
Monte Carlo: Algorithm and Performance Overview

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Outline



- **Monte Carlo Transport Methods**
 - **General Algorithm Description**
- **Neutron Monte Carlo – Criticality**
- **Implicit Monte Carlo (IMC) Radiation Transport**
 - **Photon Transport vs. Neutron Transport**
 - **The IMC algorithm: Fleck and Cummings, JCP 8, 313 (1971)**
 - **IMC vs. MC**
- **Performance of IMC**
- **Problems/Research Directions for Monte Carlo Radiation Transport**

The Monte Carlo Method of Particle Transport



- The Monte Carlo method of simulating particle transport is a *statistical* approach to “solving” the linearized Boltzmann equation, shown here for neutrons:

- While the spatial domain is divided into cells or regions, and energy may be divided into groups, this method does *not* employ a *continuum* approach to solve this integro-differential equation, as is the case in deterministic transport methods (S_N , P_N , etc)
- The essence of the Monte Carlo method of particle transport is to follow, or *track*, the trajectory of *individual* particles through this seven-dimensional phase space in an *analog* fashion.

The Monte Carlo Method of Particle Transport



- Particles undergo a series of events during tracking:
 - Streaming to the end of the time step: *Census Event* (**Temporal Streaming**)
 - Streaming to the boundary of a neighboring cell, region or system boundary: *Facet Crossing Event* (**Spatial Streaming**)
 - Streaming to the system boundary results in leakage: *Escape Event*
 - Interaction with an atom or nucleus in the background medium: *Collision Event* (Collisional **Absorption**, **Collisional Scattering**)
 - Collisional interactions may result in the production of secondary particles (**Collisional Fission Source**)
 - Streaming to the lower-energy group boundary or thermal energy of the medium during charged-particle slowing down: *Energy-Boundary Crossing or Thermalization*
- The trajectory, or track, of each particle through phase space is comprised of several segments.
- Each Monte Carlo simulation particle represents an *ensemble* of physical particles.

The Monte Carlo Method of Particle Transport



Mesh-Based Monte Carlo Particle Tracking

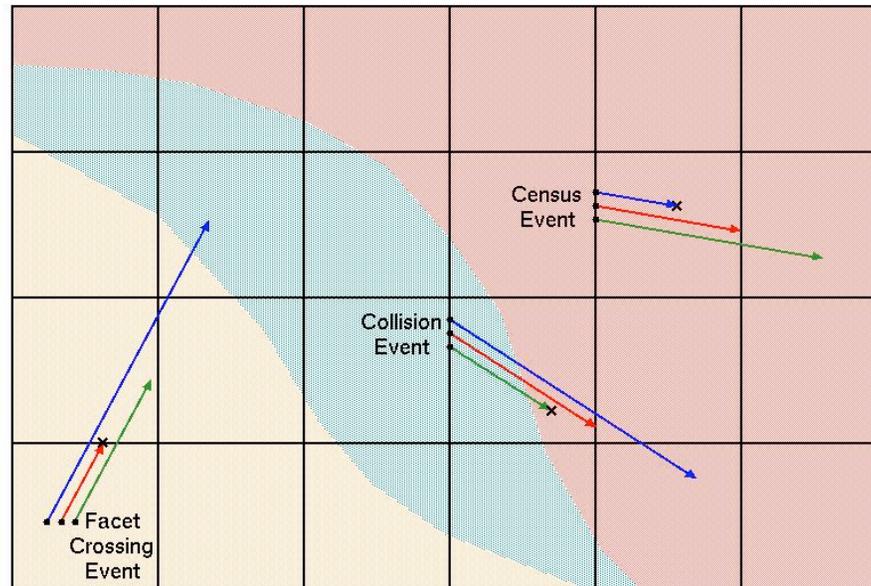
Each particle track is comprised of several segments.

Single segments from the tracks of three particles are shown.

The event chosen for each segment is the one with the shortest distance.

Note: The event distances are actually colinear.

- Distance to Census
- Distance to Facet Crossing
- Distance to Collision



Material A

Material B

Material C

The Monte Carlo Method of Particle Transport



- Tracking of particles in three-dimensional Cartesian space is independent of the problem geometry or mesh: a particle travels in a straight line until it intersects a facet/surface of first order (plane), second order (sphere, cylinder, cone, ellipsoid), etc.
- While the particles have discrete energies, the multigroup treatment of energy employs cross sections which are constant within a group.
- Collisions are point events which may result in the production of secondary particles:
 - Particles which are being tracked are placed in the vault for subsequent tracking
 - Particles which are *not* being tracked are assumed to be locally deposited
- The flux in a given cell (c) and energy group (g) is sum of the particle (i) path lengths (l) through the volume (V) in a given time step (Δt):

$$\phi = \sum_i l_i \Delta t$$

- These fluxes are multiplied by the number densities of background isotopes and the relevant cross sections to produce rates of energy deposition and isotopic burnup.

The Monte Carlo Method of Particle Transport



- Each Monte Carlo particle is defined by the following attributes:
 - Spatial coordinates: (x, y, z)
 - Velocities or Direction Cosines: (v_x, v_y, v_z) or $(\cos(\alpha), \cos(\beta), \cos(\gamma))$
 - Kinetic Energy: E
 - Weight: $W = (N_{phys} / N_{sim})$
 - Time to Census: t_{cens}
 - Number of Mean-Free Paths to Collision: N_{mfp}
 - Random Number Seed: R_{seed}
 - Miscellaneous Attributes: number of collisions, last event, breed, domain, cell, facet, etc.
- These particles are usually tracked in the seven-dimensional phase space comprised of three spatial coordinates (x, y, z) , three velocities (v_x, v_y, v_z) , energy (E) and time (t) .

Monte Carlo Criticality Eigenvalue Algorithms



- Two eigenvalue forms of the Boltzmann equation are used to define the criticality of a system:
 - The (ν/k_{eff}) static form describes a balance between neutron production and removal in a source-free multiplying medium:

 - The (α/ν) “static” form is derived from the separability of variables ansatz $\psi(\vec{r}, \Omega) = \psi(\vec{r}) \zeta(\Omega)$ and the assumption that the system is in the fundamental eigenmode $\zeta(\Omega) = \zeta(\Omega)^\alpha$, to give:

Monte Carlo Criticality Eigenvalue Algorithms



- Some *static* algorithms for calculating the k_{eff} or α eigenvalues of a system include:
 - *Static k*: “Solves” the (ν/k_{eff}) form of the Boltzmann equation by iterating to convergence over many generations
 - *Static α* : “Solves” the (α/ν) form of the Boltzmann equation by adding “time absorption” (“time production”) of neutrons in supercritical (subcritical) systems and iterating to convergence
 - *Pseudo-dynamic α* : “Solves” the Boltzmann equation for a fixed background medium, evolving the neutron distribution to convergence *in time* over many *settle* cycles
- These static k_{eff} and α eigenvalues are calculated from iteration/cycle average values of the neutron production (P), absorption (A), leakage (L) and removal lifetime (τ_{rem}):

$$k_{eff} = \frac{\langle P \rangle}{\langle A \rangle + \langle L \rangle}$$

and

$$\alpha = \frac{\langle P \rangle}{\langle A \rangle + \langle L \rangle} - \frac{1}{\langle \tau_{rem} \rangle}$$

Monte Carlo Criticality Eigenvalue Algorithms



- A *dynamic* algorithm for calculating the α eigenvalue of a system is:
 - *Dynamic* α : Uses the separability of variables and fundamental mode ansatz to give α at cycle n :

$$\alpha = \frac{\Delta}{N(t^n)}$$

where $N(t^n)$ is the particle population at the end of cycle n

- Averaged quantities are employed in the calculation the static k_{eff} or α eigenvalues in order to reduce the stochastic noise by averaging over many settle iterations/cycles.
- The logarithm of the population ratio used in the calculation of the *dynamic* α eigenvalue can lead to increased stochastic noise. This occurs as Δ , which results in $\left(\begin{matrix} \\ \end{matrix} \right)$ and $\left(\begin{matrix} \\ \end{matrix} \right)$

Accuracy Considerations of Monte Carlo Calculations



- Since the Monte Carlo method does not solve the Boltzmann equation via use of numerical differences and quadratures, it does not incur many of the accuracy and stability limitations which are faced by deterministic methods such as S_N and P_N .
- However, there are several issues which need to be considered when modeling particle transport with the Monte Carlo method:
 - *Given enough particles* the Monte Carlo method is capable of sampling all of the seven-dimensional phase space
($x, y, z, \cos(\alpha), \cos(\beta), \cos(\gamma), E, t$)
(In this regard, there is no such concept as “enough particles”!)
 - Accurate modeling of collision interaction and flux attenuation requires zone spacings comparable to, or small than, a mean-free path length $\Delta x \leq \lambda_{mfp}$
 - The multigroup energy treatment limits the resolution of cross section resonances, which leads to inaccuracies in the calculation of resonant self-shielding
 - Approximations may be used when sampling the energy and angle of secondary particles emerging from collision events

Accuracy Considerations of Monte Carlo Calculations



- The number of simulation particles (N_{sim}) required for static k_{eff} or α eigenvalue calculations can be as low as 10^3 to 10^5 , since:
 - The production, removal and lifetime components used to calculate the eigenvalues are average over many settle iterations/cycles
 - Static eigenvalues are *global* quantities which *do not* require large per-zone particle counts
- The number of simulation particles (N_{sim}) required for time-dependent depletion calculations (such as a reactor depletion calculation) *must be significantly larger*, of order 10^5 to 10^9 , since:
 - Energy deposits and isotopic depletion/production require a sufficient number of particles per zone, or order 10 to 1000, in order to reduce stochastic fluctuations in those quantities

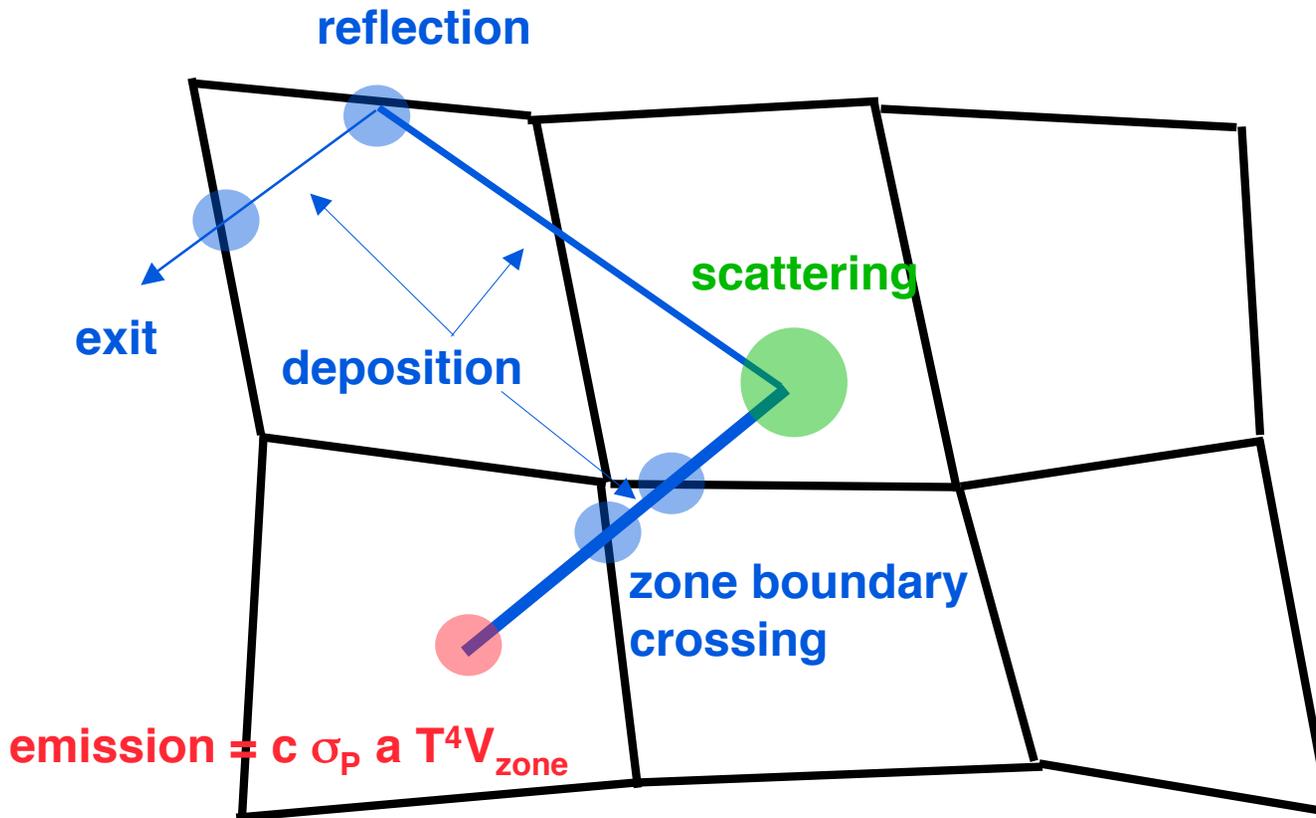
Monte Carlo solves transport equation by tracking particles which behave like photons



- The problem is cut up into a mesh as in hydrodynamics simulations
- Particles are created in zones from thermal or other sources
 - Initial positions, times and directions are sampled using random numbers
- Particles are tracked through mesh
- Particles deposit energy into matter at rate $\exp(-\sigma_a d_{path})$
- Particles scatter after traveling $d = -\ln(\text{random number} \in [0,1]) / \sigma_s$
 - new angle and frequency determined by sampling from scattering kernel

Random numbers are used in simulating photon position and scattering

Illustration of Monte Carlo Simulation



Random numbers are used in **emission** and **scattering**

- Photons are created with a position, energy and direction
- They are tracked to zone boundaries, where material properties change
- They proceed into the new zone in the same direction until they scatter or are reflected
- They deposit energy into the zones along their path
- They are tracked until their energy reaches a lower limit or they leave the mesh

The largest difference between photon and neutron Monte Carlo is coupling with matter



- Radiation and matter usually interact more strongly than neutrons
 - Matter emits radiation and cools $\sim T^4$ thermal source term
 - T^4 source term is very non-linear
 - Radiation is absorbed by matter, which heats it $\sim \sigma_a$
 - The photon mean free path is usually much shorter than neutron mean free path
- Matter-radiation coupling results in:
 - Stability problems from T^4 term
 - Numerical expense from many short photon paths
- Photons only move with speed c , not a range of speeds
 - This is unimportant; only effects tracking through mesh

Techniques for dealing with matter radiation coupling are the most important difference between photon and neutron codes

T⁴ coupling makes explicit solution for *I* difficult



- **The T⁴ source term makes the photon transport equation stiff**
 - **If we use time n value for T in a zone which changing rapidly, oscillations can occur**
- **We really want to use the future matter temperature in transport equation**
- **We have 3 choices:**
 - **Use small Δt so that T doesn't change much (Monte Carlo)**
 - **Solve equations implicitly: non-linear system (SIMC)**
 - **Cheat – use a guess for future matter temperature (IMC)**
- **Implicit Monte Carlo (IMC) is cheating**
 - **The energy equation is used to get a guess for T at time n+1**

Implicit Monte Carlo (IMC) is a way of avoiding solving multiple linear systems while still attaining stability

Radiation transport problems require the solution of 2 coupled equations for I and ϵ



- $I(\mathbf{x}, \Omega, t, \nu)$ = radiation specific intensity – cgs units erg/(cm² Hz str s)
- $\epsilon(\mathbf{x}, t)$ = matter energy density – cgs units erg/cm³

Scattering from/to direction Ω

$$\frac{1}{c} \frac{\partial I}{\partial t} + \Omega \cdot \nabla I = -(\sigma_s + \sigma_a) I + \frac{1}{4\pi} c \sigma_a a T^4 b(\nu, T) + \int \sigma_s I d\nu d\Omega + S_I$$

Photons are absorbed and heat matter

Matter radiates photons and loses energy

Photons stream in direction Ω with speed c

$$\frac{\partial \epsilon}{\partial t} = \int \sigma_a I d\nu d\Omega - \sigma_c a T^4 + S_\epsilon$$

- $\sigma_a(\mathbf{x}, t, \nu)$ = absorption opacity - cgs units cm⁻¹; σ_s = scattering opacity; σ_p = Planck mean opacity; $b(\nu, T)$ = normalized Planck function; S_I = photon sources(e.g, lasers); S_ϵ = thermal sources(e.g, chemical reactions);

Coupling between I and ϵ is through T^4 and σ_a terms

IMC uses estimate for future T from ϵ equation to estimate T^4 term in transport equation



- There are 3 steps in this procedure:
 1. The matter energy equation is manipulated to get an expression for the time derivative of T^4
 2. This derivative is approximated to get an expression for T^4 at the end of the time step in terms of current T , absorption, etc.
 - Note – expression – not a value
 3. This expression for T^4 is substituted into the transport equation and the matter energy equation
 - We end up with altered equations for I and ϵ , not the same equations with a different value for T
- The end result is new equations with some fraction of the absorption replaced by scattering, called “effective scattering”

The new equations for I and ϵ are (usually) more stable

1. Solve equation for time derivative of ε to get time derivative of aT^4



- First, define $\varepsilon_r \equiv aT^4$
- Use chain rule to get derivative $\frac{\partial \varepsilon_r}{\partial t} = \frac{\partial \varepsilon_r}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial t}$
- Use chain rule again

$$\frac{\partial \varepsilon_r}{\partial \varepsilon} = \frac{4aT^3 \frac{\partial T}{\partial t}}{\rho c_v \frac{\partial T}{\partial t}} = \frac{4aT^3}{\rho c_v} \equiv \beta$$

- This gives an equation for the time derivative of $\varepsilon_r = aT^4$:

$$\frac{\partial \varepsilon_r}{\partial t} = \beta \frac{\partial \varepsilon}{\partial t} = \beta \int \sigma_a I d\Omega dv - c\sigma_p \varepsilon_r + \beta S_\varepsilon$$

2. Use approximation for derivative of ε_r to approximate aT^4 at end of time step



- Estimate derivative of ε_r :

$$\frac{\varepsilon_r^{n+1} - \varepsilon_r^n}{\Delta t} \approx \beta \int \sigma_a I d\Omega d\nu - \beta c \sigma_p \varepsilon_r^{n+1} + \beta S_\varepsilon$$

- Solve for ε_r at time n+1 from

$$\varepsilon_r^{n+1} = \frac{1}{1 + \beta c \sigma_p \Delta t} \varepsilon_r^n + \frac{\beta c \Delta t}{1 + \beta c \sigma_p \Delta t} \int \sigma_a I d\Omega d\nu + \frac{1}{1 + \beta c \sigma_p \Delta t} \beta \Delta t S_\varepsilon$$

- Define “Fleck factor”

$$f = \frac{1}{1 + \beta c \sigma_p \Delta t}$$

This is the factor which multiplies the absorption opacity in the new transport equation

3. Use equation for $\epsilon_r = T^4$ at end of time step in aT^4 source term of transport equation



Transport equation becomes

$$\frac{1}{c} \frac{\partial I}{\partial t} + \Omega \cdot \nabla I = -(\sigma_s + \sigma_a)I + \frac{1}{4\pi} \int \sigma_a b_\nu aT^4 b(\nu, T) d\nu + \frac{1}{4\pi} (1-f) \sigma_a b(\nu, T) \int \sigma_a I d\nu d\Omega + \int \sigma_s I d\nu d\Omega + \frac{1}{4\pi} (1-f) \frac{\sigma_a b(\nu, T)}{\sigma_p} S_\epsilon + S_I$$

Emission reduced by f

Scattering with value (1-f) σ_a added

(1-f) of matter source appears as photons during the time step

3. (continued) Use expression for $\epsilon_r = T^4$ at end of time step in matter energy equation



Matter energy equation becomes

$$\frac{\partial \epsilon}{\partial t} = \int f \sigma_a I d\nu d\Omega - fc \sigma_a b_\nu a T^4 b(\nu, T)^n + f S_\epsilon$$

Absorption
reduced by f

Emission
reduced by f

Matter energy source
reduced by f

What is the result of all of this algebra?



- Transport equation has absorption and thermal emission term multiplied by fraction f in $[0,1]$
- Effective scattering is added, with opacity $(1-f)\sigma_a$
- Matter energy equation also has absorption and emission reduced
- $(1-f)$ of the material energy source appears as photons

- Effect is that
 - A fraction $(1-f)$ of absorption and emission has been replaced by scattering
 - A fraction $(1-f)$ of the material energy source now goes into radiation

What does this correspond to physically?

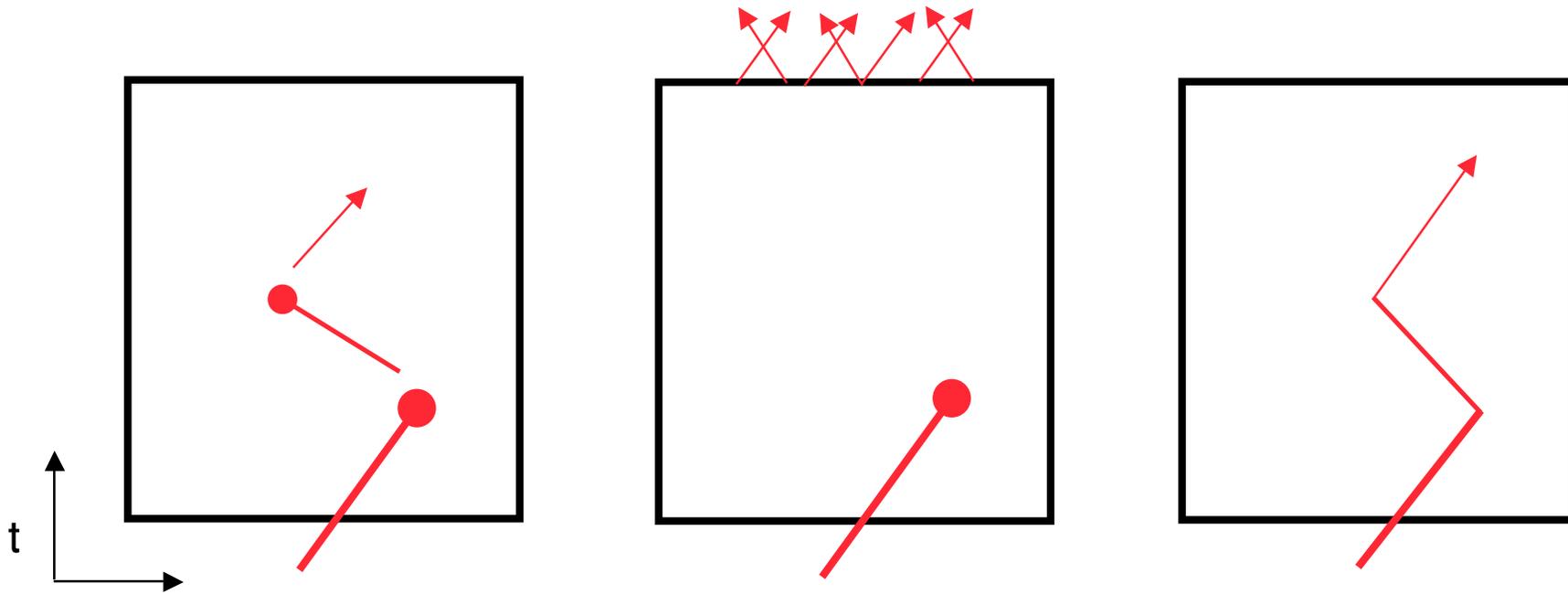


- In reality, absorption heats material, which then reemits and cools
- We don't know the correct future T at which emission occur, so we underestimate the emission
- By replacing some absorption with scattering, we simulate the reemission, even though we still don't know the future T

- Matter energy source heats material, which should radiate
- We can't simulate that until next time step, when T changes
- Putting some of this energy directly into photons allows us to simulate that emission in the current time step

Effective scattering imitates the physical process of absorption and nearby re-emission during a time step

Effective scattering approximates physical emission and absorption during a time step



Physics:

- photons enter cold zone and heat it
- hot matter near absorption events radiates new photons
- zone temperature rises continuously and smoothly

Monte Carlo:

- photons enter cold zone and heat it
- zone doesn't radiate until next time step
- zone temperature rises too much
- possible instability

Implicit Monte Carlo:

- photons enter cold zone and heat it
- Physical radiation from hot matter near absorption is simulated by scattering existing photons
- zone temperature changes more smoothly

IMC behaves differently in limits of large and small f



- When $f \approx 1$, IMC converges to MC
 - Large c_v : $f \approx 1$ when T is slowly varying
 - small σ_p : $f \approx 1$ when very little radiation is absorbed
 - When Δt is small, $f \approx 1$, and IMC becomes MC
- $f \approx 0$ implies lots of effective scatters
 - $f \approx 0$ occurs when c_v small and/or σ_p large and/or Δt large
 - Photons lose little energy because $f\sigma_a$ is small
 - Calculation becomes expensive because photons take many expensive trajectories as they execute many effective scatters without depositing much energy

IMC “stability” comes at the cost of increased cycle times in problems with $f \approx 0$ – usually when σ is large

When IMC works well, and when it doesn't



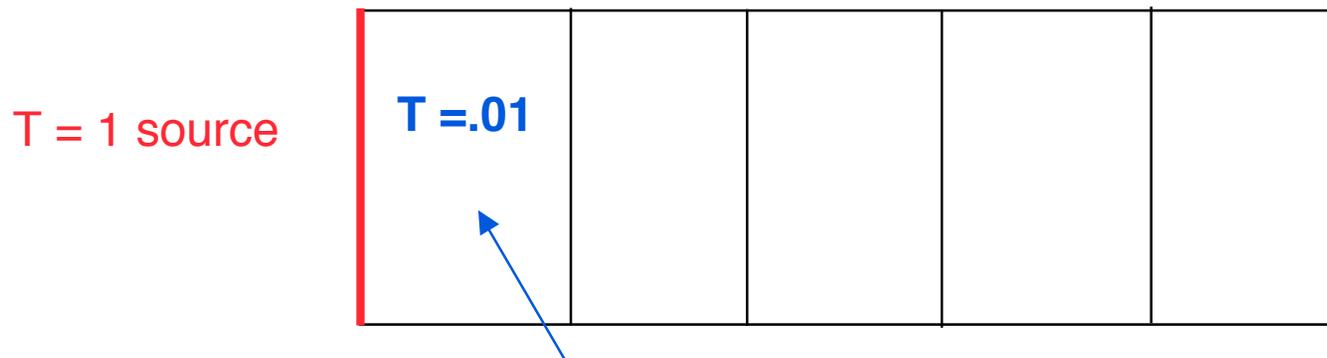
- **IMC is useful when most of problem has $f \cong 1$**
 - This happens when most material is not opaque
 - Even a small opaque region requires small Δt in MC
 - IMC runs slowly in opaque regions, but Δt can be larger everywhere
- **IMC is expensive when $f \cong 0$ in most of problem**
 - When much of material is opaque, or c_v is small
 - Almost all absorption is replaced with effective scatters
 - photons that would be absorbed scatter instead
 - They take many expensive trajectories

IMC “stability” comes at the cost of increased cycle times in problems with large amounts of opaque material

Cold matter heated by temperature source illustrates behavior of IMC vs. MC

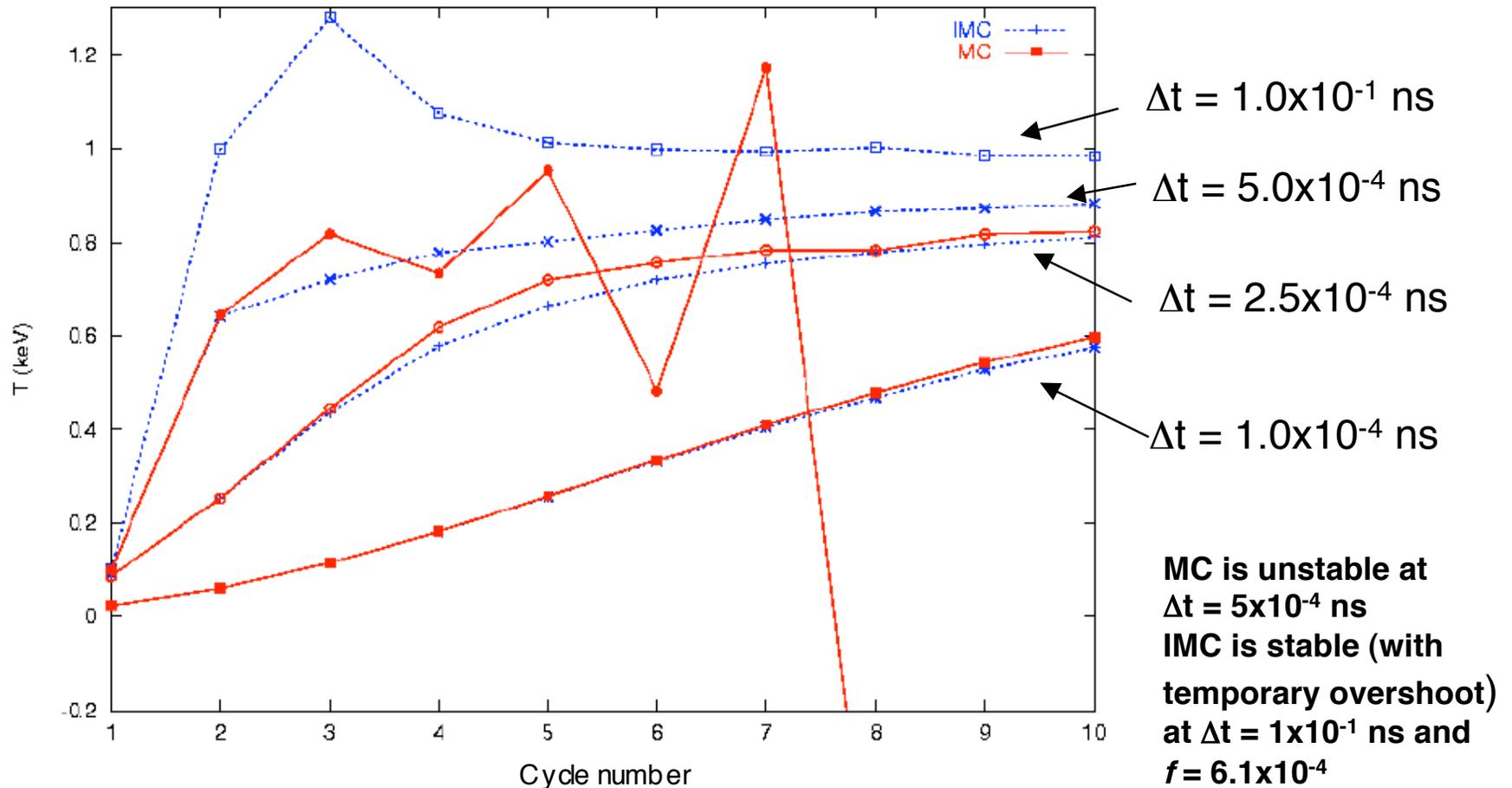


- Material with initial T of .01 keV heated with source of T = 1.0 keV
- Equation of state is ideal gas with $c_v = 10^{14} \text{ erg cm}^{-3} \text{ keV}^{-1}$, $\sigma = 100 \text{ cm}^{-1}$
- 200 zones with $\Delta x = .01 \text{ cm}$
- Using 10000 photons with IMC and MC
- Diagnostic is T vs. cycle number in first zone for various time steps



Look at T in first zone as time advances

Implicit Monte Carlo allows a much larger time steps than MC on this opaque problem

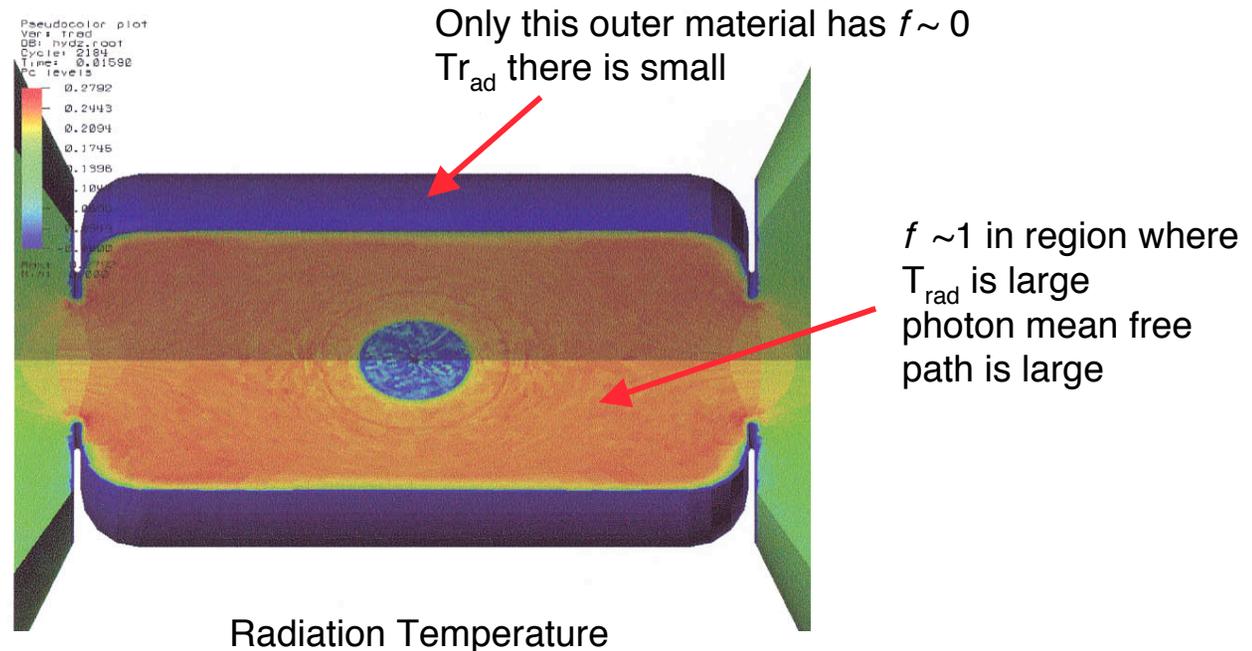


IMC runs with Δt over 500 times larger than MC on this problem



IMC is useful for ICF simulations

- Large mean free path in most of problem makes diffusion inaccurate
- Only a small amount of dense, opaque matter, so effective scattering is small in most places

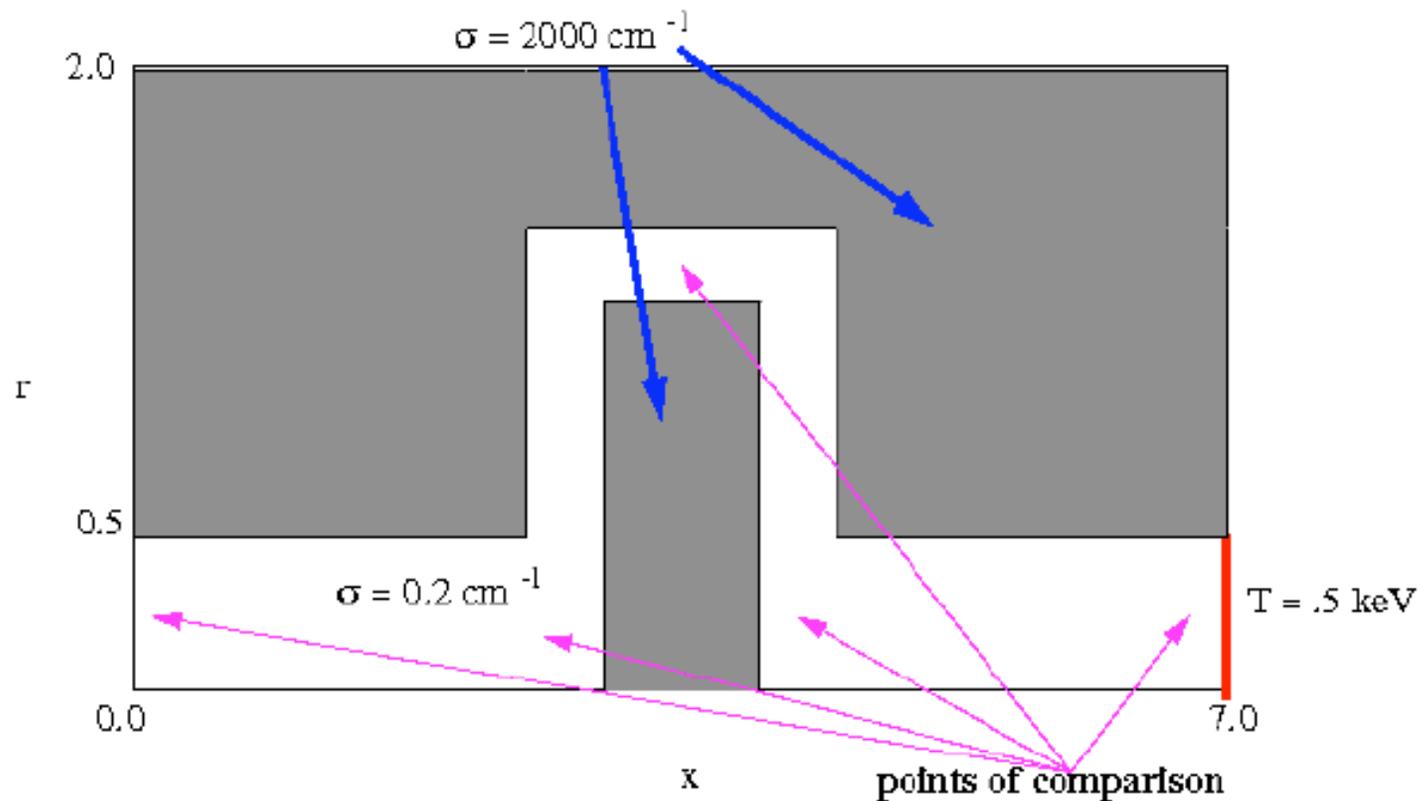


Implicit Monte Carlo is accurate and fast for simulations with large mean free paths in most zones

Crooked pipe test has opaque regions near source and large Δt so f is ~ 0 in a lot of material



• Graziani and LeBlanc, UCRL-MI-143393 (2000)



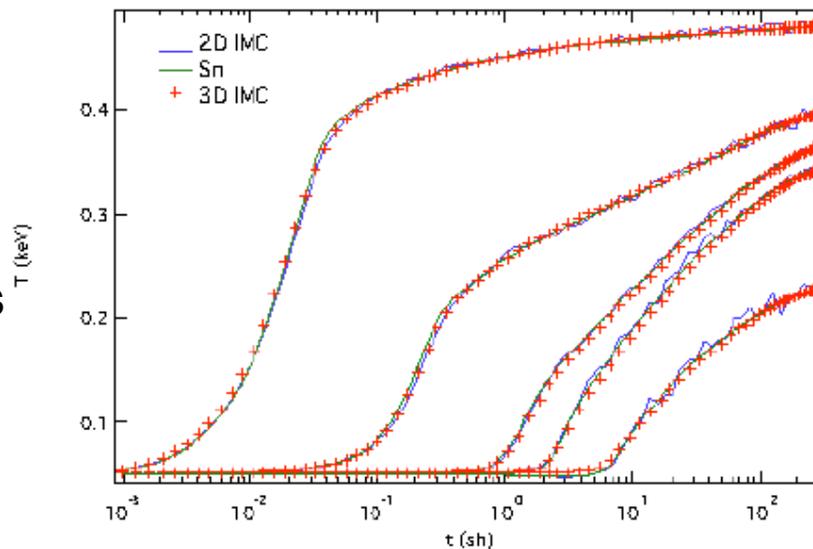
Heat flows around corners through optically thin region

Crooked pipe test illustrates slow IMC run times



- IMC gets correct answer
- Run time is long:
 - 6 days on one proc
- This happens because
 - Large amounts of opaque material heats
 - Δt is large since problem runs to $t > 100$
- This makes $f \sim 0$ in many zones

Matter Temperature vs. time for 5 points in Crooked Pipe



IMC is accurate but simulation takes a long time when much of problem is hot and opaque ($f \sim 0$)

IMC run times in opaque systems can be improved by using the diffusion equation



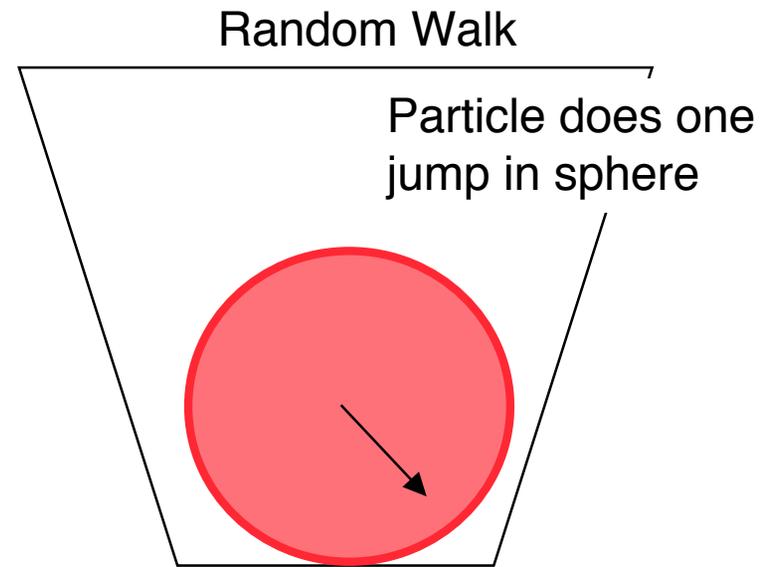
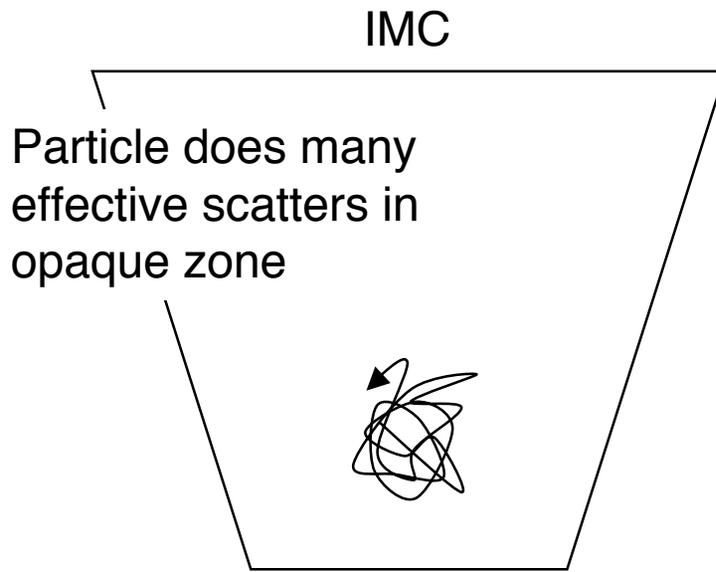
- If there are many effective scatters in a zone, the photons execute random walks, losing all angular information
- In that case, the diffusion equation is a good approximation to the transport equation
- We can use solutions to the diffusion equation to accelerate IMC
- “Random Walk” – Fleck and Canfield, J. Comput. Phys 54, 508 (1984)
 - Advance selected particles inside a zone with local solution of diffusion equation
- Hybrid techniques
 - Solve diffusion equation in opaque regions of the problem, and IMC in others (see Gentile, J. Comput. Phys 172, 543 for a summary)

Diffusion is used where IMC is slow, and IMC is used where transport is necessary for correct answer (where IMC is fast enough)

“Random Walk” procedure advances individual particles inside of a zone



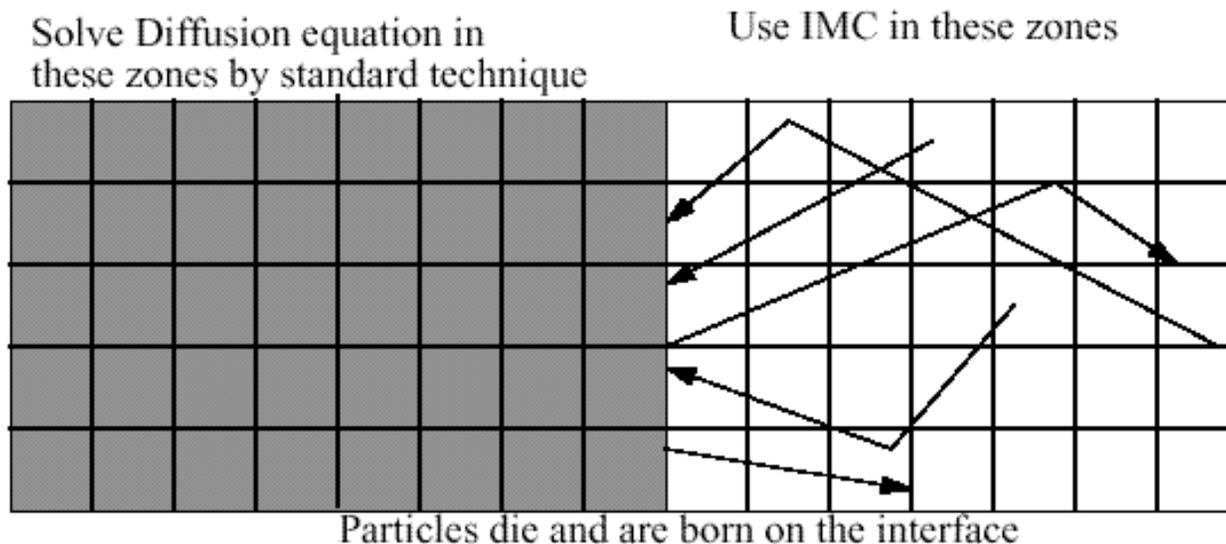
- Inscribe a sphere centered on particle in a zone
- Use analytic series solution of diffusion equation on sphere to get a probability for new particle position
- This turns many effective scatters into one jump
- But it is more computationally expensive than calculating a particle track, so it is only worth doing in very highly scattering problems



Hybrid Methods split up problem into diffusion and IMC regions



- Hybrid methods use diffusion equation in parts of problem where effective scattering opacity is large
- Energy from IMC particles entering diffusion region are converted into an approximate boundary flux for diffusion boundary condition
- Solution of diffusion equation gives a flux of particles into IMC region
- Coupling is approximate and instabilities can occur



Difficulties with IMC



- **Random Walk and hybrid methods have drawbacks**
 - Random Walk only speeds up particles far away from zone boundaries in very opaque zones
 - Hybrid methods are difficult to implement and sometimes inaccurate because IMC and diffusion treat boundaries differently
- **Teleportation error – photons heat one end of a zone, but aT^4 source term creates thermal photons everywhere in the zone**
 - Can cause unphysically fast transfer of energy through zones
- **Domain Decomposition for parallel runs has bad load balance**
 - If only one part of a problem is hot, all the work is there
 - Other processors contribute nothing
 - See Brunner, Urbatsch, Evans, Gentile, this conference

IMC is an active research area

Symbolic IMC (SIMC) produces an implicit solution for the temperatures



- The updated temperatures T_i remains unspecified
- Photons emitted in zone i during a timestep are tracked using unknown (symbolic) weights proportional to T_i^4
- A non-linear set of equations coupling all zones results
 - Bandwidth is governed by $c\Delta t$ and τ_ν

Advantages

- No linearization error
- (Almost) fully implicit => very stable

Disadvantages

- Requires full (NxN) matrix solve

E.D. Brooks III, JCP 83 (1989) 433

T. N'kaoua, SIAM J. Sci. Stat. Comput. 12 (1991) 505

The difference formulation for radiation transport



- Transport equation (without scattering)

$$\frac{1}{c} \frac{\partial I}{\partial t} + \Omega \cdot \nabla I = -\sigma_a (I - B) \quad \frac{\partial \varepsilon}{\partial t} = \int \sigma_a (I - B) d\nu d\Omega + S_\varepsilon$$

- Define the difference intensity

$$D(\mathbf{x}, t; \nu, \Omega) \equiv I(\mathbf{x}, t; \nu, \Omega) - B(\nu, T(\mathbf{x}, t))$$

- Transport equation for the difference intensity

$$\frac{1}{c} \frac{\partial D}{\partial t} + \Omega \cdot \nabla D = -\sigma_a D - \frac{1}{c} \frac{\partial B}{\partial t} + \Omega \cdot \nabla B \quad \frac{\partial \varepsilon}{\partial t} = \int \sigma_a D d\nu d\Omega + S_\varepsilon$$

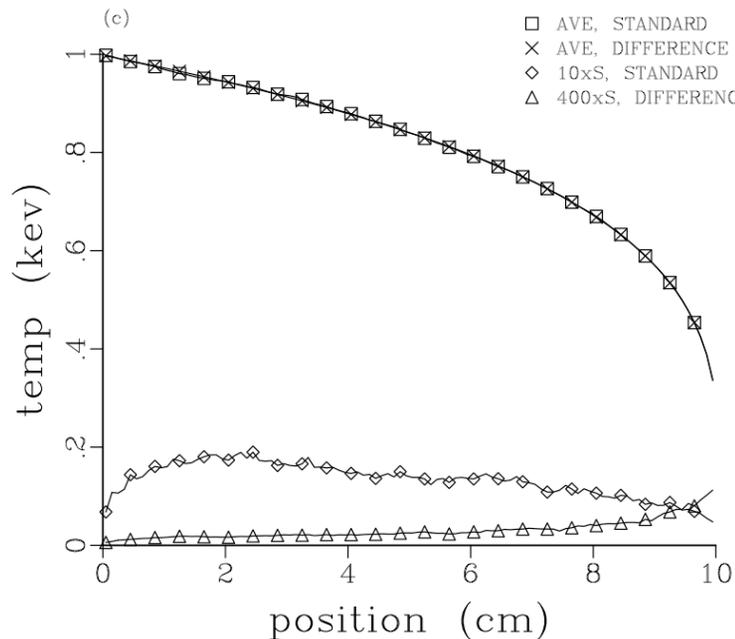
- In a thick, thermalized system $D \rightarrow 0$

The transformed equation contains only terms that are small and slowly varying in thick media

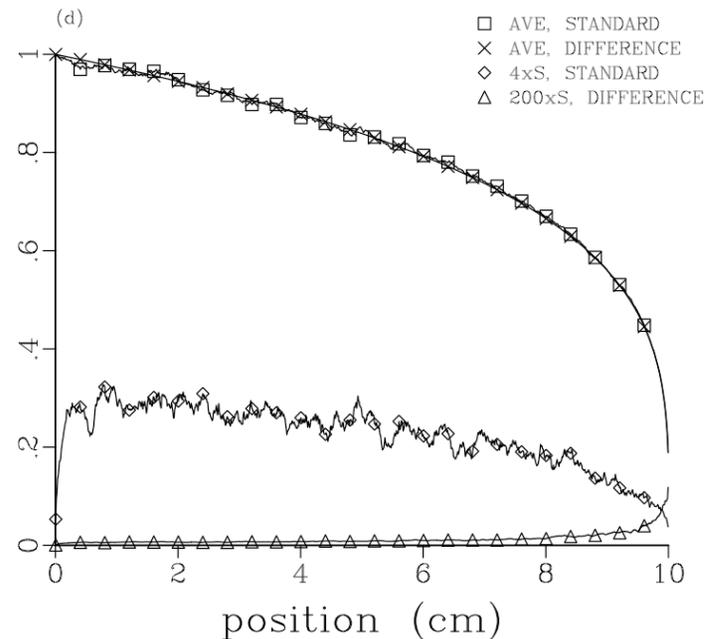
The difference formulation decreases noise dramatically in thick regions



- Test problem: slab heated from one side
- Implemented using SIMC for transport
- Comparison of temperatures and standard deviations



$\tau=100$

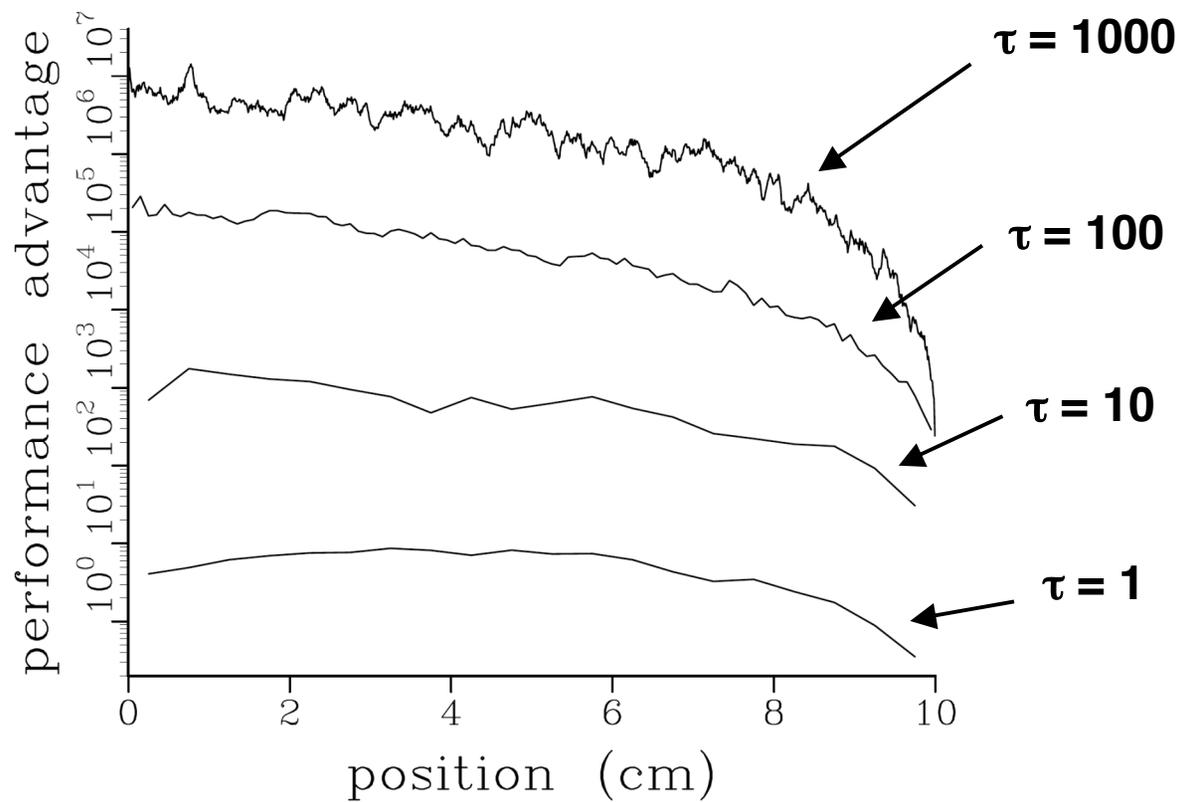


$\tau=1000$

Performance advantage at $\tau=1,10,100,1000$



$$PA = \sqrt{\frac{\sigma(\text{standard})}{\sigma(\text{difference})}}$$



Notes on the difference formulation



- **Rigorously equivalent to standard formulation**
 - similar boundary conditions
 - includes scattering
- **Rapid frequency variations appear only in opacity, not in source terms**
- **Has been formulated for non-LTE (2 level) system**
- **Suffers from same discretization errors as the standard formulation, e.g., teleportation**
- **Developed in SIMC with non-linear solution for temperatures smoothness**
 - **IMC version now being developed using minimum of initial zone temperatures from surrounding zones to get the T used in B(T) derivative sources**

A. Szoke and E.D. Brooks III, JQSRT 91 (2005) 95
E.D. Brooks III *et al*, JCP 205 (2005) 734

The difference formulation with IMC



- Less accurate, but avoids non-linear solution needed in SIMC
 - Answer is smoother than IMC for same number of particles

