

# 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*:

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

where

$N dVd\nu d\Omega =$  number of photons ...

$\mathbf{x} = (x, y, z) =$  location vector ,

$\boldsymbol{\Omega} = (\phi, \theta) =$  direction vector ,

$\nu =$  frequency ,

$\mathbf{t} =$  time .

# 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 / anisotropies, 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”



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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:

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

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

# Theory

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

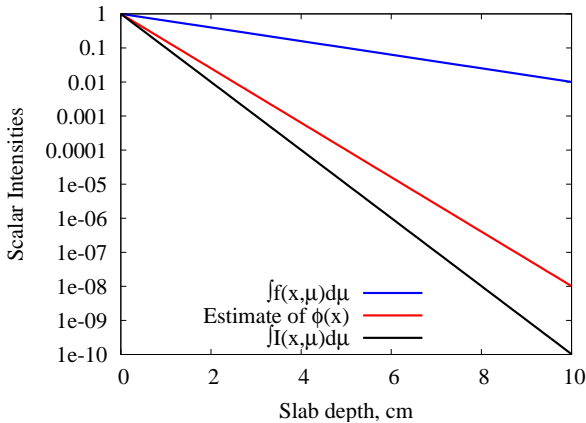
$$\frac{1}{c} \frac{\partial f}{\partial t} + \mu \frac{\partial f}{\partial x} + \left( \sigma_t + \mu \frac{\partial}{\partial x} \ln \hat{\phi} \right) f = \frac{\sigma_s}{2} \int f d\mu + \frac{\sigma_a c \eta U_m}{2 \hat{\phi}}$$

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

# 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



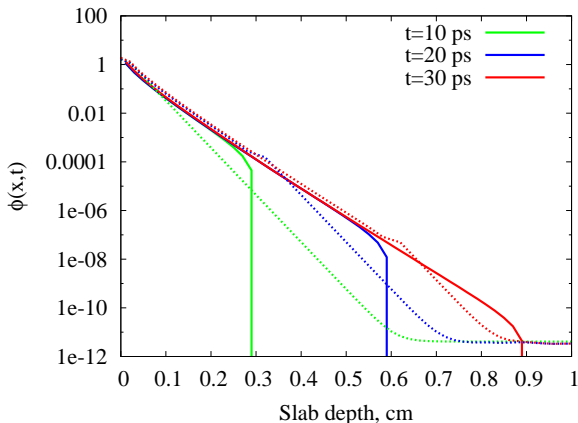
- Exact solution decays by 10 orders of magnitude
- $\hat{\phi}$  decays by 8
- $\int f d\mu$  only decays by 2

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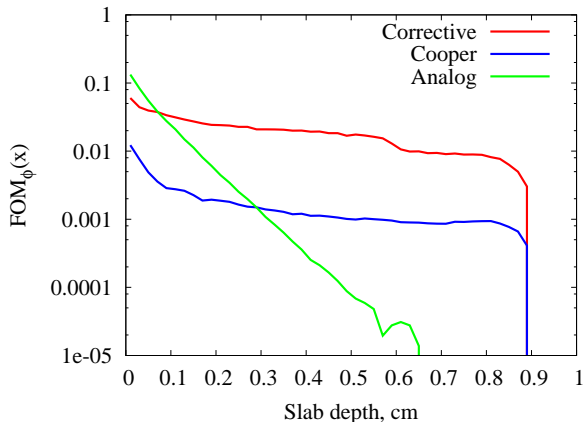


# Scalar intensity profiles



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

# 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

- Advisor: Edward Larsen
- LANL CCS-4 Advisor: Todd Urbatsch
- DOE CSGF

# 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