

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

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MC 2015 - April 22



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 (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
- 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

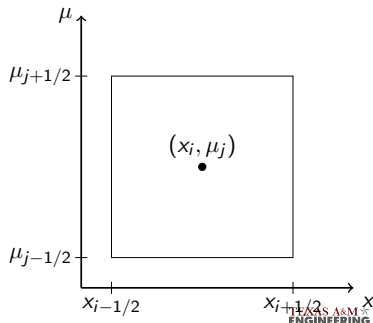
Basic Idea

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

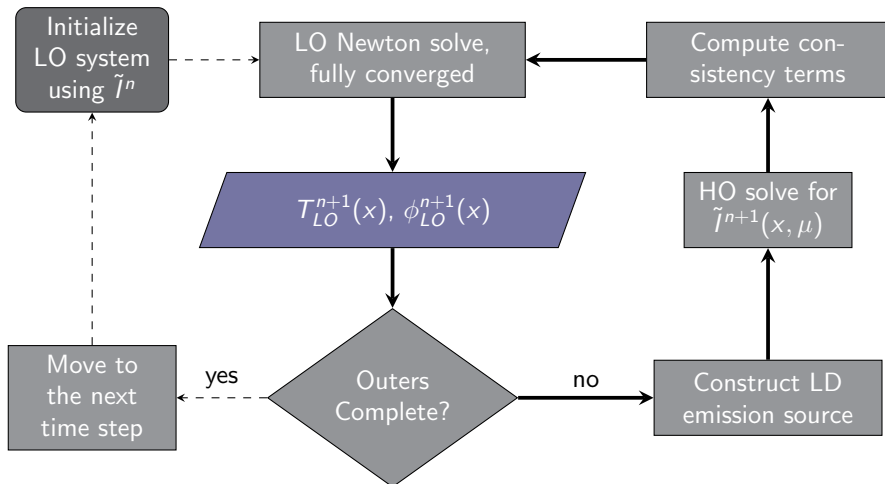
- Useful when global solution of particle density needed
- The LO solution preserves moments of the HO solution upon convergence
- The LO solver resolves non-linear temperature dependence with Newtons method
 - Lower dimensional problem in angular variable
 - Produces a linear-discontinuous (LD) finite element representation of sources
- The HO system is a fixed-source, pure-absorber transport problem, which we solve with ECMC
 - No effective scattering events

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
 - Projection computed using path-length estimators of moments of I



High-Order Low-Order Algorithm

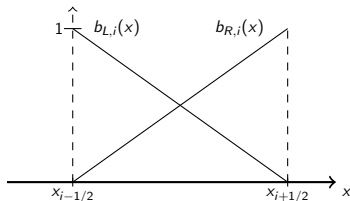
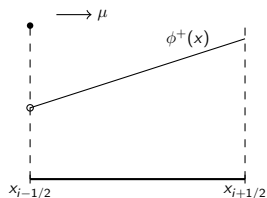


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LO Discretization & Space-Angle Moments

- Backward Euler discretization in time
- Linear discontinuous (LD) FE in space for ϕ and T



- 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 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: $\langle \phi \rangle_{L,i}^{n+1,+}$, $\langle \phi \rangle_{R,i}^{n+1,+}$, $\langle \phi \rangle_{L,i}^{n+1,-}$, $\langle \phi \rangle_{R,i}^{n+1,-}$, $T_{L,i}$, $T_{R,i}$
- The global system for radiation, **fully implicit** in time, is

$$\mathbf{D}^{n+1} \underline{\Phi}^{n+1} = \underline{B}(T^{n+1}) + \frac{\Phi^n}{c\Delta t}$$

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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High Order System and ECMC Algorithm

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

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

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

ECMC Algorithm

- 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

Other MC Implementation Details

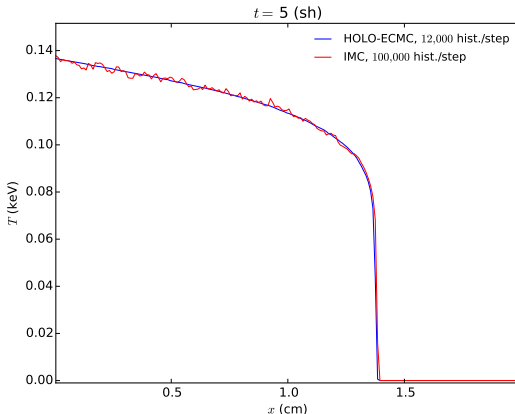
- The LO solver provides the scattering and emission source, producing a pure absorber, fixed-source transport problem.
- Discrete in time, resulting in a modified source and removal cross section
- Particles are allowed to stream, $w(s) = w_0 e^{-\Sigma_t s}$
- LDFE and upwinding **eliminates** surface 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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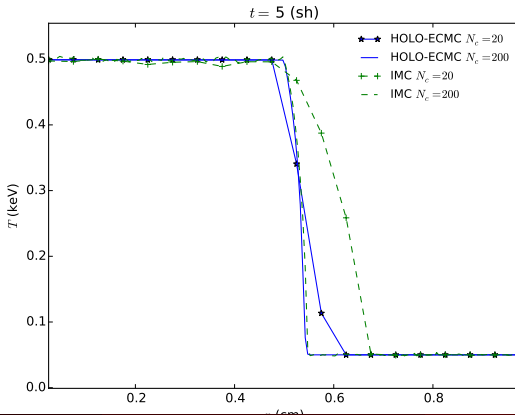
Marshak Wave Test Problem

- 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



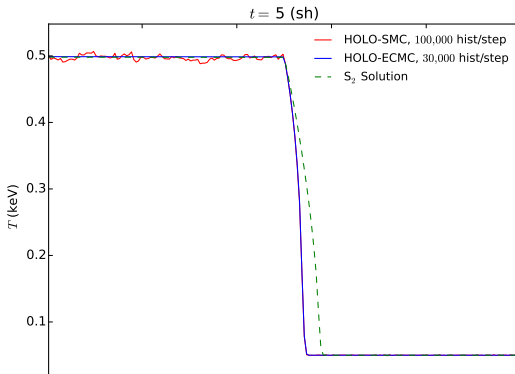
Two Material Problem, Comparison of Spatial Convergence

- 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?

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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 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 $\|\tilde{\epsilon}\|_2 < \text{tol} \times \|\psi\|_2$

Algorithm

- ➊ Initialize $\langle \mu \rangle^\pm$ parameters to S_2
- ➋ Solve LO system using power iteration
- ➌ Build q^{LD} for HO solver, and set $\tilde{\psi}$ to latest HO estimate on coarsest $x-\mu$ mesh
- ➍ Solve $\tilde{\psi}(x, \mu) = \mathbf{L}^{-1} q^{LO}$ using ECMC
- ➎ Compute new $\langle \mu \rangle^\pm$ parameters using $\tilde{\psi}^{HO}$ over LO mesh
- ➏ Repeat 2-5 until Φ^{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