A Hybrid Monte Carlo-Deterministic Method for Global, Time-Dependent Transport Calculations

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Outline

1. Introduction
   - Radiation Transport
   - Solution Schemes
2. Analysis
   - Theory
3. Results
4. Summary

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Radiation Transport Applications

High Energy Density Physics (HEDP):

- Stellar regimes
- Inertial Confinement Fusion (ICF)

Fission reactors, shielding

Medical physics:

- Radiation beams
- Nuclear medicine

Unknown(Phase space)

For HEDP problems, we use the *specific intensity*:

$$I \equiv ch\nu N(\mathbf{x}, \mathbf{\Omega}, \nu, t)\,,$$

where

$$N\ dVd\nu d\Omega = \text{ number of photons } \ldots$$

$$\begin{aligned}\mathbf{x} &= (x, y, z) = \text{location vector}\,,\\ \mathbf{\Omega} &= (\phi, \theta) = \text{direction vector}\,,\\ \nu &= \text{frequency}\,,\\ \mathbf{t} &= \text{time}\,.\end{aligned}$$

A mathematical model

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega} \cdot \nabla I + \sigma_t I = \iint \sigma_s I \, d\nu d\Omega + \sigma_a B$$

$$c_v \frac{\partial T}{\partial t} + \iint \sigma_a B \, d\nu d\Omega = \iint \sigma_a I \, d\nu d\Omega$$

Properties:

- Time change + removal = source
- Nonlinear in temperature, integro-differential in intensity
- Reduces to an elliptic, parabolic, and hyperbolic PDE in various regimes
- Neglects quantum effects, polarity, material motion / anistropies, stochasticity ...
- Generally no "detector" region: need a global solution

Deterministic vs. Monte Carlo

- Always provides a global solution
- Discretize everything: ($\approx 300 \times 10^6 \times 10^3$) per time step
- Angle: Gauss-Legendre. Space: FE. Frequency: Multigroup. Time: Implicit
- No general parallel scheme since information propagation varies highly by problem data

State of the art: flux-limited diffusion (no angles, reduced space)

Deterministic vs. **Monte Carlo**

- Statistical error reduces as $C/\sqrt{M}$
- All current methods are essentially physical analogs – straightforward to implement, expensive to ensure adequate problem population in physically important regions
- Variance reduction requires human experience
- "Embarassingly parallel"

A Hybrid Scheme

What about a hybrid method, a.k.a. "automatic variance reduction"?

- Should be hands-off, efficient, and not require exotic changes to existing methods
- Recent, excellent success with local problems
- Our new method is one of two known global methods

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Theory

We have results for this new, hybrid method on the following, simplified thermal radiative transport equations:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial x} + \sigma_t I = \frac{\sigma_s}{2}\int I \, d\mu + \frac{\sigma_a c\eta U_m}{2}$$

$$\frac{\partial U_m}{\partial t} + \sigma_a c\eta U_m = \sigma_a \int I \, d\mu$$

These are 1-D, frequency-integrated, and linearized over a time step.

Theory

- Perform a cheap, deterministic method to obtain an estimate of the scalar intensity $\hat{\phi}(x, t)$
- Define the multiplicative correction $f(x, \mu, t)$:

$$I(x, \mu, t) = \hat{\phi}(x, t) f(x, \mu, t)$$

Theory

- Inserting this into the previous equations and rearranging, we form an exact transport equation for the multiplicative correction:

$$\frac{1}{c}\frac{\partial f}{\partial t} + \mu\frac{\partial f}{\partial x} + \left(\sigma_t + \mu\frac{\partial}{\partial x}\ln\hat{\phi}\right) f = \frac{\sigma_s}{2}\int f\; d\mu + \frac{\sigma_a c\eta U_m}{2\hat{\phi}}$$

$$\frac{\partial U_m}{\partial t} + \sigma_a c\eta U_m = \sigma_a\hat{\phi}\int f\; d\mu$$

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Theory

- Inserting this into the previous equations and rearranging, we form an exact transport equation for the multiplicative correction:

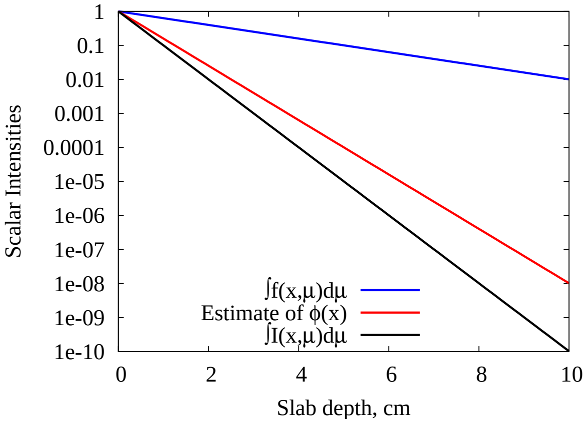
$$\frac{1}{c}\frac{\partial f}{\partial t} + \mu\frac{\partial f}{\partial x} + \left(\sigma_t + \mu\frac{\partial}{\partial x}\ln\hat{\phi}\right) f = \frac{\sigma_s}{2}\int f\ d\mu + \frac{\sigma_a c\eta U_m}{2\hat{\phi}}$$

$$\frac{\partial U_m}{\partial t} + \sigma_a c\eta U_m = \sigma_a\hat{\phi}\int f\ d\mu$$

Theory

- Solving this transport equation is advantageous because:
  - The correction f should be more uniform than I; “correctons” are therefore more uniformly distributed than photons (reduces variance)
  - The angle-dependent opacity encourages particles to move along gradients (increases efficiency, reduces variance)
  - For decent $\hat{\phi}$, the average particle weight is constant (reduces variance)
  - Provided that $\hat{\phi}$ has a simple form and the collision term is positive, f may found using known MC techniques (eases implementation)

Theory



- Exact solution decays by 10 orders of magnitude
- $\hat{\phi}$ decays by 8
- $\int f \, d\mu$ only decays by 2

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Figure of Merit (FOM)

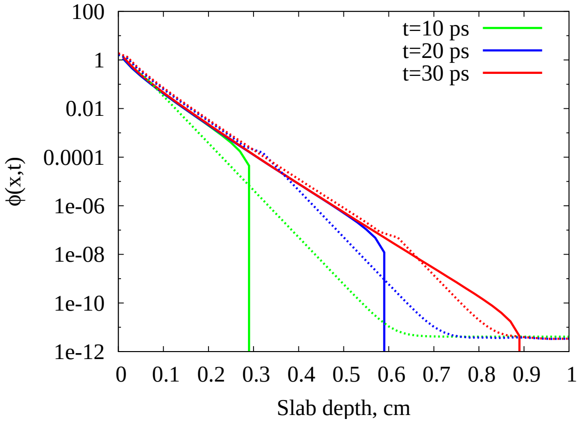
- The *Figure of Merit* (FOM) is a metric to compare Monte Carlo methods:

$$FOM(x) = \frac{1.0}{R^2(x)T_{cpu}}$$

R = relative statistical error (standard deviation / mean)
T_{cpu} = processor time

- Large FOM = good method

Scalar intensity profiles



- Solid = Hybrid solution
- Dashed = $\hat{\phi}(x, t)$
- Snapshots in time
- $\sigma_t = 25.0$, $c_v = 0.1$, 10^9 histories

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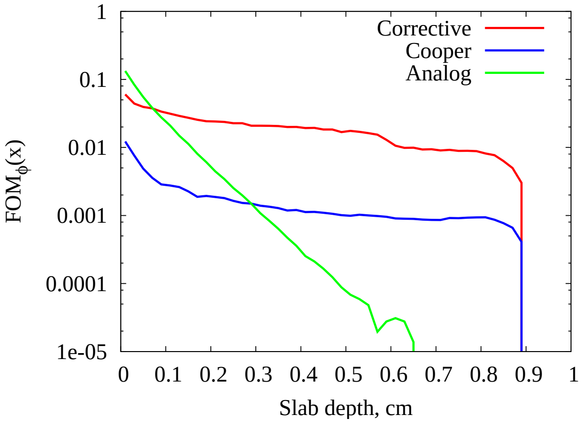
Intensity Figure of Merit



- $t = 30$ ps
- $\sigma_t = 25.0$,
  $c_v = 0.1$,
  10^9 histories

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Summary

- Radiation transport is a computationally challenging, multi-faceted problem
- New methods that are hybrids of totally different approaches are having great success
- Here, a new hybrid deterministic-Monte Carlo method was implemented in which a transport equation for the *multiplicative correction* to a deterministic estimate is solved
- The correcton method is very competitive for problems with large spatial gradients, and requires little change to existing algorithms

Acknowledgments

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Implementation

Object-oriented C++ driven by a Python GUI (wxPython).

- C++ exposed to Python via SWIG
- Object example: Problem is composed of Mesh, Materials, BCs, Fields; a Method (MC, Diffusion) solves a Problem
- Monte Carlo is parallel through MPI
- Version control using SVN
- Python regression testing
- To be "documented" via Doxygen