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research note

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Subject: 1-D Equilibrium Discrete Diffusion Monte Carlo

Executive Summary

We present a derivation and a demonstration of the Equilibrium Discrete Diffusion Monte Carlo (EqDDMC) method for 1-D diffusion problems in which the radiation field coexists with matter in local thermodynamic equilibrium. Our goal is to demonstrate the efficacy of the EqDDMC method on simple slab problems as a first step toward applying Discrete Diffusion Monte Carlo to non-equilibrium diffusion.

1. Introduction

Urbatsch, Morel and Gulick [1,2] have developed a spatially discretized, hybrid diffusion Monte Carlo method for neutronics calculations. This method has been called Discrete Diffusion Monte Carlo (DDMC). The general description of this method is that Monte Carlo particles traverse discrete space according to a single-cell, deterministic, diffusion solution. The intent has always been to apply this method to diffusive regions of thermal radiative transfer problems. In particular, we have hypothesized that this method could prove to be an effective replacement for the Random Walk method [3] in Implicit Monte Carlo [4]. This study represents the first effort at applying the DDMC method to radiative transfer problems.

In this research note, we derive an Equilibrium Discrete Diffusion Monte Carlo (EqDDMC) method and demonstrate its properties on simple slab problems. This study foreshadows the development of multidimensional DDMC in general thermal radiation-hydrodynamics problems.

2. The Equilibrium Diffusion Equations

Morel, Wareing, and Smith [5] have derived asymptotically the equilibrium diffusion equation,

$$(C_v + 4aT^3)\frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\frac{4acT^3}{3\sigma_{\mathrm{R}}}\frac{\partial T}{\partial x} = 0 \,, \tag{1}$$

where $C_v \equiv C_v(x, T(x,t))$ [jerks $\cdot$ cm^{-3} $\cdot$ keV^{-1}] is the specific heat capacity of the material, $a = 0.01372$ [jerks $\cdot$ cm^{-3} $\cdot$ keV^{-4}] is the radiation constant, $c = 299.79$ [cm $\cdot$ sh^{-1}] is the vacuum light speed, and $T \equiv T(x,t)$ [keV] is the temperature that characterizes both the radiation and the material. The opacity, $\sigma_{\mathrm{R}} \equiv \sigma_{\mathrm{R}}(x, T(x,t))$ [cm^{-1}], is the Rosseland Mean opacity. Equation (1) is defined without external sources. Additionally, we can define a diffusion coefficient, $D \equiv D(x, T(x,t))$ [cm],

as follows,

$$D = \frac{1}{3\sigma_{\mathrm{R}}} \ .$$

(2)

The left-most term in Eq. (1) represents the radiation-material coupling. The equation is non-linear in temperature, both from terms containing T explicitly and implicitly through σ_{R} and C_v.

The diffusion approximation results by assuming that the radiation intensity, ψ, is linear in angle such that the first two angular moments of the radiation intensity are conserved,

$$\psi(x,\nu,\mu,t) \rightarrow \frac{1}{2}[\phi(x,\nu,t) + 3\mu F(x,\nu,t)] \ ,$$

(3)

where $\phi(x,\nu,t)$ is the scalar radiation intensity and $F(x,\nu,t)$ is the radiation flux, defined as the zeroth and first angular moments, respectively, of the radiation intensity,

$$\phi(x,\nu,t) = \int_{-1}^{1} \psi(x,\nu,\mu,t)d\mu \ ,$$

(4a)

$$F(x,\nu,t) = \int_{-1}^{1} \mu\psi(x,\nu,\mu,t)d\mu \ .$$

(4b)

When the radiation field coexists with matter in complete thermodynamic equilibrium at temperature T, the radiation intensity is independent of space, direction, and time, and is given by the Planck function

$$\psi(\nu) = B(\nu,T) \ .$$

(5)

The Planck function (or Planckian) is defined as,

$$B(\nu,T) = \frac{2h\nu^3}{c^2}\left(e^{\frac{h\nu}{kT}} - 1\right)^{-1} \ ,$$

(6)

where h is Planck's constant and k is the Boltzmann constant.

In *local* thermodynamic equilibrium (LTE), when gradients are small over characteristic lengths and time (a condition that is valid in the diffusion approximation), the radiation intensity can be written as (see [6], p.328)

$$\psi(x,\nu,t) = B(\nu,T) \ ,$$

(7)

where $T \equiv T(x,t)$. The assumption of LTE will continue to hold through the remainder of this note.

Using Eqs. (4) and (7), we define the gray (*i.e.*, integrated over all photon frequencies ν) scalar radiation intensity; this links the scalar intensity to the fourth power of the temperature,

$$\phi(x,t) = \int_{\nu} 4\pi B(\nu,T)d\nu$$
$$= acT^4 \ .$$

(8)

The Marshak boundary condition [7] suffices for this work,

$$4F^{(-)}(x) = \phi(x) + \frac{2}{3\sigma_{\mathrm{R}}}\frac{d\phi(x)}{dx}\mathbf{n}\cdot\mathbf{i} \, . \tag{9}$$

We consider the incoming partial flux for three specific conditions: (1) if the boundary condition is reflecting, the incoming partial flux is equal to the outgoing partial flux; (2) if the boundary condition is vacuum, the incoming partial flux is zero; (3) if the boundary condition is defined by a black body at temperature T_B at the boundary, the incoming intensity is Planckian and the incoming partial flux is σT_B^4 [6], where $\sigma = \frac{1}{4}ac$ is the Stefan-Boltzmann constant. In summary,

$$F^{(-)} = \begin{cases} F^{(+)} & \text{reflecting} \\ 0 & \text{vacuum} \\ \sigma T_B^4 & \text{black body} \end{cases} . \tag{10}$$

Finally, Fick's Law relates the radiation flux and the gray scalar radiation intensity,

$$F(x,t) = -D\frac{\partial\phi(x,t)}{\partial x} \, . \tag{11}$$

Fick's law will be used extensively in the derivation that follows in § 3.1.

In what follows, we shall define Eq. (1) in terms of T^4 instead of T. Thus, using the transform

$$\partial T = \frac{1}{4acT^3}\partial\phi \, , \tag{12}$$

we write Eq. (1) in the following form,

$$\left(\frac{C_v}{4acT^3} + \frac{1}{c}\right)\frac{\partial\phi}{\partial t} - \frac{\partial}{\partial x}D\frac{\partial\phi}{\partial x} = 0 \, , \tag{13}$$

whereby Eq. (1) is transformed into a 1-D equilibrium diffusion equation for the gray scalar radiation intensity. Equation (13) will be used in the following section to derive the 1-D EqDDMC method.

3. 1-D EqDDMC Method

In this section we shall derive the EqDDMC method. The first part will consist of deriving the 1-D EqDDMC equation from the equilibrium diffusion equation, Eq. (13), given in § (2). The second part will describe the Monte Carlo implementation of the method.

3.1. 1-D EqDDMC Equations

Equation (13) must be linearized before it can be solved with standard Monte Carlo techniques. We shall linearize the equilibrium diffusion equation by using the following time discretization,

$$\left(\frac{C_v^n}{4acT^{n\,3}} + \frac{1}{c}\right)\frac{\phi^{n+1} - \phi^n}{\Delta t} - \frac{d}{dx}D^n\frac{d\phi^{n+1}}{dx} = 0 \tag{14}$$
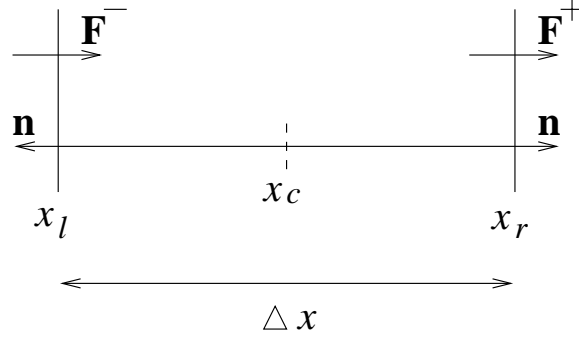
FIG. 1: Spatially discretized cell. Fluxes superscripted by a (-) sign are incoming, and fluxes superscripted by a (+) sign are outgoing.

and by evaluating T^3, C_v, and D at the beginning of the timestep, t^n. Thus, Eq. (14) is time-implicit in ϕ, but it is time-explicit in T^3, C_v, and D. Also, Eq. (14) is linear in each timestep, where the $(n+1)^{th}$ timestep is defined over a time $\Delta t = t^{n+1} - t^n$.

The time-derivative of ϕ on the left-hand side of Eq. (14) can be subdivided into an implicit and explicit portion. The explicit portion, which is evaluated at t^n, can be moved to the right-hand side of Eq. (14) as an explicit source,

$$\left(\frac{C_v^n}{4acT^{n\,3}\Delta t} + \frac{1}{c\Delta t}\right)\phi^{n+1} - \frac{d}{dx}D^n\frac{d\phi^{n+1}}{dx} = \left(\frac{C_v^n}{4acT^{n\,3}\Delta t} + \frac{1}{c\Delta t}\right)\phi^n \; . \tag{15}$$

To begin a spatial treatment of Eq. (15), consider the 1-D cell shown in Fig. 1. First, D and C_v are defined constant in a cell. Operating on Eq. (15) with $\int_{x_l}^{x_r}(\cdot)dx$ and utilizing Fick's Law, Eq. (11), yields

$$\left(\frac{C_v^n}{4acT_c^{n\,3}\Delta t} + \frac{1}{c\Delta t}\right)\phi_c^{n+1}\Delta x + \int_{x_l}^{x_r} dF^{n+1} = \left(\frac{C_v^n}{4acT_c^{n\,3}\Delta t} + \frac{1}{c\Delta t}\right)\phi_c^n\Delta x \; , \tag{16}$$

where $\phi_c^{n+1} = \frac{1}{\Delta x}\int_{x_l}^{x_r}\phi^{n+1}dx$, $\phi_c^n = \frac{1}{\Delta x}\int_{x_l}^{x_r}\phi^n dx$, and $T_c^n = \frac{1}{\Delta x}\int_{x_l}^{x_r}T^n dx$. Evaluating the integral term and recognizing that the parenthetical expression is a material coupling coefficient that acts like an absorption/emission cross section, Eq. (16) becomes

$$\tilde{\sigma}_c^n\phi_c^{n+1}\Delta x + F_r^{n+1} - F_l^{n+1} = \tilde{\sigma}_c^n\phi_c^n\Delta x \; , \tag{17}$$

where

$$\tilde{\sigma}_c^n = \left(\frac{C_v^n}{4acT_c^{n\,3}\Delta t} + \frac{1}{c\Delta t}\right)\;[\text{cm}^{-1}] \; , \tag{18}$$

$$\phi_c^n = acT_c^{n\,4}\;[\text{jerks}\cdot\text{cm}^{-2}\cdot\text{sh}^{-1}] \; , \tag{19}$$

$$D^n = \frac{1}{3\sigma_{\text{R}}^n}\;[\text{cm}] \; . \tag{20}$$

Equation (17) is a photon balance equation, which states that the photon absorption at time t^{n+1} and the sum of the net (outgoing) fluxes on the cell-edges is equal to the material radiation emission

in the cell at time t^n. To complete the EqDDMC description, we must derive expressions for the cell-edge fluxes. In particular, we want the cell-edge fluxes to be defined in terms of the incoming partial fluxes at the cell-edges. The incoming partial fluxes will be represented in the EqDDMC algorithm by the weights of Monte Carlo particles entering a cell.

We can write discretized expressions for the cell-edge fluxes by utilizing Fick's Law. We apply forward-differencing to Eq. (11) yielding

$$F_r^{n+1} = \frac{-2D_c^n}{\Delta x}(\phi_r^{n+1} - \phi_c^{n+1}) \, , \tag{21a}$$

$$F_l^{n+1} = \frac{-2D_c^n}{\Delta x}(\phi_c^{n+1} - \phi_l^{n+1}) \, . \tag{21b}$$

Discretizing the Marshak boundary condition, Eq. (9), while considering Fick's Law, Eq. (11), yields expressions for the cell-edge incoming fluxes at each side of the cell

$$F_r^{(-)n+1} = \frac{1}{4}\phi_r^{n+1} - \frac{1}{2}F_r^{n+1} \, , \tag{22a}$$

$$F_l^{(-)n+1} = \frac{1}{4}\phi_l^{n+1} + \frac{1}{2}F_l^{n+1} \, . \tag{22b}$$

Eliminating the cell-edge scalar intensities between Eqs. (22) and (21) results in the following expressions for the cell-edge fluxes,

$$F_r^{n+1} = \frac{2D^n}{\Delta x + 4D^n}\phi_c^{n+1} - \frac{8D^n}{\Delta x + 4D^n}F_r^{(-)n+1} \, , \tag{23a}$$

$$F_l^{n+1} = \frac{8D^n}{\Delta x + 4D^n}F_l^{(-)n+1} - \frac{2D^n}{\Delta x + 4D^n}\phi_c^{n+1} \, . \tag{23b}$$

Thus, forms for F_r^{n+1} and F_l^{n+1} have been derived that are functions of the incoming partial fluxes.

Using Eqs. (23) and (17), an expression for the cell-centered scalar radiation intensity, in terms of the incoming partial fluxes, is

$$\boxed{\phi_c^{n+1} = \left[\tilde{\sigma}_c^n\Delta x + \frac{4D^n}{\Delta x + 4D^n}\right]^{-1}\left[\tilde{\sigma}_c^n\phi_c^n\Delta x + \frac{8D^n}{\Delta x + 4D^n}(F_r^{(-)n+1} + F_l^{(-)n+1})\right] \, .} \tag{24}$$

In the EqDDMC algorithm, partial incoming fluxes, $F_r^{(-)n+1}$ and $F_l^{(-)n+1}$, will be represented on the fly by Monte Carlo particles. The other quantities in Eq. (24), $\tilde{\sigma}_c^n$, ϕ_c^n, and D^n, are all explicit at time t^n and can be calculated using Eqs. (18), (19), and (20), respectively, with the results from the previous timestep.

Equation (17) shows that knowledge of the cell-edge fluxes is required to solve the diffusion problem. Since incoming partial fluxes are represented by Monte Carlo particles, expressions for the outgoing cell-edge partial fluxes are necessary to solve the balance equation. Using the definition of the radiation flux in Eq. (4), the net flux (in the forward or $\mu > 0$ direction) can be defined as

$$F(x) = \int_{-1}^{1} \mu\psi(x,\mu)d\mu$$
$$= -\int_{-1}^{0} |\mu|\psi(x,\mu)d\mu + \int_{0}^{1} |\mu|\psi(x,\mu)d\mu \, . \tag{25}$$

Applying Eq. (25) at the right- and left-hand boundaries of a cell produces the following discrete expressions for the cell-edge fluxes:

$$F_r^{n+1} = F_r^{(+)n+1} - F_r^{(-)n+1} \ , \tag{26a}$$

$$F_l^{n+1} = F_l^{(-)n+1} - F_l^{(+)n+1} \ . \tag{26b}$$

Equations for the outgoing cell-edge fluxes can now be formulated by use of Eqs. (26) and (23),

$$F_r^{(+)n+1} = \frac{2D^n}{\Delta x + 4D^n} \phi_c^{n+1} + \frac{\Delta x - 4D^n}{\Delta x + 4D^n} F_r^{(-)n+1} \ , \tag{27a}$$

$$F_l^{(+)n+1} = \frac{2D^n}{\Delta x + 4D^n} \phi_c^{n+1} + \frac{\Delta x - 4D^n}{\Delta x + 4D^n} F_l^{(-)n+1} \ . \tag{27b}$$

Note that, aside from physical and computational parameters, these expressions for the outgoing partial fluxes are dependent only upon the cell-centered scalar intensity and incoming partial fluxes.

To complete the derivation of the EqDDMC equations, the net cell-edge fluxes in Eq. (17) must be evaluated in terms of incoming and outgoing partial fluxes. This is accomplished by substituting Eq. (26) into (17) yielding

$$\tilde{\sigma}_c^n \phi_c^{n+1} \Delta x + F_r^{(+)n+1} + F_l^{(+)n+1} = \tilde{\sigma}_c^n \phi_c^n \Delta x + F_r^{(-)n+1} + F_l^{(-)n+1} \ . \tag{28}$$

This balance equation states that the effective absorption of photons through the $\tilde{\sigma}_c^n$ term and the sum of the outgoing partial fluxes are equal to the contributions from the time-explicit source and the incoming partial fluxes. Equations (24), (27), and (28) form the basis of the EqDDMC method. We will now explain how these equations are used to solve the 1-D equilibrium diffusion problem stochastically.

3.2. EqDDMC Implementation

The source terms are represented by the particle weights, w, of the Monte Carlo particles. Relying on the linearity of the solution in each source term, the particle weight can be written as

$$w = F_r^{(-)n+1} + F_l^{(-)n+1} + \tilde{\sigma}_c^n \phi_c^n \Delta x \ , \tag{29}$$

where only one of the three terms on the right-hand side is nonzero at any given time in the life of the particle:

$$F_r^{(-)n+1} = \begin{cases} w & \text{if entering from the right,} \\ 0 & \text{otherwise;} \end{cases} \tag{30}$$

$$F_l^{(-)n+1} = \begin{cases} w & \text{if entering from the left,} \\ 0 & \text{otherwise;} \end{cases} \tag{31}$$

$$\tilde{\sigma}_c^n \phi_c^n \Delta x = \begin{cases} w & \text{if born in the cell at time } t^n, \\ 0 & \text{otherwise.} \end{cases} \tag{32}$$

Dividing Eq. (28) by the total source in the cell (*i.e.*, RHS of equation) yields the following probability equation,

$$\frac{\tilde{\sigma}_c^n \phi_c^{n+1} \Delta x}{S_{total}} + \frac{F_r^{(+)n+1}}{S_{total}} + \frac{F_l^{(+)n+1}}{S_{total}} = 1 \tag{33}$$

where $S_{total} \equiv \tilde{\sigma}_c^n \phi_c^n \Delta x + F_r^{(-)n+1} + F_l^{(-)n+1}$. The probability equation can also be expressed as

$$P_{\text{abs}} + P_{\text{leak r}} + P_{\text{leak l}} = 1 \tag{34}$$

where the probabilities for absorption and leakage are as follows:

$$P_{\text{abs}} = \frac{\tilde{\sigma}_c^n \phi_c^{n+1} \Delta x}{S_{total}} \, , \tag{35}$$

$$P_{\text{leak r}} = \frac{F_r^{(+)n+1}}{S_{total}} \, , \tag{36}$$

$$P_{\text{leak l}} = \frac{F_l^{(+)n+1}}{S_{total}} \, . \tag{37}$$

This probability equation completes the mathematical description of the EqDDMC method. We shall now proceed to outline the method.

We have derived the EqDDMC equations such that the problem is linear in a single timestep. Thus, N particles are sampled each timestep and the cell-centered scalar intensities are output at the end of each timestep. In a timestep, the EqDDMC method is performed in the following steps:

1. sample one particle (cell and weight) from the source:
    (a) time-explicit volume emission from $\tilde{\sigma}_c^n \phi_c^n \Delta x$;
    (b) surface source boundary condition, $F_{boundary}^{(-)n+1}$;
2. calculate ϕ_c^{n+1} using Eq. (24);
3. calculate the outgoing partial fluxes using Eqs. (27);
4. calculate the probabilities for effective absorption, right-, and left-leakage using Eqs. (35), (36), and (37), respectively;
5. accumulate the cell-centered scalar intensities at time t^{n+1};
6. if the particle is absorbed or leaks out of the system, the particle history is complete; start a new particle (go to step 1);
7. if the particle leaks into an adjacent cell, go to step 2;
8. When all the particles have been processed, divide the accumulated cell-centered scalar intensities by the total weight of source particles (*i.e.*, the total energy in the system at time t^n) to get the total cell-centered scalar radiation intensity.

This concludes the description of the 1-D EqDDMC method.

4. 1-D EqDDMC Test Code

We have implemented the EqDDMC method, as outlined in the foregoing section, in a Fortran 1-D test code. This so-called "eqddmc" test code is an adaptation and extension of the analogous "ddmc" suite of Fortran routines developed by Urbatsch, Morel and Gulick [1, 2] for neutronics calculations.

The eqddmc code retains the geometry capability, an adaptation of the source normalization, and an adaptation of the Monte Carlo estimation algorithms of the ddmc routines. Additionally, eqddmc incorporates new algorithms required by EqDDMC, including the time-stepping and all the necessary updating of time-explicit quantities.

5. 1-D EqDDMC Test Problems

The EqDDMC method was tested on two simple, degenerate problems.

Test Problem 1. Initial Uniform Nonzero Temperature in a Homogeneous Infinite Medium.
The problem specification is modeled by a finite slab, with reflecting boundary conditions, at a given temperature. As defined, this problem is in steady-state. Computationally, the temperature should not change over time except for statistical fluctuation.

Test Problem 2. Spatial and Temporal Equilibration of Temperature.
This test problem is somewhat less degenerate and, as such, more interesting and evaluative than the first problem. Again, the boundary conditions are reflecting, but the initial temperature is not uniform. Over time, the temperature should equilibrate to a temperature that is characteristic of the total energy in the system. The detailed problem specifications are as follows:

Geometry: 10 cells in a one-region homogeneous slab;

Dimensions: $0 < x < 2$ [cm]; $\Delta x_{cell} = 0.2$ [cm];

Boundary Condition: reflecting on both sides of slab;

Initial Condition: $T_{initial}(x) = 0.8 + 0.1x$ [keV];

Physical Properties: $\sigma_{\mathrm{R}} = 10.0$ [cm^{-1}]; $\rho = 1.0$ [g $\cdot$ cm^{-3}]; $C_v = 0.01$ [jerks $\cdot$ cm^{-3} $\cdot$ keV^{-1}];

Execution Parameters: 500 timesteps; $\Delta t_{step} = 0.001$ [sh]; 10^6 particles per step.

6. Results and Discussion

Test Problem 1 was run with the eqddmc code. Except for statistical fluctuation, the temperature remained constant over time, as required.

Test Problem 2 was run with the eqddmc code, and, for comparison, with the Milagro IMC code [8]. Figure 2 focuses on the spatial equilibration of temperature as computed by the eqddmc code. The results of both runs are compared in Fig. 3, focusing on the temporal equilibration of the temperature in the first and last (tenth) cells.
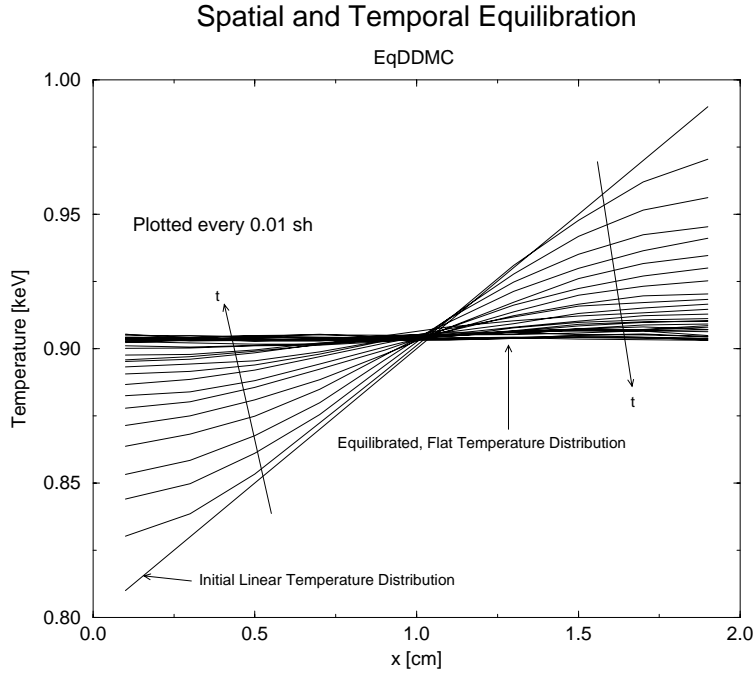
FIG. 2: Temporal equilibration of temperature as a function of position, as computed by EqDDMC.

The analytical final equilibrated temperature was computed to be $T_f = 0.906$ [keV], and is represented in Fig. 3 as the solid horizontal line. Recall that the final temperature should *not* be the average of the initial-condition temperature profile, because it is the *energy* ($\sim aT^4$) that is being conserved.

At 0.3 sh, the Milagro IMC result had a 1.02% energy error (gain). The temperature corresponding to the total initial energy plus a 1.02% gain is 0.908 keV and is plotted as a dashed line in Fig. 3.

The eqddmc code converges to the equilibrium temperature. Moreover, the temporal equilibration for the eqddmc-code result compares favorably with its Milagro benchmark counterpart, which lends credence to the EqDDMC method.

7. Conclusion

The Discrete Diffusion Monte Carlo (DDMC) method, a hybrid Monte Carlo method for time-independent neutronics calculations, has been applied to equilibrium diffusion radiative transfer. This new method, Equilibrium Discrete Diffusion Monte Carlo (EqDDMC), has been derived and outlined for one-dimensional, slab geometry. The new method has been successfully tested on two different benchmark problems and showed good agreement with analytical results and with an existing, verified Implicit Monte Carlo radiative transfer code.

The EqDDMC method, when extended to multidimensions, may be a competitive tool compared to deterministic diffusion, especially since EqDDMC is a candidate for exponential convergence with residual methods. Finally, EqDDMC is the first significant step toward applying DDMC to

Spatial and Temporal Equilibration
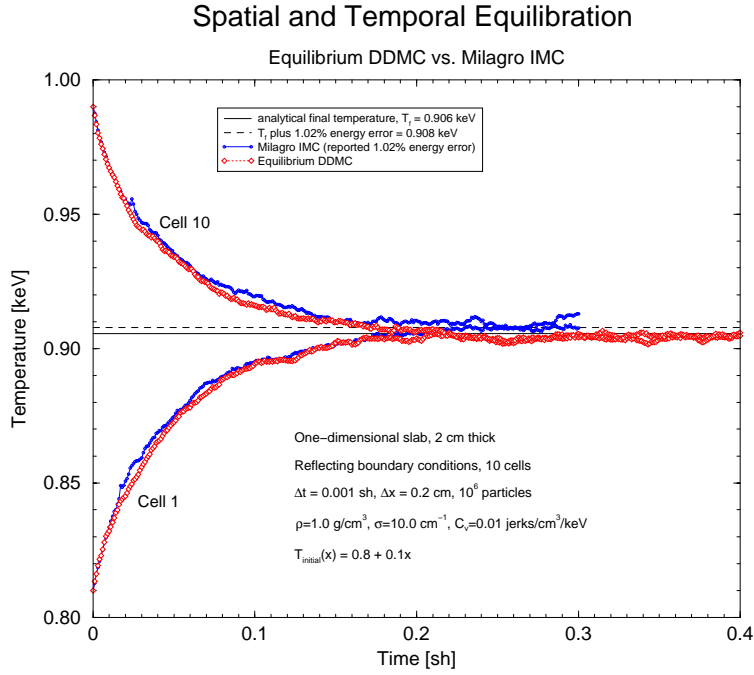
Equilibrium DDMC vs. Milagro IMC

FIG. 3: Spatial and temporal equilibration of temperature, as computed by EqDDMC and by Milagro IMC.

non-equilibrium diffusion and coupling it to Implicit Monte Carlo.

8. Acknowledgements

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