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Monte Carlo Chord Length Sampling for *d*-dimensional Markov binary mixtures

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A B S T R A C T

The Chord Length Sampling (CLS) algorithm is a powerful Monte Carlo method that models the effects of stochastic media on particle transport by generating on-the-fly the material interfaces seen by the random walkers during their trajectories. This annealed disorder approach, which formally consists of solving the approximate Levermore–Pomraning equations for linear particle transport, enables a considerable speed-up with respect to transport in quenched disorder, where ensemble-averaging of the Boltzmann equation with respect to all possible realizations is needed. However, CLS intrinsically neglects the correlations induced by the spatial disorder, so that the accuracy of the solutions obtained by using this algorithm must be carefully verified with respect to reference solutions based on quenched disorder realizations. When the disorder is described by Markov mixing statistics, such comparisons have been attempted so far only for one-dimensional geometries, of the rod or slab type. In this work we extend these results to Markov media in two-dimensional (extruded) and three-dimensional geometries, by revisiting the classical set of benchmark configurations originally proposed by Adams, Larsen and Pomraning [1] and extended by Brantley [2]. In particular, we examine the discrepancies between CLS and reference solutions for scalar particle flux and transmission/reflection coefficients as a function of the material properties of the benchmark specifications and of the system dimensionality.

1. Introduction

Several applications in nuclear science and engineering involve linear particle transport theory in stochastic media. Examples include neutron diffusion in pebble-bed reactors or randomly mixed water–vapor phases in boiling water reactors [3–7], and inertial confinement fusion [8–10]. Particle propagation in random media emerges more broadly in material and life sciences and in radiative transport [11–17]. Assuming that particles undergo single-speed transport with isotropic scattering, the angular particle flux $\varphi(\mathbf{r}, \boldsymbol{\omega})$ for each physical realization of the system obeys the linear Boltzmann equation

$$\boldsymbol{\omega} \cdot \nabla\varphi + \Sigma(\mathbf{r})\varphi = \frac{\Sigma_s(\mathbf{r})}{\Omega_d} \int \varphi(\mathbf{r}, \boldsymbol{\omega}')d\boldsymbol{\omega}' + S. \quad (1)$$

Here $\mathbf{r}$ and $\boldsymbol{\omega}$ denote the position and direction variables, respectively, $\Sigma(\mathbf{r})$ being the total cross section and $S = S(\mathbf{r}, \boldsymbol{\omega})$ the source term. The quantity $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface area of the unit sphere in dimension d, $\Gamma(a)$ being the Gamma function. The quantities $\Sigma(\mathbf{r})$, $\Sigma_s(\mathbf{r})$ and $S(\mathbf{r}, \boldsymbol{\omega})$ are in principle random variables, since the materials composing the traversed medium are assumed to be possibly distributed according to some statistical law. The physical observable of interest is typically the ensemble-averaged angular particle flux $\langle\varphi(\mathbf{r}, \boldsymbol{\omega})\rangle$, or more generally some ensemble-averaged functional $\langle F[\varphi]\rangle$ of the particle flux, namely,

$$\langle\varphi(\mathbf{r}, \boldsymbol{\omega})\rangle = \int \mathcal{P}(q)\varphi^{(q)}(\mathbf{r}, \boldsymbol{\omega})dq, \quad (2)$$

where $\varphi^{(q)}(\mathbf{r}, \boldsymbol{\omega})$ is the solution of the Boltzmann equation (1) corresponding to a single realization q, and $\mathcal{P}(q)$ is the stationary probability of observing the state q for the functions $\Sigma^{(q)}(\mathbf{r})$, $\Sigma_s^{(q)}(\mathbf{r})$ and $S^{(q)}(\mathbf{r}, \boldsymbol{\omega})$ [3,18].

Exact solutions for $\langle F[\varphi]\rangle$ can be in principle obtained in the following way: first, a realization of the medium is sampled from the underlying mixing statistics; then, the linear transport equation (1) corresponding to this realization is solved by either deterministic or Monte Carlo methods, and the physical observables of

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interest $F[\varphi]$ are determined; a sufficiently large collection of realizations is produced; and ensemble averages are finally taken for the physical observables.

Reference solutions are very demanding in terms of computational resources, especially if transport is to be solved by Monte Carlo methods in order to preserve the highest possible accuracy in solving the Boltzmann equation. In principle, it would be thus desirable to directly derive a single equation for the ensemble-averaged flux $\langle\varphi\rangle$. A widely adopted model of random media is the so-called binary stochastic mixing, where only two immiscible materials (say α and β) are present [3]. Then, by averaging Eq. (1) over realizations having material α at $\mathbf{r}$, we obtain the following equation for $\langle\varphi_\alpha(\mathbf{r},\boldsymbol{\omega})\rangle$

$$[\boldsymbol{\omega}\cdot\nabla+\Sigma_\alpha]p_\alpha\langle\varphi_\alpha\rangle=\frac{p_\alpha\Sigma_{s,\alpha}}{\Omega_d}\int\langle\varphi_\alpha(\mathbf{r},\boldsymbol{\omega}')\rangle d\boldsymbol{\omega}'$$
$$+p_{\beta,\alpha}\langle\varphi_{\beta,\alpha}\rangle-p_{\alpha,\beta}\langle\varphi_{\alpha,\beta}\rangle+p_\alpha S_\alpha \quad (3)$$

where $p_i(\mathbf{r})$ is the probability of finding the material of index i at position $\mathbf{r}$. Here $p_{i,j}=p_{i,j}(\mathbf{r},\boldsymbol{\omega})$ represents the probability per unit length of crossing the interface from material i to material j for a particle located at $\mathbf{r}$ and travelling in direction $\boldsymbol{\omega}$. The quantity $\langle\varphi_{i,j}\rangle$ denotes the angular flux averaged over those realizations where there is a transition from material i to material j for a particle located at $\mathbf{r}$ and travelling in direction $\boldsymbol{\omega}$. The cross sections Σ_α and $\Sigma_{s,\alpha}$ are those of material α. The equation for $\langle\varphi_\beta(\mathbf{r},\boldsymbol{\omega})\rangle$ is immediately obtained from Eq. (3) by permuting the indices α and β. Excluding the special case of particle transport in the absence of scattering, we are thus led to an infinite hierarchy for $\langle\varphi_\alpha\rangle$ in Eqs. (3).

In order to explicitly derive the ensemble-averaged flux $\langle\varphi_\alpha\rangle$, it is therefore necessary to introduce a closure formula, which will in general depend on the underlying mixing statistics [3,18,19]. The celebrated Levermore–Pomraning model assumes for instance $\langle\varphi_{\alpha,\beta}\rangle=\langle\varphi_\alpha\rangle$ for homogeneous Markov mixing statistics, with

$$p_{i,j}(\mathbf{r},\boldsymbol{\omega})=\frac{p_i}{\Lambda_i(\boldsymbol{\omega})}, \quad (4)$$

where $\Lambda_i(\boldsymbol{\omega})$ is the mean chord length for trajectories crossing material i in direction $\boldsymbol{\omega}$ [3]. Several generalisations of this model have been later proposed, including higher-order closure schemes [3,19].

In parallel, a family of Monte Carlo algorithms have been conceived in order to approximate the ensemble-averaged solutions to various degrees of accuracy [9,20,21]. Their common feature is that they allow a simpler treatment of transport in stochastic mixtures (typically by neglecting the correlations on particle trajectories induced by the spatial disorder), which might be convenient in practical applications. In this context, a prominent role is played by the so-called Chord Length Sampling (CLS) algorithm, which is supposed to solve the Levermore–Pomraning model for Markovian binary mixing [9,22,23]. The basic idea behind CLS is that the interfaces between the constituents of the stochastic medium are sampled on-the-fly during the particle displacements by drawing the distances to the following material boundaries from a distribution depending on the mixing statistics. The free parameters of the CLS model are the average chord length Λ_i through each material and the volume fraction p_i. Since the spatial configuration seen by each particle is regenerated at each particle flight, the CLS corresponds to an annealed disorder model, as opposed to the quenched disorder of the reference solutions, where the spatial configuration is frozen for all the traversing particles. Generalization of these Monte Carlo algorithms including partial memory effects due to correlations for particles crossing back and forth the same materials have been also proposed [9].

In order to quantify the accuracy of the various approximate models, comparisons with respect to reference solutions are mandatory. For instance, although originally formulated for Markov statistics, CLS has been extensively applied also to randomly dispersed spherical inclusions into background matrices, with application to pebble-bed and very high temperature gas-cooled reactors [20,21], and several benchmark problems have been examined in two and three dimensions [20,21,24,25]. Some methods to mitigate the errors between CLS and the reference solutions have been presented in the context of eigenvalue calculations, e.g., in [26]. For Markov mixing, a number of benchmark problems comparing CLS and reference solutions have been proposed in the literature so far [1,2,18,27,28], with focus exclusively on $1d$ geometries, either of the rod or slab type. Flat two-dimensional configurations have received less attention [10].

In a series of recent papers, some of the authors have provided reference solutions for particle transport in extruded two-dimensional and full three-dimensional random media with Markov statistics [29,30], where the spatial disorder has been generated by means of homogeneous and isotropic d-dimensional Poisson tessellations [31]. In this work, we will compare the CLS simulation results to the reference solutions for the classical benchmark problem proposed by Adams, Larsen and Pomraning for transport in stochastic media [1] and revisited by Brantley [2]. The case of $1d$ slab disorder has been considered previously in the literature [1,2,18,27,28] and will be reported here for the sake of completeness. In addition, we will also consider $2d$ extruded and full $3d$ Markov mixing configurations. The physical observables of interest will be the particle flux $\langle\varphi\rangle$, the transmission coefficient $\langle T\rangle$ and the reflection coefficient $\langle R\rangle$: we will examine the discrepancies between reference and CLS simulation results as a function of the benchmark configurations and of the system dimensionality d. In order to verify the consistency of the proposed results, the CLS calculations will be performed by using two independent Monte Carlo implementations of the CLS algorithm, in the TRIPOLI-4® code [32] and in the Mercury code [33,34], respectively.

This paper is organized as follows: in Section 2 we will recall the benchmark specifications that will be used in this work. In Sections 3 and 4 we will detail the methods and the algorithms that we have adopted in order to produce reference and CLS results, respectively. Simulation findings will be illustrated and discussed in Section 5. Conclusions will be finally drawn in Section 6.

2. Benchmark specifications

In order for the paper to be self-contained, we start by recalling the benchmark specifications that have been selected for this work, which are essentially taken from those originally proposed in [1,18], and later extended in [2,27,28].

We consider single-speed linear particle transport through a stochastic binary medium with homogeneous Markov mixing. The medium is non-multiplying, with isotropic scattering. The geometry consists of a cubic box of side $L=10$ (in arbitrary units), with reflective boundary conditions on all sides of the box except two opposite faces (say those perpendicular to the x axis), where leakage boundary conditions are imposed.[1] Two kinds of non-stochastic sources will be considered: either an imposed normalized incident angular flux on the leakage surface at $x=0$ (with zero interior sources), or a distributed homogeneous and isotropic normalized interior source (with zero incident angular flux on the leakage surfaces). Following the notation in [2], the benchmark configurations pertaining to the former kind of source will be called *suite* I, whereas those pertaining to the latter will be called *suite* II. The material properties for the Markov mixing are entirely

[1] In [1,18], system sizes $L=0.1$ and $L=1$ were also considered, but in this work we will focus on the case $L=10$, which leads to more physically relevant configurations.