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A hybrid transport-diffusion Monte Carlo method for frequency-dependent radiative-transfer simulations

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ABSTRACT

Discrete Diffusion Monte Carlo (DDMC) is a technique for increasing the efficiency of Implicit Monte Carlo radiative-transfer simulations in optically thick media. In DDMC, particles take discrete steps between spatial cells according to a discretized diffusion equation. Each discrete step replaces many smaller Monte Carlo steps, thus improving the efficiency of the simulation. In this paper, we present an extension of DDMC for frequency-dependent radiative transfer. We base our new DDMC method on a frequency-integrated diffusion equation for frequencies below a specified threshold, as optical thickness is typically a decreasing function of frequency. Above this threshold we employ standard Monte Carlo, which results in a hybrid transport-diffusion scheme. With a set of frequency-dependent test problems, we confirm the accuracy and increased efficiency of our new DDMC method.

1. Introduction

Implicit Monte Carlo (IMC) is an accurate and robust method for performing nonlinear, time-dependent radiative-transfer calculations via Monte Carlo simulation [1]. An important component of IMC is "effective" scattering, which represents radiation absorption and re-emission within a time step. Unfortunately, in optically thick media not only is the mean-free path between collisions small, but also collisions are primarily effective scatters. In this situation, the transport process can be described as *diffusive*, particle histories consist of an excessive number of steps, and the resulting IMC calculation is inefficient.

The diffusive nature of IMC in optically thick media has lead to the development of several hybrid transport-diffusion methods for improving the efficiency of IMC in this regime. These techniques replace a portion of the standard Monte Carlo procedure with an alternate one based on the diffusion approximation, which is accurate in optically thick media for IMC. One such method is Random Walk (RW) [2,3]. In RW, several Monte Carlo steps are replaced by a larger step over a sphere centered about the particle's current position, thus increasing the efficiency of the simulation. The radius of the sphere is limited such that the sphere lies inside the particle's current spatial cell, while the step is governed by an analytic diffusion solution within the sphere. In order to ensure the accuracy of this solution, the radius of the sphere is further required to be greater than a specified minimum as measured in mean-free paths. If it is not possible to satisfy this minimum-radius criterion, the particle instead transports according to standard Monte Carlo. This situation occurs not only in optically thin media, where the mean-free path is large and the diffusion approximation is not appropriate, but also in optically thick media when a particle is near a cell boundary.

Discrete Diffusion Monte Carlo (DDMC) is another technique for increasing the efficiency of IMC in optically thick media [4,5]. In DDMC, particles take discrete steps between spatial cells according to a discretized diffusion equation. Each discrete

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step replaces many smaller Monte Carlo steps, which, as with RW, improves the efficiency of the IMC calculation. In practice, DDMC is combined with standard Monte Carlo to form a hybrid transport-diffusion method, with DDMC used in optically thick media and standard Monte Carlo employed elsewhere. Because a particle can travel to a new cell each DDMC step (whereas an RW step is limited to within a cell) and transports according to DDMC exclusively in optically thick media (whereas standard Monte Carlo is used with RW to some extent in optically thick media), DDMC typically provides greater efficiency gains over standard Monte Carlo than RW.

In this paper, we present an extension of DDMC for frequency-dependent radiative transfer [6]. Because the opacity is typically a decreasing function of frequency, a spatial region can be optically thick for low frequencies but optically thin for high frequencies. Therefore, we base our new DDMC method on a grey (frequency-integrated) diffusion equation for frequencies below a specified threshold. Above this threshold we employ standard Monte Carlo. This approach is similar to that taken by Clouët and Samba [7] in their hybrid transport-diffusion scheme for the Symbolic Monte Carlo method [8].

Cleveland, Gentile, and Palmer [9] have also recently developed a version of DDMC (which they refer to as Implicit Monte Carlo Diffusion) that accounts for frequency dependence. However, our new DDMC method differs from theirs in two important ways. First, in terms of efficiency, their technique is based on a frequency-dependent diffusion equation that still contains a term corresponding to effective scattering. As with standard Monte Carlo, the presence of effective scattering can lead to extremely long particle histories and thus degrade the efficacy of DDMC. The grey diffusion equation that we use greatly reduces this effective scattering. Second, in terms of accuracy, we employ standard Monte Carlo for sufficiently high frequencies where the diffusion approximation is not appropriate, whereas Cleveland, Gentile, and Palmer use DDMC for all frequencies.

We begin the remainder of this paper by presenting a concise review of radiative transfer and IMC. Next, we develop our grey diffusion equation along with a corresponding boundary condition. We then use this diffusion equation and boundary condition to form our new DDMC method and demonstrate how it is coupled to standard Monte Carlo. With a set of frequency-dependent test problems, we demonstrate the accuracy and improved efficiency, as compared to both standard Monte Carlo and RW, of our new DDMC method. We conclude with a brief discussion.

2. Radiative transfer and Implicit Monte Carlo

In the absence of internal sources and scattering, the equations governing frequency-dependent radiative transfer are [10–12]

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega}\cdot\nabla I + \sigma I = \sigma B \tag{1}$$

and

$$C_v\frac{\partial T}{\partial t} = \int_{4\pi}\int_0^\infty \sigma(I - B)\,dv\,d\mathbf{\Omega}. \tag{2}$$

Here, $\mathbf{r}$ is the spatial variable, $\mathbf{\Omega}$ is the angular variable, v is the frequency variable, t is the temporal variable, $I(\mathbf{r},\mathbf{\Omega},v,t)$ is the radiation intensity, $T(\mathbf{r},t)$ is the material temperature, $\sigma(\mathbf{r},v,T)$ is the opacity, $C_v(\mathbf{r},T)$ is the heat capacity, and c is the speed of light. In addition, the Planck function $B(v,T)$ is defined by

$$B(v,T) = \frac{2hv^3}{c^2}\frac{1}{e^{hv/kT}-1}, \tag{3}$$

where h is Planck's constant and k is Boltzmann's constant. Also of interest are the normalized Planck function,

$$\begin{aligned} b(v,T) &= \frac{B(v,T)}{\int_0^\infty B(v,T)dv} \\ &= \frac{15}{\pi^4}\left(\frac{h}{kT}\right)^4\frac{v^3}{e^{hv/kT}-1}, \end{aligned} \tag{4}$$

which follows from Eq. (3), and the Planck-mean opacity,

$$\sigma_P(\mathbf{r},T) = \int_0^\infty \sigma(\mathbf{r},v,T)b(v,T)dv. \tag{5}$$

Appropriate boundary and initial conditions for the radiation intensity and material temperature also accompany Eqs. (1) and (2).

The IMC method for Eqs. (1) and (2) is based on semi-implicitly approximating the temperature dependence of the Planck function using the latter expression. The resulting equations within each time step are [1]

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega}\cdot\nabla I + \sigma_n I = \frac{\chi_n}{4\pi}\int_{4\pi}\int_0^\infty (1-f_n)\sigma_n(v')I(\mathbf{r},\mathbf{\Omega}',v',t)dv'd\mathbf{\Omega}' + \frac{\chi_n}{4\pi}f_n\sigma_{P,n}acT_n^4 \tag{6}$$

and