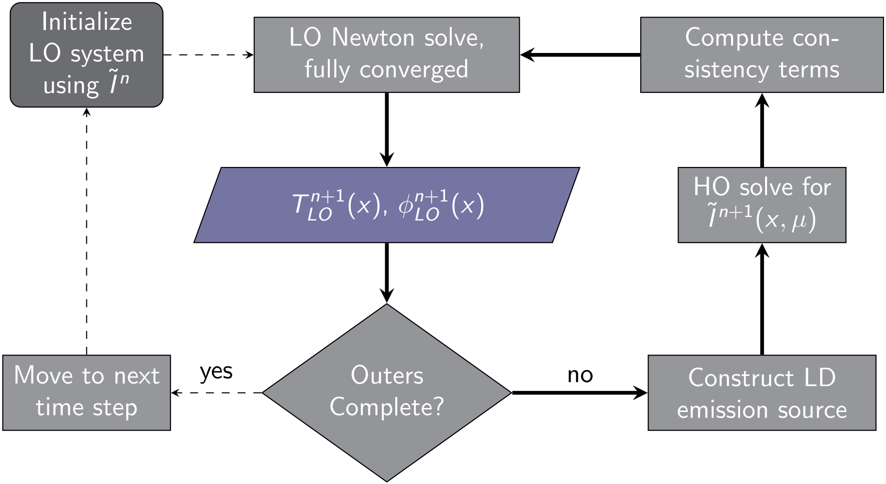
High-Order Low-Order Algorithm



Relevant Implementation Specifics

- Monte Carlo details:
  - Particles are allowed to stream along path s, $w(s) = w_0 e^{-\sigma_t s}$
  - Cell-wise, global representation allows for easy stratified sampling
    - $N_{i,j} \propto |r_i(x, \mu)|$
- LO system is fully converged each solve
- Difficulties in resolving the solution near the wave-front
  - The LD representation for I results in negativite values within a cell
  - In these results, no correction is applied to the HO solution, and the LO solution uses a lumped LD closure and S_2 equivalent terms in these cells
- For all results, one HO solve per time step

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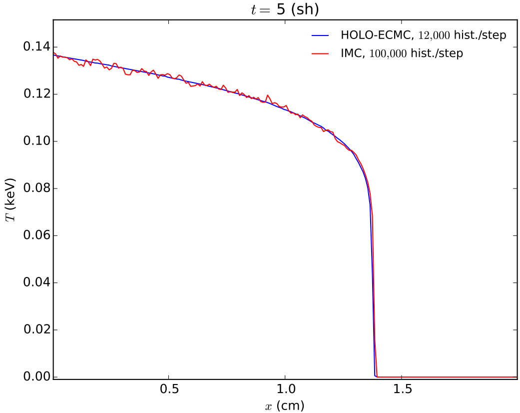
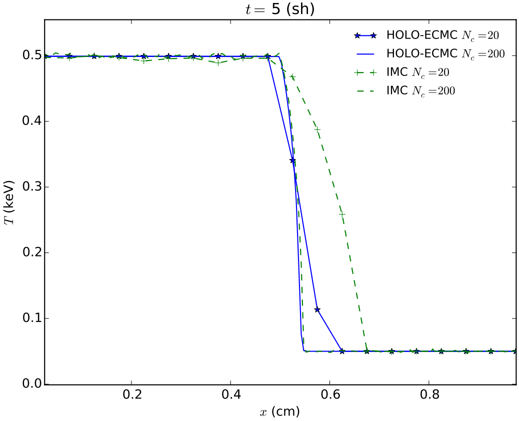
Marshak Wave Test Problem

- From equilibrium, a radiation source is applied at the left boundary at $t = 0$. With $\sigma_a \propto T^{-3}$, energy slowly moves across the system.
- Transient solution after 5 shakes plotted as $T_r = \sqrt[4]{\phi/ac}$, with 200 x cells



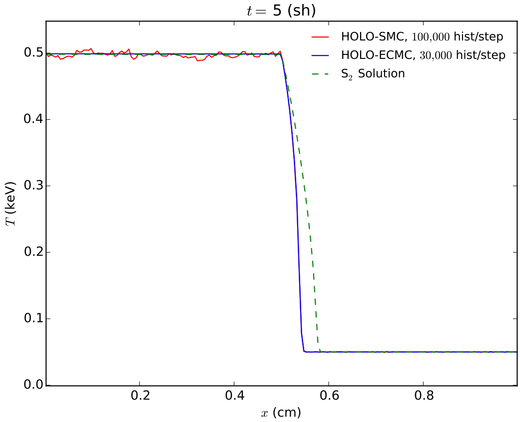
Two Material Problem, Comparison of Spatial Convergence

- Problem the same as Marshak Wave, but with constant opacities and an optically thin (left) and optically thick (right) region



Comparison of statistical noise for standard and ECMC HO solvers

- One HO solve, with a *fixed number of histories* per time step, for two different HO solvers: a comparison of ECMC with 3 batches and standard MC (SMC), as well as S_2 solution



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Current & Future Development

- Can accurately reproduce IMC results with HOLO method
  - ECMC requires significantly less particles
  - LO solver determines non-linear Material temperature distribution
  - Linear shape within a cell mitigates teleportation error
  - Very efficient for diffusive problems
- Currently developing strategies for dealing with unresolvable solutions
- Next step will be to implement in 2 spatial dimensions

Questions?

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ECMC procedure

Algorithm

1. Intialize $\tilde{I}^{n+1,(0)} := \tilde{I}^{n}$
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

LO System

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

$$-2\mu_{i-1/2}^{n+1,+}\phi_{i-1/2}^{n+1,+}+\{\mu\}_{L,i}^{n+1,+}\langle\phi\rangle_{L,i}^{n+1,+}+\{\mu\}_{R,i}^{n+1,+}\langle\phi\rangle_{R,i}^{n+1,+}+\left(\sigma_t^{n+1}+\frac{}{c}\right.$$

$$-\frac{\sigma_s h_i}{2}\left(\langle\phi\rangle_{L,i}^{n+1,+}+\langle\phi\rangle_{L,i}^{n+1,-}\right)=\frac{h_i}{2}\langle\sigma_a^{n+1}acT^{n+1,4}\rangle_{L,i}+\frac{h_i}{c\Delta t}\langle\phi\rangle_{L,i}^{n,+}, \tag{1}$$

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

Solving LO System with Newton's Method

- Linearization: $\underline{B}(T^{n+1}) = \underline{B}(T^*) + \left(T^{n+1} - T^*\right) \left.\frac{\partial \underline{B}}{\partial t}\right|_{t^*}$
- Modified system

$$\left[\mathbf{D}(\mu^{\pm}) - \sigma_a^*(1 - f^*)\right] \underline{\Phi}^{n+1} = f^* \underline{B}(T^*) + \frac{\underline{\Phi}^n}{c\Delta t}$$

$$\boxed{\hat{\mathbf{D}}\Phi^{n+1} = \underline{Q}}$$

$$f = \left(1 + \sigma_a^* c\Delta t \frac{4aT^{*3}}{\rho c_v}\right)^{-1} \qquad T_i^* = \frac{T_{L,i}^* + T_{R,i}^*}{2}$$

- Equation for T^{n+1} based on linearization that is conservative
- Converge T^{n+1} and $\langle \phi \rangle$ with Newton Iterations
  - Spatial representation can result in negative temperatures