A Hybrid Transport-Diffusion Method for Monte Carlo Radiative Transfer Simulations

Jeffery D. Densmore, Todd J. Urbatsch,

Thomas M. Evans, and Michael W. Buksas

Los Alamos National Laboratory

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Implicit Monte Carlo

Within a time step, the transport equation governing the Implicit Monte Carlo (IMC) method for grey, slab-geometry, radiative transfer problems is

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial x} + \sigma_n I = \frac{1}{2}(1-f_n)\sigma_n \int_{-1}^{1} I(x,\mu',t)d\mu' + \frac{1}{2}f_n\sigma_n acT_n^4 \quad , \tag{1}$$

where the *Fleck factor* f_n is given by

$$f_n = \frac{1}{1+\beta_n c\sigma_n \Delta t_n} \quad , \tag{2}$$

and

$$\beta_n = \frac{4aT_n^3}{C_{v,n}} \quad . \tag{3}$$

Difficulties with IMC

The IMC method uses an effective-scatter process to approximate absorption and emission of radiation within a time step.

- The physical opacity σ_n is divided into an isotropic scattering opacity $(1 - f_n)\sigma_n$ and an absorption opacity $f_n\sigma_n$.
- Effective scattering helps stabilize the calculation, allowing the use of larger time steps.

However, as the opacity increases, standard Monte Carlo becomes inefficient.

- The mean-free path between collisions is small.
- Collisions are primarily scattering events.
- The Monte Carlo transport process can be characterized as *diffusive*.
- Particles histories are extremely long.

Discrete Diffusion Monte Carlo

Discrete Diffusion Monte Carlo (DDMC) is a hybrid transport-diffusion method for increasing the efficiency of Monte Carlo simulations in diffusive media.

- DDMC is used in diffusive regions, while standard Monte Carlo is employed in transport (i.e. optically thin) regions.
- DDMC particles take discrete steps between spatial cells according to a discretized diffusion equation.
- Each DDMC step replaces several small transport steps, and thus DDMC is more efficient than a pure standard Monte Carlo simulation.
- Since DDMC is based on the diffusion approximation, this hybrid technique should provide accurate results.

Improvements to DDMC

We extend previously developed DDMC methods in several ways that improve the accuracy and utility of DDMC for IMC calculations.

- We use a diffusion equation that is discretized in space but is continuous in time.
  - theoretically more accurate than temporally discretized implementations
  - particle time is always known
  - no ambiguity regarding what time to assign a DDMC particle that leaves a diffusive region and is converted into a Monte Carlo particle

Improvements to DDMC (continued)

- We employ an improved technique for interfacing DDMC and Monte Carlo simulations.
  - used for converting DDMC particles into Monte Carlo particles, and vice versa
  - based on the asymptotic diffusion-limit boundary condition
  - produces accurate results regardless of the angular distribution of Monte Carlo particles incident on the diffusive region
- We develop a method for estimating momentum deposition in DDMC.
  - required in coupled radiation-hydrodynamics calculations to correctly determine fluid motion

Interior Cells

We consider a region $X_L < x < X_R$ that has been designated for simulation by DDMC, and subdivide it into a spatial grid of J cells. We then derive a discretized diffusion approximation to the IMC transport equation for interior cells $2 \leq j \leq J-1$,

$$\frac{1}{c}\frac{d}{dt}\phi_j + \left(\sigma_{L,j} + \sigma_{R,j} + f_{n,j}\sigma_{n,j}\right)\phi_j = f_{n,j}\sigma_{n,j} acT_{n,j}^4 + \frac{1}{\Delta x_j}\left(\sigma_{L,j+1}\phi_{j+1}\Delta x_{j+1} + \sigma_{R,j-1}\phi_{j-1}\Delta x_{j-1}\right) \quad , \tag{4}$$

where

$$\sigma_{L,j} = \frac{2}{3\Delta x_j}\frac{1}{\sigma_{n,j}\Delta x_j + \sigma_{n,j-1}\Delta x_{j-1}} \quad , \tag{5}$$

and

$$\sigma_{R,j} = \frac{2}{3\Delta x_j}\frac{1}{\sigma_{n,j}\Delta x_j + \sigma_{n,j+1}\Delta x_{j+1}} \quad . \tag{6}$$

Interior Cells (continued)

The DDMC equation for interior cells can be viewed as a time-dependent, infinite medium transport problem in each cell.

- Particles have no angular or spatial information, but their current cell and time are always known.
- Particles stream in time (but not in space) at the speed of light.
- Particles experience not only absorption reactions, but also "left-leakage" and "right-leakage" reactions.
- Particles that undergo leakage reactions are transfered to the appropriate neighboring cell.
- The source term consists of not only the usual emission source, but also particles experiencing leakage reactions in neighboring cells.

Asymptotic Diffusion-Limit Boundary Condition

The asymptotic diffusion-limit boundary condition at $x = X_L$ is

$$2\int_0^1 W(\mu) I_b(X_L, \mu, t) d\mu = \phi(X_L, t) - \frac{\lambda}{\sigma_n} \frac{\partial \phi}{\partial x}\bigg|_{x=X_L} \quad , \tag{7}$$

where $W(\mu)$ is a transcendental function well approximated by

$$W(\mu) \approx \mu + \frac{3}{2}\mu^2 \quad , \tag{8}$$

and I_b is the incident intensity.

This boundary condition has several advantageous properties.

- It can be derived in an asymptotic analysis of the IMC transport equation as σ_n becomes large and f_n vanishes. This is exactly the situation where DDMC is employed.
- It produces an accurate interior solution regardless of the angular distribution of the incident intensity.

Interface Method

We now develop an interface method based on the asymptotic diffusion-limit boundary condition. This is equivalent to deriving a cell-centered equation for cell 1:

$$\frac{1}{c}\frac{d}{dt}\phi_1 + \left(\sigma_{L,1} + \sigma_{R,1} + f_{n,1}\sigma_{n,1}\right)\phi_1 = f_{n,1}\sigma_{n,1} a c T_{n,1}^4 + \frac{1}{\Delta x_1}\left(\sigma_{L,2}\phi_2\Delta x_2 + \int_0^1 P(\mu)\mu I_b(X_L,\mu,t)d\mu\right) \quad , \qquad (9)$$

where

$$\sigma_{L,1} = \frac{1}{\Delta x_1}\frac{2}{3\sigma_{n,1}\Delta x_1 + 6\lambda} \quad , \qquad (10)$$

and

$$P(\mu) = \frac{4}{3\sigma_{n,1}\Delta x_1 + 6\lambda}\left(1 + \frac{3}{2}\mu\right) \quad . \qquad (11)$$

Interface Method (continued)

The DDMC equation for cell 1 has a Monte Carlo interpretation similar to the equation for interior cells.

- The expression for the left-leakage opacity is different.
- The rate at which radiation energy is incident on the DDMC region for a given direction μ is $\mu I_b(\mu)$. Thus, the probability that an incident Monte Carlo particle will be converted into a DDMC particle is $P(\mu)$.
- Converted Monte Carlo particles begin transporting via DDMC in cell 1.
- Unconverted Monte Carlo particles and leaked DDMC particles are placed isotropically on the DDMC region boundary.

Momentum Deposition

The specific momentum deposition (i.e. the momentum deposited per unit volume per unit time) is given by

$$p(x,t) = \frac{\sigma}{c}\int_{-1}^{1} \mu I(\mu,x,t)d\mu \quad . \tag{12}$$

Using the flux at each cell edge,

$$F(x_{j+1/2},t) = \int_{-1}^{1} \mu I(x_{j+1/2},\mu,t)d\mu \quad , \tag{13}$$

we can estimate the specific momentum deposition in each cell using the rate at which DDMC particles travel between cells,

$$p_j = \frac{1}{2}\frac{\sigma_{n,j}}{c}\left(F_{j+1/2} + F_{j-1/2}\right) \quad . \tag{14}$$

Numerical Results

We now examine two problems with both optically thick and optically thin regions. We employ standard Monte Carlo in the optically thin region, and either standard Monte Carlo or DDMC in the optically thick region.

First Problem:

- This problem is driven by an isotropic surface source on the left boundary.
- The left-most region is 0.1 cm of optically thick material, followed by a 0.4 cm optically thin region.
- The DDMC simulation was approximately 20 times faster than standard Monte Carlo.

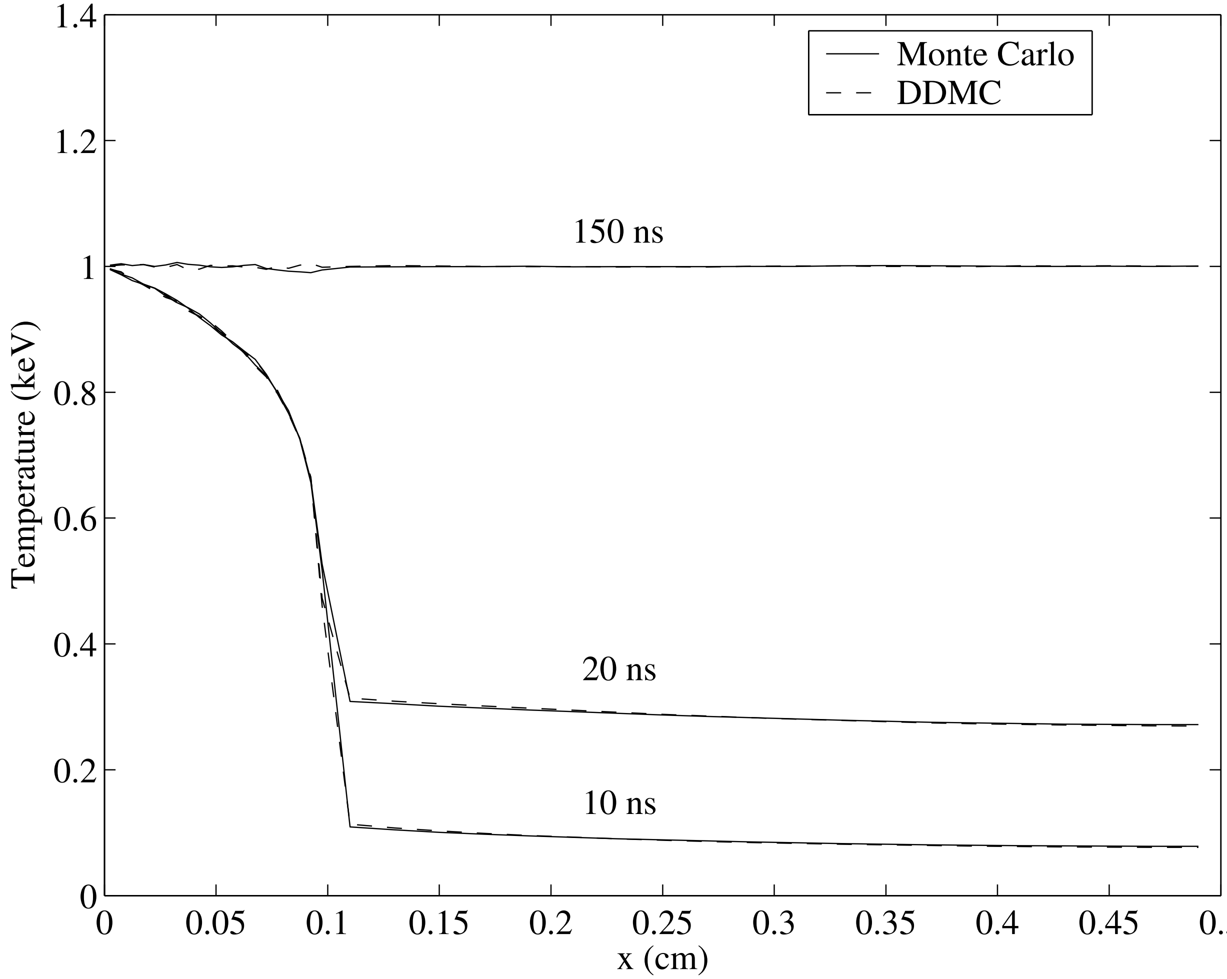

Figure 1: First Problem Material Temperature

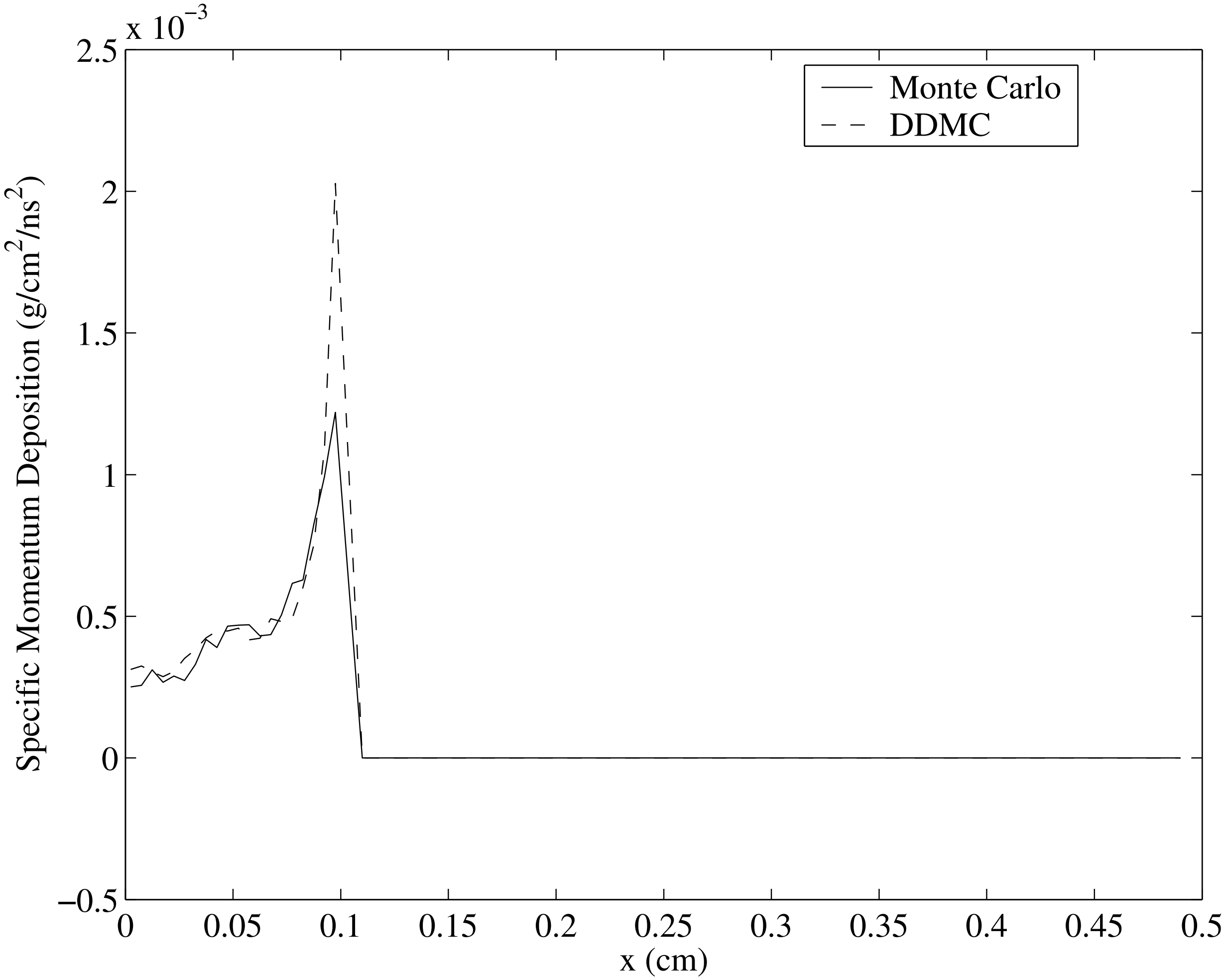

Figure 2: First Problem Momentum Deposition at 10 ns

Numerical Results (continued)

Second Problem:

- This problem is driven by a normal surface source on the left boundary.
- The left-most region is 1.0 cm of optically thin material, followed by a 0.5 cm optically thick region.
- The radiation reaching the optically thick region is fairly anisotropic. Thus, using our improved interface method is important.
- The DDMC simulation was approximately 13 times faster than standard Monte Carlo.

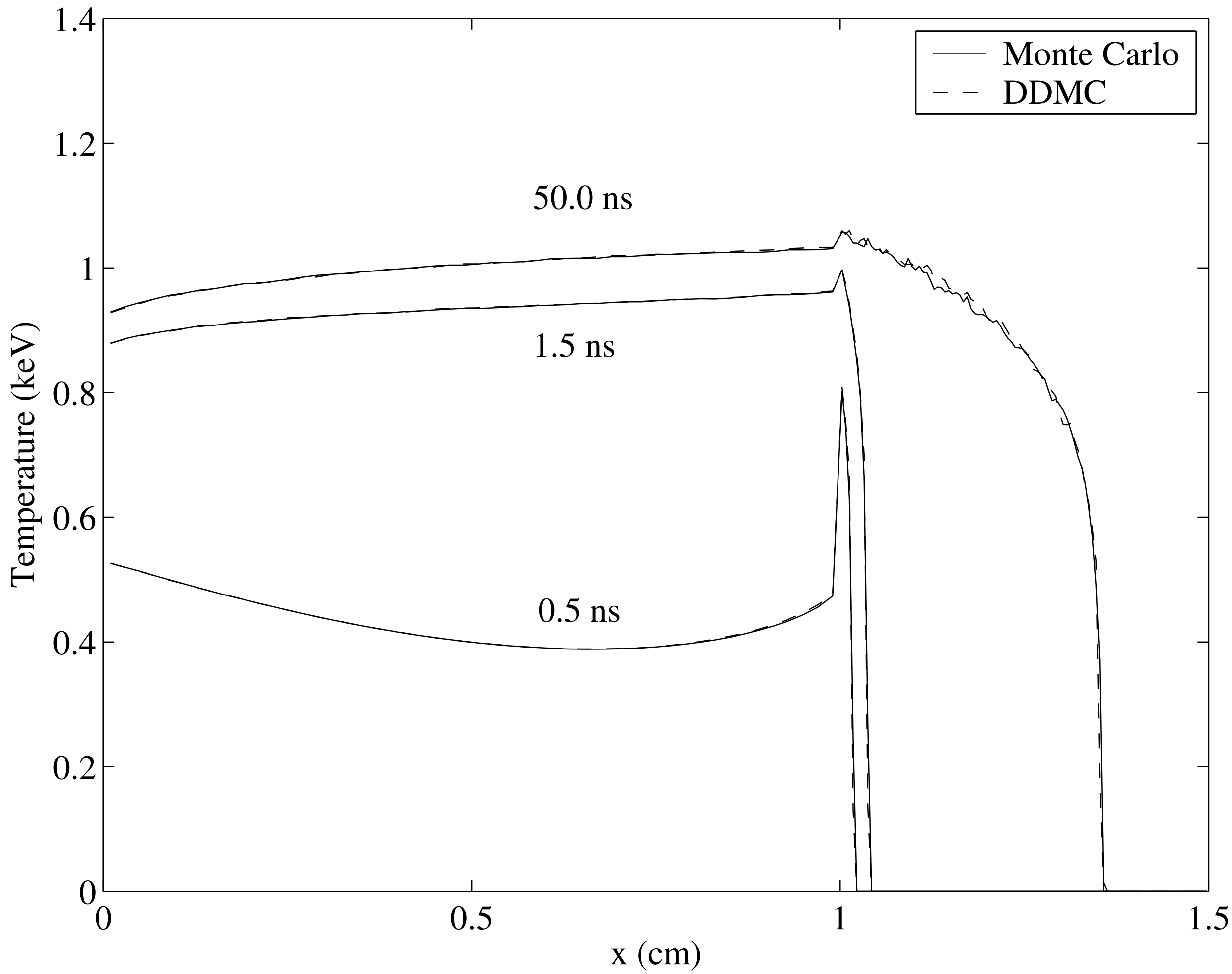

Figure 3: Second Problem Material Temperature

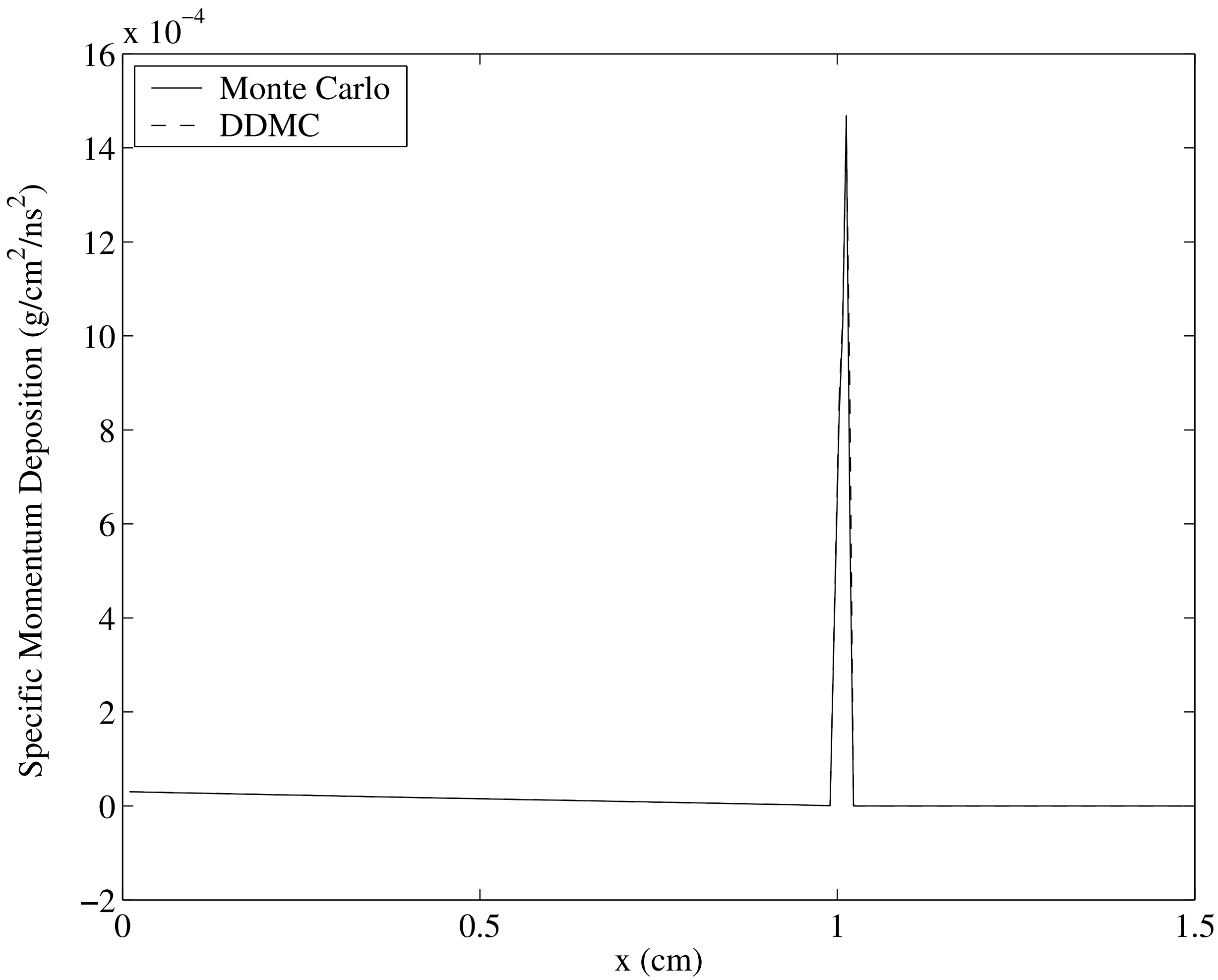

Figure 4: Second Problem Momentum Deposition at 0.5 ns

Conclusions

We have extended previously developed DDMC methods in several ways that improve the accuracy and utility of DDMC for grey IMC calculations.

- We base our method on a temporally continuous diffusion equation.
- We use an interface technique that is derived from the asymptotic diffusion-limit boundary condition.
- We have developed a method for estimating momentum deposition during the DDMC simulation.

Conclusions (continued)

However, several issues remain for future work.

- The statistical error in momentum deposition estimates must be reduced, both for DDMC and standard Monte Carlo.
- We must be able to determine when and where to employ DDMC *a priori*.
- Our improved DDMC method must be extended to frequency-dependent, multi-dimensional simulations.