Title: **1-D Equilibrium Discrete Diffusion Monte Carlo**

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Submitted to:

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1-D Equilibrium Discrete Diffusion Monte Carlo

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Abstract. We present a new hybrid Monte Carlo method for 1-D equilibrium diffusion problems in which the radiation field coexists with matter in local thermodynamic equilibrium. This method, the Equilibrium Discrete Diffusion Monte Carlo (EqDDMC) method, combines Monte Carlo particles with spatially discrete diffusion solutions. We verify the EqDDMC method with computational results from three slab problems. The EqDDMC method represents an incremental step toward applying this hybrid methodology to non-equilibrium diffusion, where it could be simultaneously coupled to Monte Carlo transport.

1   Introduction and Motivation

Urbatsch, Morel and Gulick [1] 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 multiple single-cell, deterministic, diffusion solutions. The intent has always been to apply this method to diffusive regions of thermal radiative transfer problems. In particular, we have hypothesized that the DDMC method could prove to be an effective replacement for the Random Walk method [2] in Implicit Monte Carlo (IMC) [3].

   This paper describes the first effort at applying the DDMC method to radiative transfer problems. We derive an Equilibrium Discrete Diffusion Monte Carlo (EqDDMC) method in one-dimensional, slab geometry for the equilibrium diffusion equation, an approximation to the radiative transfer equation, where the radiation and material are in local thermodynamic equilibrium. We demonstrate the method's properties and verify its correctness by successfully running three benchmarked problems.

2   1-D EqDDMC Method

We begin with the equilibrium diffusion equation [4] with no external sources,

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

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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, $\sigma_R \equiv \sigma_R(x, T(x,t))$ [cm^{-1}], is the Rosseland Mean opacity.

After recasting Eq. (1) in terms of the equilibrium radiation energy density, $\phi = acT^4$, we discretize over a timestep and over a spatial cell to obtain a discrete equation that is nonlinear in temperature. We linearize the equation by evaluating the coefficients at the beginning of the timestep, time t^n. Utilizing discrete expressions for Fick's Law, the Marshak boundary condition, and the definition of the net flux, we obtain the EqDDMC balance equation,

$$\tilde{\sigma}_c^n \phi_c^{n+1} \Delta x + F_r^{(+)n+1} + F_l^{(+)n+1} = \tilde{\sigma}_c^n \phi_c^n \Delta x + F_r^{(-)n+1} + F_l^{(-)n+1} \,, \qquad (2)$$

where $F_r^{(-)n+1}$ and $F_l^{(-)n+1}$ are the incoming partial fluxes and where the cell-centered scalar radiation intensity and outgoing partial fluxes at the end of the timestep are

$$\phi_c^{n+1} = \left[\tilde{\sigma}_c^n \Delta x + 2\lambda \right]^{-1} \left[\tilde{\sigma}_c^n \phi_c^n \Delta x + 4\lambda (F_r^{(-)n+1} + F_l^{(-)n+1}) \right] \,, \qquad (3)$$

$$F_r^{(+)n+1} = \lambda \phi_c^{n+1} + (1 - 4\lambda) F_r^{(-)n+1} \,, \qquad (4)$$

$$F_l^{(+)n+1} = \lambda \phi_c^{n+1} + (1 - 4\lambda) F_l^{(-)n+1} \,, \qquad (5)$$

where $\tilde{\sigma}_c^n = \left(\frac{C_v^n}{4acT_c^{n\,3}\Delta t} + \frac{1}{c\Delta t} \right)$, $D^n = \frac{1}{3\sigma_R^n}$, and $\lambda = \frac{2D^n}{\Delta x + 4D^n}$.

3   EqDDMC Implementation

In practice, each piece of the source on the right hand side of the balance equation, Eq. (2), is modeled with particles. When a particle enters or is born in a cell, the cell-centered scalar radiation intensity and the exiting partial fluxes are solved for that particular particle. When divided through by the source, the balance equation with its newly calculated solutions provides a probability equation that can be sampled to determine whether the particle is absorbed in the cell or leaks out one of the sides of the cell. This process is repeated while a particle goes from one cell to another until it escapes the system or is absorbed. The temperature at the end of the timestep is obtained from the cell-centered scalar radiation intensity, which is accumulated each time Eq. 3 is solved (i.e. whenever a particle is born in or enters a cell).

For wave propagation through cold slabs, we implemented a treatment that enables transmission through their opaque cells. This commenly used treatment is necessary when the opacity is proportional to T^{-3}. The idea amounts to utilizing an *opacity-defining* cell temperature, which is simply taken as the larger of the two cell-edge values. Each edge value is taken to be the average of the two cell-centered values on either side of the edge.

4 EqDDMC Verification Results

The EqDDMC method ('the method') was successfully tested in a FORTRAN code ('**eqddmc**' or 'the code') for three test cases. Most aspects of the test cases have analytic solutions to which the **eqddmc** results were compared. In one case, the **eqddmc** results were compared to a well-verified IMC code.

4.1 Homogeneous, Infinite Medium in Steady State

One early test was a steady-state, homogeneous, infinite medium problem. The result was that, except for statistical fluctuation, the computed temperature remained constant over time, as expected.
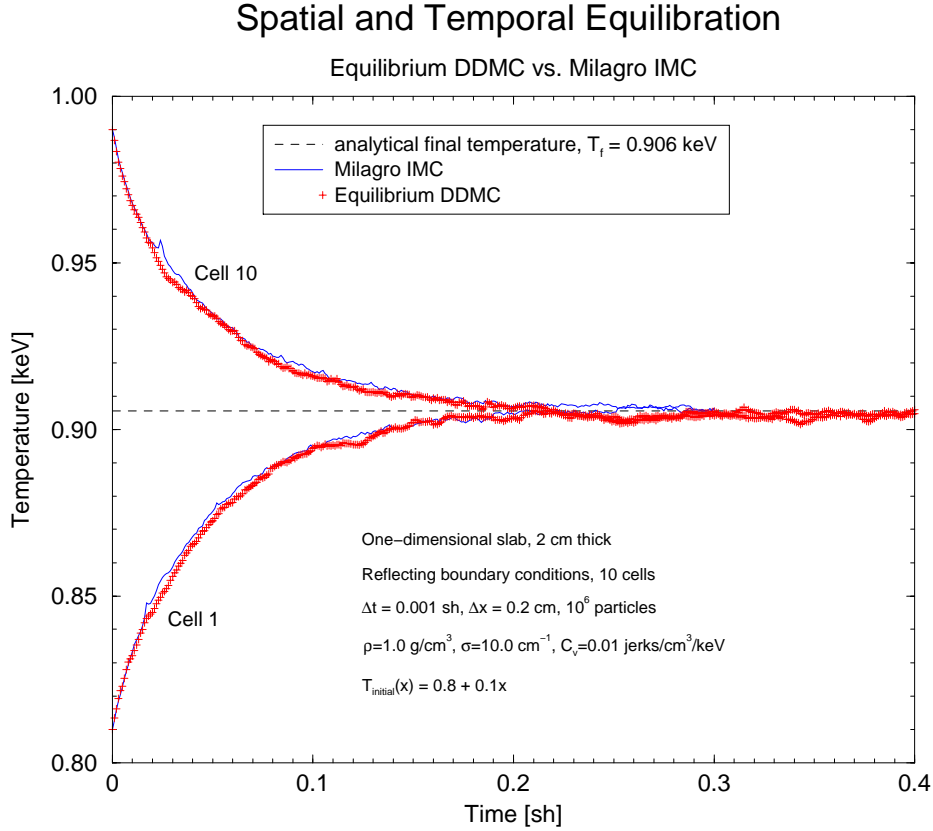
4.2 Spatial and Temporal Equilibration

The method was also tested on a finite slab of 10 uniform cells with reflecting boundaries and a sloped initial temperature. Figure 1 shows the equilibration over time of the temperatures in the left-most and right-most cells. The code produced the correct analytic equilibrium temperature of 0.906 keV. The temporal equilibration matched that of a verified Implicit Monte Carlo code, Milagro [5], which is also depicted in Fig. 1.

4.3 Marshak Wave Solution

This particular Marshak benchmark [6] is in slab geometry, with a delta-function source of 0.01 Jerks at $x = 0$ cm and at $t = 0$ shakes. The actual modeling of the delta-function source was finessed starting the problem at $t = 0.1$ shake with the analytic solution as the initial-condition temperature profile. The analytical data used to compare output and to produce the initial source (*i.e.*, based on the temperature distribution at 0.1 shake) was obtained from the LANL Transport Methods Group Analytical Test Suite [7]. We used a slab material opacity of $10/T^3$ cm^2/g, a specific heat of 0.1 Jerks/g/keV, and a density of 3.0 g/cm^3. Figure 2 shows the results of a series of **eqddmc** calculations for this Marshak benchmark.

The final profile computed by **eqddmc** is the computed mean (with 1-standard-deviation precision error bars) for 11 uncorrelated runs, accomplished by varying the random number seed for each run. It must be noted, however, that this estimated precision does not include any inaccuracy (*i.e.*, difference from true physical quantity being estimated) inherent in the calculation as a result of modeling approximations. One such approximation is that the initial **eqddmc** temperature profile, with its 20 values, can not resolve accurately the initial wavefront. This approximation introduces a systematic error that propagates along with the wavefront and is *not* accounted for by the Monte-Carlo estimated precision for the calculation. For further discussion of the difference between the precision and accuracy of a Monte Carlo calculation see Ref. [8].

Spatial and Temporal Equilibration

Fig. 1. Spatial and temporal equilibration of temperature, as computed by EqDDMC and by Milagro IMC.

Of the 15 non-zero mean-value estimates, 7 were within 1 standard deviation (1σ) of estimated precision from the corresponding analytic values, 11 were within 2σ, and 13 were within 3σ. The two estimates in the knee of the propagated wave were within 8σ. It should be noted, however, that the knee of the propagated wave is difficult to resolve with such a small number of discrete points, especially when modeling approximations are known to contribute a systematic error (inaccuracy).

In order to analyze these results statistically, let us assume that each cell's results are independent and that we may collapse the independent results over space and treat this ensemble as if it represented a set of estimates for one stochastic quantity. In so doing, the 15 estimated non-zero mean values and associated σs (corresponding to the first 15 points of the spatial temperature profile) produce coverage rates of 47%, 73%, and 87% for 1σ, 2σ, and 3σ, respectively. Eliminating the 2 estimates around the knee of the profile, results in coverage rates of 54%, 85%, and 100%, for 1σ, 2σ, and 3σ, respectively. These

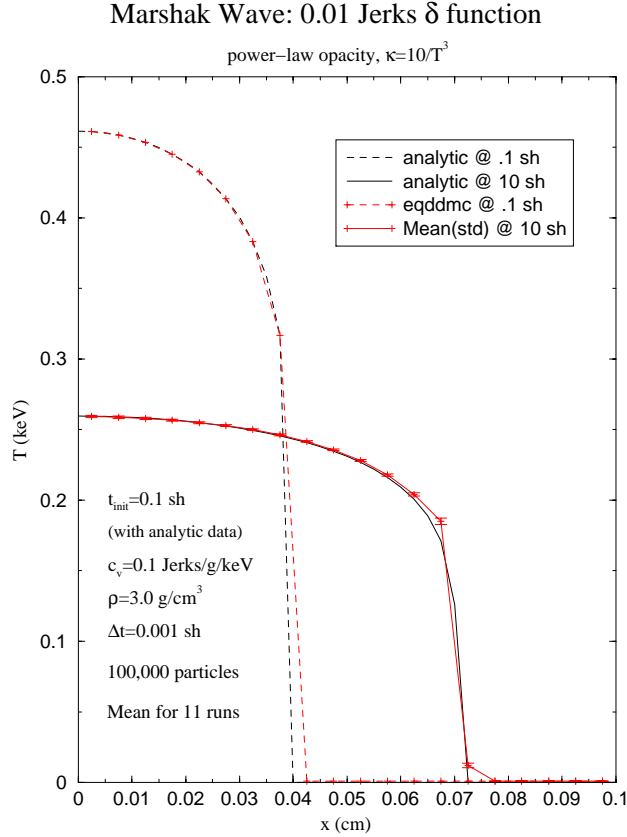**Fig. 2.** Propagation of a δ-function-driven Marshak wave through a slab.

coverage rates compare reasonably well with the theoretically expected coverage rates of 67%, 95%, and 99%, respectively, bearing in mind the impact on our computed results from the inherent modeling errors noted above.

5   Conclusion

This new method, Equilibrium Discrete Diffusion Monte Carlo (EqDDMC), has been derived for one-dimensional equilibrium diffusion radiative transfer in slab geometry. The new method has been successfully tested on three benchmark problems. The EqDDMC results agreed with analytical results and with the results from 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 non-equilibrium diffusion and coupling it to Implicit Monte Carlo.

6   Acknowledgements

We thank Jim Morel and Dimitri Mihalas (both in LANL Transport Methods Group) for fruitful discussions during the development of the method. We also thank John McGhee (LANL Transport Methods Group) for suggesting the test problem whose results are depicted in Fig. 1 and Mark Gray (LANL Transport Methods Group) for providing his Analytical Test Suite, which we relied on for our Marshak wave propagation benchmark.

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