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A Nonclassical Monte Carlo Algorithm for Transport Problems in Diffusive Binary Stochastic Media

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1. INTRODUCTION

The Levermore–Pomraning (LP) model is a well-known approach for solving linear particle transport problems in a heterogeneous physical system consisting of two (or more) materials [1]. For binary systems, the model is represented by coupled transport equations for the two materials in the problem and can be solved using Monte Carlo algorithms [2]. While the LP model is exact for purely absorbing non-participating media, it is generally inaccurate in diffusive systems.

For physical systems in which absorption and sources are weak and the solution varies slowly over the distance of a mean free path, the diffusion equation has been shown to be an asymptotic limit of the transport equation [3]. However, considering these same assumptions, the standard LP model reduces to a diffusion equation with an incorrect diffusion coefficient [4, 5]. Adjusted models of the LP equations with modified closures have been proposed to mitigate this issue [6].

The theory of nonclassical particle transport describes processes in which the particle's free-path s (the particle's distance between interactions) is not exponentially distributed. Instead, it is given by [7]

$$p(s) = \Sigma_t(s) e^{-\int_0^s \Sigma_t(s')ds'} \,. \tag{1}$$

Here, $\Sigma_t(s)$ represents the nonclassical macroscopic total cross section, which depends upon the free-path variable s.

Recently, it has been shown that certain diffusion approximations to the transport equation can be represented exactly by a nonclassical transport equation [8]. This is done by obtaining explicit expressions for the free-path distribution $p(s)$ and the corresponding $\Sigma_t(s)$ such that the nonclassical equation can be converted to an integral equation for the scalar flux that is identical to the integral formulation of the diffusive approximation. Moreover, the sampling of s from nonexponential probability functions $p(s)$ allows the use of Monte Carlo methods to solve these nonclassical transport equations. In particular, it is possible to solve *diffusion* problems using a nonclassical Monte Carlo *transport* method [9].

The goal of this work is to introduce a nonclassical Monte Carlo transport approach to solve the LP equations in diffusive binary stochastic media. The full version of this work will present the following original content:

1. We will derive explicit expressions for $p(s)$ and $\Sigma_t(s)$ such that the diffusion equations for the LP model (and its adjusted models) can be exactly represented by a nonclassical transport equation.
2. We will consider transport problems in diffusive binary stochastic media and perform nonclassical Monte Carlo simulations in which the free-paths are sampled from the appropriate nonexponential distributions. Numerical results will be presented.
3. We will investigate the effectiveness of the nonclassical Monte Carlo algorithm in approximating the results of the classical LP Monte Carlo algorithms. Numerical results will be presented.
4. We will analyze the advantages and disadvantages of the nonclassical Monte Carlo approach when compared to standard LP Monte Carlo algorithms.

The remainder of this summary is organized as follows. In Section 2, we sketch the integral formulation of the LP diffusion equation and compare it to the integral formulation of the nonclassical transport equation. This allows us to determine the free-path distribution $p(s)$ from which s will be sampled in the nonclassical Monte Carlo algorithm. In Section 3 we present a brief discussion of what will be included in the full work.

2. INTEGRAL FORMULATION OF THE LP DIFFUSION EQUATION

Consider the following LP formulation for transport in a binary stochastic medium:

$$\begin{aligned}\mu\frac{\partial\Psi_i}{\partial x}(x,\mu)+\Sigma_{ti}\Psi_i(x,\mu) &= \frac{\Sigma_{si}}{2}\int_{-1}^{1}\Psi_i(x,\mu')d\mu' \\ &+|\mu|\left(\frac{\Psi_j(x,\mu)}{\lambda_j}-\frac{\Psi_i(x,\mu)}{\lambda_i}\right)+\frac{P_iQ_i}{2}, \quad -X\le x\le X, -1\le\mu\le 1,\end{aligned} \tag{2}$$

where $i,j\in\{1,2\}$ with $j\neq i$; $\Psi_i(x,\mu)=P_i(x)\psi_i(x,\mu)$; $P_i(x)$ is the volume fraction for material i at location x; and $\psi_i(x,\mu)$ is the material averaged flux in direction μ at location x conditioned on the location being in material i. Here, Σ_{ti} and Σ_{si} are the macroscopic total and isotropic scattering cross sections for material i, and λ_i is the mean chord length value of a segment of material i.

For diffusive systems that (I) have weak absorption and sources; (II) are optically thick; and (III) consist of a large number of material layers with mean thicknesses comparable to (or small compared to) a mean free path, the LP formulation above has been shown to asymptotically limit to the LP diffusion equation [4, 5]

$$-\frac{\beta}{3\Sigma_t}\frac{d^2\phi}{dx^2}(x)+\Sigma_a\phi(x)=Q. \tag{3}$$

Here, $\phi(x)$ is the scalar flux at location x, and

$$\Sigma_{ai} = \Sigma_{ti} - \Sigma_{si}, \qquad \Sigma_m = P_1\Sigma_{m1} + P_2\Sigma_{m2} \text{ for } m = t, s, a, \qquad Q = P_1 Q_1 + P_2 Q_2,$$
$$\beta = \int_0^1 3\mu^2 \alpha(\mu) d\mu, \qquad \alpha(\mu) = \frac{\lambda_1\lambda_2\Sigma_t(P_1\Sigma_{t2} + P_2\Sigma_{t1}) + (\lambda_1\Sigma_{t1} + \lambda_2\Sigma_{t2})\mu}{\lambda_1\lambda_2\Sigma_{t1}\Sigma_{t2} + (\lambda_1\Sigma_{t1} + \lambda_2\Sigma_{t2})\mu}.$$

If $\Sigma_{t1} \neq \Sigma_{t2}$, $\beta > 1$ and the diffusion coefficient is unphysically large. Modified closures of the LP formulation lead to different values of β.

Let us define the scattering source $S(x) \equiv \Sigma_s\phi(x) + Q(x)$. We can now rewrite Eq. (3) as

$$-\frac{d^2\phi}{dx^2}(x) + \frac{3\Sigma_t^2}{\beta}\phi(x) = \frac{3\Sigma_t}{\beta}S(\boldsymbol{x})\,. \tag{4}$$

The Green's function for the operator on the left hand side of Eq. (4) is:

$$G(|x - x'|) = \frac{e^{-\frac{\sqrt{3}\Sigma_t}{\sqrt{\beta}}|x-x'|}}{4\pi|x - x'|}. \tag{5}$$

Therefore, we can solve Eq. (4) for $\phi(x)$ by taking

$$\phi(x) = \int \frac{3\Sigma_t|x - x'|e^{-\frac{\sqrt{3}\Sigma_t}{\sqrt{\beta}}|x-x'|}}{4\pi\beta|x - x'|^2}S(x')dx', \tag{6}$$

and the collision rate density $f = \Sigma_t\phi$ is given by

$$f(x) = \Sigma_t\phi(x) = \int \frac{3\Sigma_t^2|x - x'|e^{-\frac{\sqrt{3}\Sigma_t}{\sqrt{\beta}}|x-x'|}}{4\pi\beta|x - x'|^2}S(x')dx'\,. \tag{7}$$

The integral formulation of the nonclassical transport equation yields the collision rate [8, 9]

$$f(x) = \int S(x')\frac{p(|x' - x|)}{4\pi|x' - x|^2}dx', \tag{8}$$

where p is the free-path distribution given by Eq. (1). This result agrees with Eq. (7) iff

$$p(s) = \frac{3\Sigma_t^2 s}{\beta}e^{-\frac{\sqrt{3}\Sigma_t}{\sqrt{\beta}}s}. \tag{9}$$

If we define

$$\xi = \int_0^s p(s')ds' = 1 - \left(1 + \frac{\sqrt{3}\Sigma_t}{\sqrt{\beta}}s\right)e^{-\frac{\sqrt{3}\Sigma_t}{\sqrt{\beta}}s}, \tag{10}$$

the nonclassical Monte Carlo algorithm can sample the free-path s using

$$s = \frac{\sqrt{\beta}}{\sqrt{3}\Sigma_t}\tau^{-1}(\xi), \tag{11a}$$

where

$$\tau(z) = (1 + z)e^{-z}. \tag{11b}$$

The solution obtained by this Monte Carlo procedure should match the solution of Eq. (3), which should converge to the solution of Eq. (2) in diffusive systems.

3. DISCUSSION

The goal of this work is to introduce a nonclassical Monte Carlo algorithm to address transport problems in diffusive binary stochastic media. In the full version, we will expand on the theory sketched in Section 2 and provide full details on the exact representation of the LP diffusion equation as a nonclassical transport equation. We will include similar results to the adjusted LP equations with modified closures.

We will present a full set of numerical results for problems in slab geometry, in which we will compare the results of the nonclassical Monte Carlo algorithm with those obtained through classical LP Monte Carlo algorithms. The effectiveness of the proposed approach will be investigated, and the advantages and disadvantages of the method will be analyzed.

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