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Poisson-Box Sampling algorithms for three-dimensional Markov binary mixtures

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ABSTRACT

Particle transport in Markov mixtures can be addressed by the so-called Chord Length Sampling (CLS) methods, a family of Monte Carlo algorithms taking into account the effects of stochastic media on particle propagation by generating on-the-fly the material interfaces crossed by the random walkers during their trajectories. Such methods enable a significant reduction of computational resources as opposed to reference solutions obtained by solving the Boltzmann equation for a large number of realizations of random media. CLS solutions, which neglect correlations induced by the spatial disorder, are faster albeit approximate, and might thus show discrepancies with respect to reference solutions. In this work we propose a new family of algorithms (called 'Poisson Box Sampling', PBS) aimed at improving the accuracy of the CLS approach for transport in d-dimensional binary Markov mixtures. In order to probe the features of PBS methods, we will focus on three-dimensional Markov media and revisit the benchmark problem originally proposed by Adams, Larsen and Pomraning [1] and extended by Brantley [2]: for these configurations we will compare reference solutions, standard CLS solutions and the new PBS solutions for scalar particle flux, transmission and reflection coefficients. PBS will be shown to perform better than CLS at the expense of a reasonable increase in computational time.

1. Introduction

Linear particle transport theory in random media is key to several applications in nuclear science and engineering, such as neutron diffusion in pebble-bed reactors or randomly mixed water-vapour phases in boiling water reactors [3–7], and inertial confinement fusion [8–10]. Material and life sciences as well as radiative transport also often involve particle propagation in random media [11–17].

In this context, the material cross sections composing the traversed medium and the particle sources are distributed according to some statistical laws, and the physical observable of interest is typically the ensemble-averaged angular particle flux $\langle\varphi(\mathbf{r},\boldsymbol{\omega})\rangle$, namely,

$$\langle\varphi(\mathbf{r},\boldsymbol{\omega})\rangle = \int \mathcal{P}(q)\varphi^{(q)}(\mathbf{r},\boldsymbol{\omega})dq, \tag{1}$$

where $\varphi^{(q)}(\mathbf{r},\ \boldsymbol{\omega})$ satisfies the linear Boltzmann equation corresponding to a single realization q, and $\mathcal{P}(q)$ is the stationary probability of observing the state q for the material cross sections and/or the sources [3,18]. In the following, we consider linear particle transport in binary stochastic mixing composed of two immiscible random media (say α and β).

Exact solutions for $\langle\varphi\rangle$, or more generally for some ensemble-averaged functional $\langle F[\varphi]\rangle$ of the particle flux, can be obtained using a so-called quenched disorder approach: an ensemble of medium realizations are first sampled from the underlying mixing statistics; then, the linear transport equation is solved for each realization by either deterministic or Monte Carlo methods, and the physical observables of interest $F[\varphi]$ are determined; ensemble averages are finally computed. In a series of recent papers, we have provided reference solutions for particle transport in d-dimensional random media with Markov statistics [19,20], where the spatial disorder has been generated by means of homogeneous and isotropic d-dimensional Poisson tessellations [21].

Reference solutions for particle transport in stochastic media are computationally expensive, so faster but approximate methods have been therefore proposed. A first approximate approach consists in deriving an expression for the ensemble-averaged flux $\langle\varphi\rangle$ in each material: this generally leads to an infinite hierarchy of equations, which ultimately requires a closure formula, such as in the celebrated Levermore-Pomraning model [3,5,22]. A second approach is based on Monte Carlo algorithms that reproduce

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the ensemble-averaged solutions to various degrees of accuracy by modifying the displacement laws of the simulated particles in order to take into account the effects of spatial disorder [9,23,24]. The Chord Length Sampling (CLS) algorithm is perhaps the most representative and best-known example of such algorithms: 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. It has been shown that the CLS algorithm formally solves the Levermore-Pomraning model for Markovian binary mixing [9,25,26]. 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. This means that the correlations on particle trajectories induced by the spatial disorder are neglected in the standard implementation of CLS. Generalization of these Monte Carlo algorithms including partial memory effects due to correlations for particles crossing back and forth between the same materials have been also proposed [9].

CLS, which had been originally formulated for Markov statistics, 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 [23,24]. In order to quantify the accuracy of CLS with respect to reference solutions for spherical inclusions, several comparisons have been proposed in two and three dimensions [23,24,27–29]. Some methods to mitigate the errors between CLS and the reference solutions have been presented in the context of eigenvalue calculations, e.g., in [30]. For Markov mixing specifically, a number of benchmark problems comparing CLS and reference solutions have been proposed in the literature so far [1,2,18,31,32] with focus on $1d$-geometries (either of the rod or slab type); flat $2d$ geometries have been considered in [10]. These benchmark comparisons have been recently extended to d-dimensional Markov geometries, for $d = 2$ (extruded) and $d = 3$ [33].

Not surprisingly, CLS solutions may display discrepancies as compared to reference solutions, whose relevance varies strongly with the system dimensionality, the average chord length and the material volume fraction [33]. For the case of $1d$ slab geometries with Markov mixing, possible improvements to the standard CLS algorithm accounting for partial memory effects for particle trajectories have been detailed [9], and numerical tests have revealed that these corrections contribute to palliating the discrepancies [2], although a generalization to higher dimensions seems hardly feasible with reasonable computational burden [9].

In this work we propose a new family of Monte Carlo algorithms aimed at improving the standard CLS for d-dimensional Markov media, yet keeping the increase in algorithmic complexity to a minimum. Inspiration comes from the observation that the physical observables related to particle transport through quasi-isotropic Poisson tessellations based on Cartesian boxes are almost identical to those computed for isotropic Poisson tessellations, for any dimension d [20,34], which confirms the considerations in [35]. This quite remarkable property suggests that the standard CLS algorithm can be extended by replacing the memoryless sampling of material interfaces by the sampling of d-dimensional Cartesian boxes sharing the statistical features of quasi-isotropic Poisson tessellations, so as to mimic the spatial correlations that would be induced by isotropic Poisson tessellations. We will call this class of algorithms Poisson Box Sampling (PBS).

In order to illustrate the behaviour of the PBS with respect reference solutions and to CLS, we will revisit the classical benchmark problem for transport in Markov binary mixtures proposed by Adams, Larsen and Pomraning [1] and revisited by Brantley [2]. The physical observables of interest will be the particle flux $\langle\varphi\rangle$, the transmission coefficient $\langle T\rangle$ and the reflection coefficient $\langle R\rangle$, for incident flux conditions and for uniform interior sources.

Table 1
Material parameters for the three cases of the benchmark configurations.

Case	Σ_α	Λ_α	Σ_β	Λ_β
1	10/99	99/100	100/11	11/100
2	10/99	99/10	100/11	11/10
3	2/101	101/20	200/101	101/20

This paper is organized as follows: in Section 2 we will recall the benchmark specifications that will be used for our analysis in dimension $d = 3$. In Section 3 we will illustrate the reference solutions for the benchmark problem obtained by using isotropic and quasi-isotropic Poisson tessellations: this preliminary investigation will allow establishing that quasi-isotropic tessellations yield results very close to those of isotropic tessellations, as expected based on previous investigations. Then, in Section 4 we will describe in detail the PBS algorithms, compare these methods to the reference solutions and to the standard CLS approach, and discuss their respective merits and drawbacks. Conclusions will be finally drawn in Section 5.

2. Benchmark specifications

In order for this paper to be self-contained, we briefly recall here the benchmark specifications that have been selected for this work, which are essentially drawn from those originally proposed in [1] and [18], and later extended in [2,31,32].

We consider mono-kinetic linear particle transport through a stochastic binary medium with homogeneous and isotropic 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. Two kinds of 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). 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 [2]. Markov mixing statistics are entirely defined by assigning the average chord length for each material $i = \alpha, \beta,$ namely Λ_i. The (homogeneous) probability p_i of finding material i at an arbitrary location within the box follows from

$$p_i = \frac{\Lambda_i}{\Lambda_i + \Lambda_j}. \quad (2)$$

By definition, the material probability p_i yields the volume fraction for material i. The cross sections for each material will be denoted as customary Σ_i for the total cross section and $\Sigma_{s,i}$ for the scattering cross section. The average number of particles surviving a collision in material i will be denoted by $c_i = \Sigma_{s,i}/\Sigma_i \le 1$. The physical parameters for the benchmark configurations are recalled in Tabs. 1 and 2: the benchmark specifications include three cases (numbered 1, 2 and 3, corresponding to different materials), and three sub-cases (noted *a, b* and *c*, corresponding to different c_i for a given material) for each case [1].

Following [2], the physical observables of interest for the benchmark will be the ensemble-averaged outgoing particle currents $\langle J\rangle$ on the two surfaces with leakage boundary con-