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

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SIAM CSE 2015

Outline

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

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Overview

Thermal radiative transfer is relevant in very high temperature heat transfer scenarios, representing a complicatedn 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. Time dependent, radiative transfer simulations are important in:

- Inertial confinement fusion
- High energy plasma calculations
- Astrophysics calculations

The thermal radiative transfer equations

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

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

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

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

- Fundamental unknowns are the radiation intensity $I(x,\mu)$ and material temperature T
- Cross sections (σ) can be a strong function of T
- Equations are tightly coupled through source terms and contain the non-linear Planckian emission source acT^4

The implicit Monte Carlo method

- These equations are typically 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 an effective source and scattering cross section for a linear transport problem
  - 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, resulting in many expensive MC scattering events
  - System is not truly implicit in time, because of linearization
  - Artificial reconstruction of linear source shape in cell

An alternative High-Order Low-Order approach

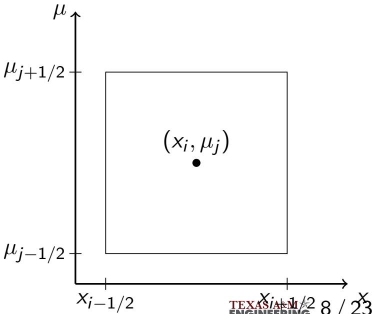
Basic Idea

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

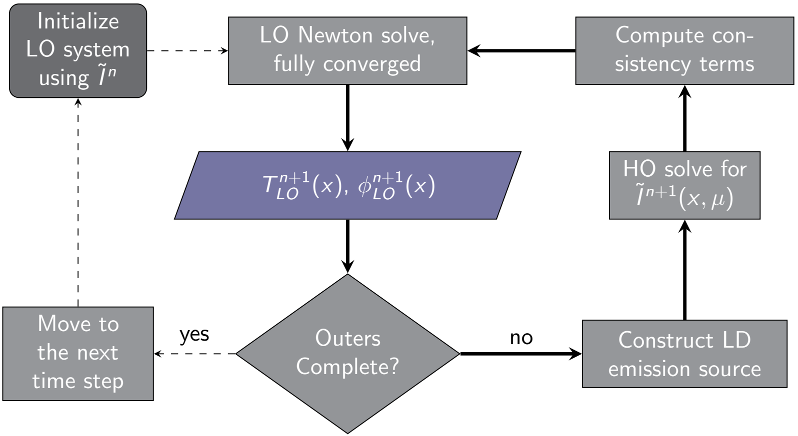
- Useful when global solution of particle density needed
- The LO solution preserves moments of the HO solution upon convergence
- The LO solver resolves non-linear temperature dependence with Newtons method
  - Lower dimensional problem in anglular variable
  - Produces a linear-discontinuous (LD) finite 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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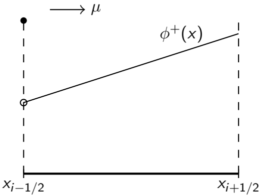
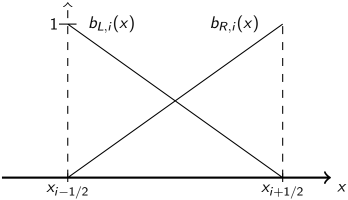
LO Discretization & Space-Angle Moments

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





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

<u>Spatial: left basis</u>

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

<u>Angular: positive flow</u>

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

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

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

Computing LO Consistency terms from HO Solution

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

$$\langle\mu\rangle^{+}_{L,i} \simeq \frac{\dfrac{2}{h_i}\displaystyle\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu \, b_{L,i}(x)\tilde{I}^{HO}(x,\mu)\mathrm{d}\mu\mathrm{d}x}{\dfrac{2}{h_i}\displaystyle\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)\tilde{I}^{HO}(x,\mu)\mathrm{d}\mu\mathrm{d}x} \tag{4}$$

- 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

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

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

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
- Repeat for fixed number of batches

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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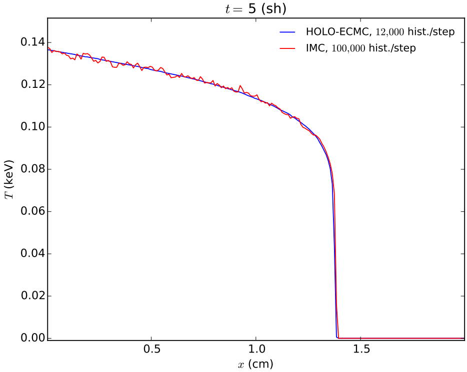
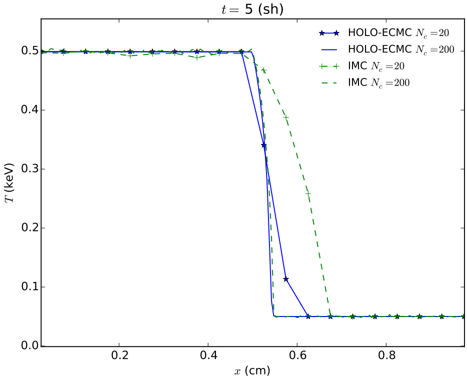
Marshak Wave Test Problem

- 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 x cells



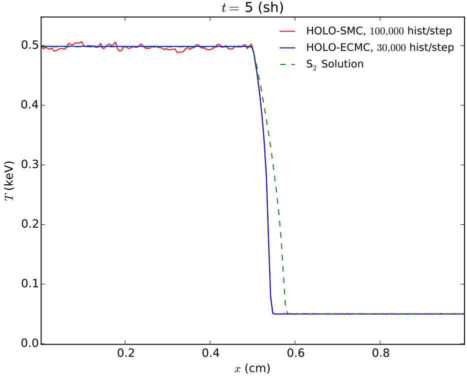
Two Material Problem, Comparison of Spatial Convergence

- 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
  - Pure absorber histories are more effecient than standard MC simulations
  - ECMC requires significantly less
  - LO solver determines non-linear Material temperature distribution
  - Linear shape within a cell mitigates teleportation error
  - Very efficient for diffusive problems
- Future work will be to implement in 2 spatial dimensions to demonstrate the elimination of ray effects

Questions?

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

Backup Slides

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

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

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

$$-2\mu_{i-1/2}^{n+1,+}\phi_{i-1/2}^{n+1,+}+\{\mu\}_{L,i}^{n+1,+}\langle\phi\rangle_{L,i}^{n+1,+}+\{\mu\}_{R,i}^{n+1,+}\langle\phi\rangle_{R,i}^{n+1,+}+\Big(\sigma_t^{n+1}$$
$$-\frac{\sigma_s h_i}{2}\left(\langle\phi\rangle_{L,i}^{n+1,+}+\langle\phi\rangle_{L,i}^{n+1,-}\right)=\frac{h_i}{2}\langle\sigma_a^{n+1}acT^{n+1,4}\rangle_{L,i}+\frac{h_i}{c\Delta t}\langle\phi\rangle_{L,i}^{n,+},$$
(5

- 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