

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

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# Outline

- 1 Introduction
- 2 Low-Order Solver
- 3 High-Order Solver
- 4 Computational Results
- 5 Conclusions

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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 gray thermal radiative transfer equations

- The 1D, frequency-integrated (grey) equations

$$\frac{1}{c} \frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial x} + \sigma_t I(x, \mu) = \frac{1}{2} \sigma_a a c T^4,$$

$$C_v \frac{\partial T}{\partial t} = \sigma_a \phi(x) - \sigma_a a c T^4,$$

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

- Fundamental unknowns are the radiation intensity  $I(x, \mu)$  and material temperature  $T$
- Absorption cross section ( $\sigma_a$ ) 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
- In IMC, the material energy equation is linearized over a time step and eliminated from the system
  - Results in effective emission and scattering terms
  - This linear transport equation is solved with standard MC particle transport algorithms
  - Continuous integration in time
- Drawbacks
  - Effective scattering cross section can be very large
  - Nonlinearities not converged
  - Reconstruction of linear source shape in cell

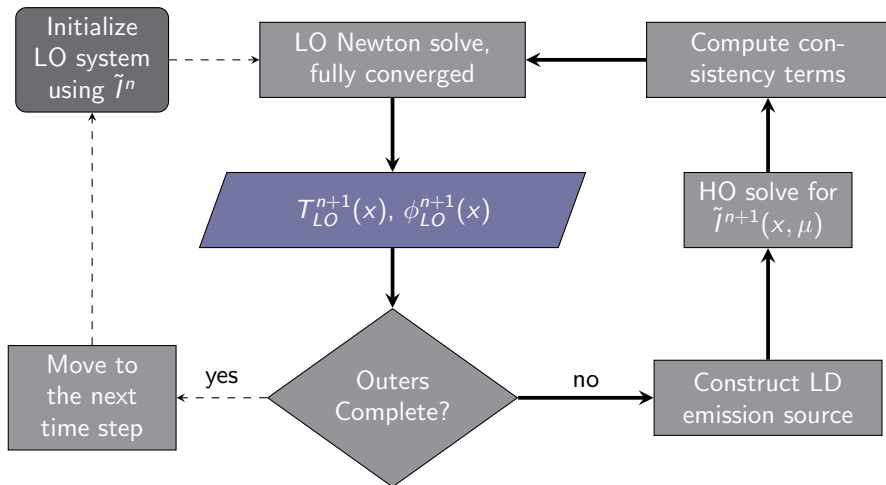
# An alternative High-Order Low-Order approach

## Basic Idea

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

- The LO system, formed over a fixed spatial finite element (FE) mesh, contains **angular consistency terms**.
- The LO solver resolves non-linear temperature dependence with Newtons method
  - **Lower dimensional** problem in angular variable
  - Produces a linear-discontinuous (LD) finite element representation of sources
- The HO system is a fixed-source, pure-absorber transport problem
  - No effective scattering events
  - Solved with ECMC for efficient reduction of statistical noise

# High-Order Low-Order Algorithm



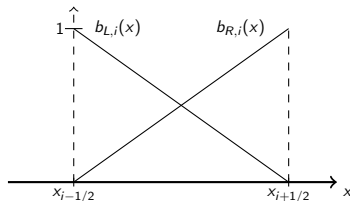
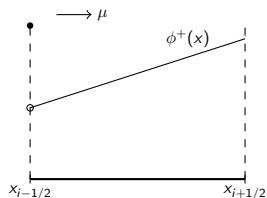


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# LO Discretization & Space-Angle Moments

- Backward Euler discretization in time
- Linear discontinuous (LD) FE in space for  $\phi$ ,  $T$ , and  $T^4$



- Half-range integrals in angle
- *Examples of moments:*

Spatial: left basis

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

Angular: positive flow

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

# Forming the LO System

- Backward Euler discretization in time
- We take half range angular integrals spatial and angular moments of the equations to reduce dimensionality.
- Taking moments of T.E. yields 4 radiation equations, and 2 material energy equations, per cell
- Conserves the total energy in the system
- Cell unknowns:  $\langle \phi \rangle_{L,i}^{n+1,+}$ ,  $\langle \phi \rangle_{R,i}^{n+1,+}$ ,  $\langle \phi \rangle_{L,i}^{n+1,-}$ ,  $\langle \phi \rangle_{R,i}^{n+1,-}$ ,  $T_{L,i}$ ,  $T_{R,i}$

# Computing LO Consistency terms from HO Solution

- The streaming operator contains generally unknown weighted angular averages, called **consistency terms**
- For  $\mu > 0$ ,  $L$  moment

$$\langle \mu \rangle_{L,i}^+ \simeq \frac{\frac{2}{h_i} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu b_{L,i}(x) \tilde{I}^{HO}(x, \mu) d\mu dx}{\frac{2}{h_i} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) \tilde{I}^{HO}(x, \mu) d\mu dx} \quad (1)$$

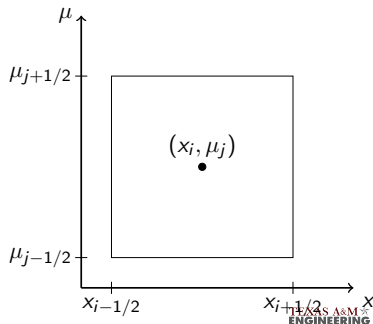
- ECMC gives LDfE  $\tilde{I}^{HO}(x, \mu)$  for computing terms directly

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# 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**  $\propto e^{-\alpha N}$
  - 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, computed with path-length estimators of moments



## High Order System and ECMC Algorithm

- **Pure absorber** transport problem because we know RHS from LO solution

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

FOR a fixed number of batches:

- Residual Equation:  $\mathbf{L} \tilde{\epsilon}^{(m)} = \tilde{r}^{(m)} = \mathbf{q} - \mathbf{L} \tilde{I}^{n+1,(m)}$
- 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  $\epsilon$  tallies, each batch
  - Issues when solution cannot be represented within a cell

## Other MC Implementation Details

- The LO solver provides the scattering and emission source, producing a pure absorber, fixed-source transport problem.
- Discrete in time, resulting in a modified source and removal cross section
- 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

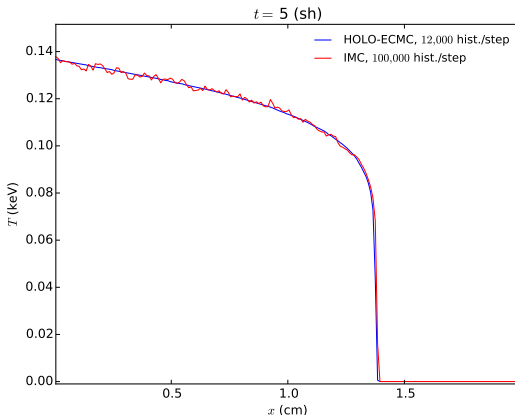


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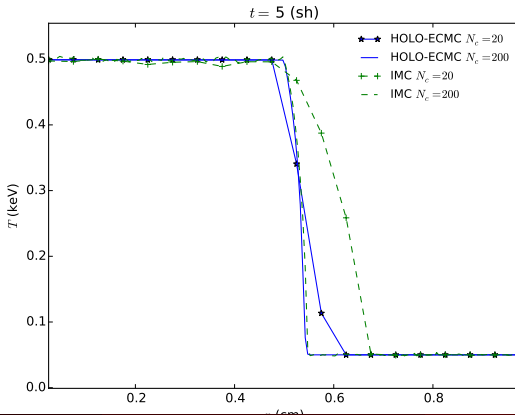
# Marshak Wave Test Problem

- From equilibrium, a radiation source is applied at the left boundary,  $\sigma \propto T^{-3}$ .
- Plot of transient solution for  $T_r = \sqrt[4]{\phi/ac}$  after 5 shakes, 200  $\times$  cells



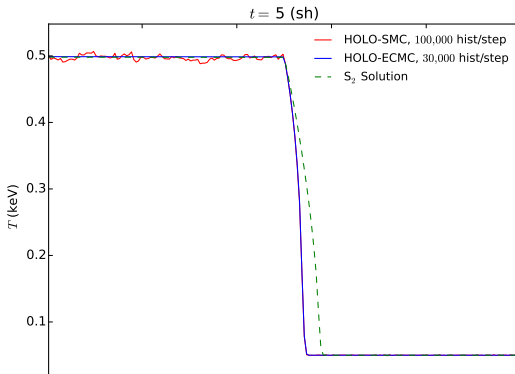
## Two Material Problem, Comparison of Spatial Convergence

- Same as Marshak Wave, but with constant opacities and an optically thin (left) and optically thick (right) region
- Convergence of spatial mesh:



# Comparison of statistical noise for standard and ECMC HO solvers

- Two material problem
- 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
- Future work will be to implement in 2 spatial dimensions to demonstrate the elimination of ray effects

# Questions?

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

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# Backup Slides

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## Algorithm

- 1 Initialize  $\tilde{I}^{n+1,(0)} := \tilde{I}^n$
- 2 Using Monte Carlo, solve  $\epsilon^{(m)} = \mathbf{L}^{-1} \tilde{r}^{(m)}$ 
  - Use volumetric tallies, weighted with  $x$  and  $\mu$  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  $\|\tilde{\epsilon}\|_2 < \text{tol} \times \|\psi\|_2$

## 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  $\Phi^{LO}$  is converged
- Use adaptive convergence criteria

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

$$\begin{aligned}
 & -2\mu_{i-1/2}^{n+1,+} \phi_{i-1/2}^{n+1,+} + \{\mu\}_{L,i}^{n+1,+} \langle \phi \rangle_{L,i}^{n+1,+} + \{\mu\}_{R,i}^{n+1,+} \langle \phi \rangle_{R,i}^{n+1,+} + \left( \sigma_t^{n+1} + \frac{h_i}{c\Delta t} \right) \\
 & - \frac{\sigma_s h_i}{2} \left( \langle \phi \rangle_{L,i}^{n+1,+} + \langle \phi \rangle_{L,i}^{n+1,-} \right) = \frac{h_i}{2} \langle \sigma_a^{n+1} a c T^{n+1,4} \rangle_{L,i} + \frac{h_i}{c\Delta t} \langle \phi \rangle_{L,i}^{n,+},
 \end{aligned} \tag{2}$$

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

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

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

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

- 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