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Monte Carlo particle transport in random media: The effects of mixing statistics

Coline Larmier [a], Andrea Zoia [a,*], Fausto Malvagi [a], Eric Dumonteil [b], Alain Mazzolo [a]

[a] Den-Service d'Etudes des Réacteurs et de Mathématiques Appliquées (SERMA), CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France
[b] IRSN, 31 Avenue de la Division Leclerc, 92260 Fontenay aux Roses, France

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ABSTRACT

Particle transport in random media obeying a given mixing statistics is key in several applications in nuclear reactor physics and more generally in diffusion phenomena emerging in optics and life sciences. Exact solutions for the ensemble-averaged physical observables are hardly available, and several approximate models have been thus developed, providing a compromise between the accurate treatment of the disorder-induced spatial correlations and the computational time. In order to validate these models, it is mandatory to use reference solutions in benchmark configurations, typically obtained by explicitly generating by Monte Carlo methods several realizations of random media, simulating particle transport in each realization, and finally taking the ensemble averages for the quantities of interest. In this context, intense research efforts have been devoted to Poisson (Markov) mixing statistics, where benchmark solutions have been derived for transport in one-dimensional geometries. In a recent work, we have generalized these solutions to two and three-dimensional configurations, and shown how dimension affects the simulation results. In this paper we will examine the impact of mixing statistics: to this aim, we will compare the reflection and transmission probabilities, as well as the particle flux, for three-dimensional random media obtained by using Poisson, Voronoi and Box stochastic tessellations. For each tessellation, we will furthermore discuss the effects of varying the fragmentation of the stochastic geometry, the material compositions, and the cross sections of the background materials.

1. Introduction

Linear transport in heterogeneous and random media emerges in several applications in nuclear reactor physics, ranging from the analysis of the effects of the grain size distribution in burnable poisons (especially Gadolinium) and of Pu agglomerates in MOX fuel pellets, the quantification of water density variations in concrete structures and in the moderator fluid during operation (e.g., steam flow in BWRs) or accidents (e.g., local boiling in PWRs), the assessment of the probability of a re-criticality accident in a reactor core after melt-down (corium), or the investigation of neutron diffusion in pebble-bed reactors [1–3]. The spectrum of applications of stochastic media is actually far reaching [4–7], and concerns also inertial-confinement fusion [8], light propagation through engineered optical materials [9–11], atmospheric radiation transport [12–14], tracer diffusion in biological tissues [15], and radiation trapping in hot atomic vapours [16], only to name a few.

The stochastic nature of particle transport stems from the materials composing the traversed medium being randomly distributed according to some statistical law: thus, the total cross section, the scattering kernel and the source are in principle random fields. Particle transport theory in random media is therefore aimed at providing a description of the ensemble-averaged angular particle flux $\langle \varphi(\mathbf{r}, \mathbf{v}) \rangle$ and related functionals. For the sake of simplicity, in the following we will focus on mono-energetic transport in non-fissile media, in stationary (i.e., time-independent) conditions. However, these hypotheses are not restrictive, as described in [1].

A widely adopted model of random media is the so-called binary stochastic mixing, where only two immiscible materials are present [1]. In principle, it is possible to formally write down a set of coupled linear Boltzmann equations describing the evolution of the particle flux in each immiscible phase. Nonetheless, it has been shown that these equations form generally speaking an infinite hierarchy (exact solutions can be exceptionally found, such as for purely absorbing media), so that in most cases it is necessary to truncate the infinite set of equations with some appropriate closure formulas, depending on the underlying mixing statistics. Perhaps the best-known of such closure formulas goes under the name of the Levermore-Pomraning model, initially developed for homogeneous Markov mixing statistics [1,17]. Several generalisations of this model have been later

* Corresponding author.
E-mail address: andrea.zoia@cea.fr (A. Zoia).

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proposed, including higher-order closure schemes [1,18]. Along the development of deterministic equations for the ensemble-averaged flux, Monte Carlo methods have been also proposed, such as the celebrated Chord Length Sampling [3,19–21]. The common feature of these approaches is that they allow a simpler, albeit approximate, treatment of transport in stochastic mixtures, which might be convenient in practical applications where a trade-off between computational time and precision is needed [22,23].

In order to assess the accuracy of the various approximate models it is therefore mandatory to compute reference solutions for linear transport in random media. Such solutions can be obtained in the following way: first, a realization of the medium is sampled from the underlying mixing statistics (a stochastic tessellation model); then, the linear transport equations corresponding to this realization are solved by either deterministic or Monte Carlo methods, and the physical observables of interest are determined; this procedure is repeated many times so as to create a sufficiently large collection of realizations, and ensemble averages are finally taken for the physical observables.

For this purpose, a number of benchmark problems for Markov mixing have been proposed in the literature so far [24–29]. In a previous work [30], we have revisited the benchmark problem originally proposed by Adams, Larsen and Pomraning for transport in binary stochastic media with Markov mixing [24], and later extended in [26–29]. In particular, while these authors had exclusively considered 1*d* slab or rod geometries, we have provided reference solutions obtained by Monte Carlo particle transport simulations through 2*d* extruded and 3*d* Markov tessellations, and discussed the effects of dimension on the physical observables.

In this work, we further generalize these findings by probing the impact of the underlying mixing statistics on particle transport. The nature of the microscopic disorder is known to subtly affect the path of the travelling particles, so that the observables will eventually depend on the statistical laws describing the shape and the material compositions of the random media [6,7,12,25]. This is especially true in the presence of distributed absorbing traps [7]. We will consider three different stochastic 3*d* tessellations and compute the ensemble-averaged reflection and transmission probabilities, as well as the particle flux. Two distinct benchmark configurations will be considered, the former including purely scattering materials and voids, and the latter containing scattering and absorbing materials. This paper is organized as follows: in Section 2 we will introduce the mixing statistics that we have chosen, namely homogeneous and isotropic Poisson (Markov) tessellations, Poisson-Voronoi tessellations, and Poisson Box tessellations, and we will show how the free parameters governing the mixing statistics can be chosen in order for the resulting stochastic media to be comparable. In Section 3 we will illustrate the statistical features of such tessellations, which is key to understanding the effects on particle transport. In Section 4 we will propose two benchmark problems, provide reference solutions by using the Tripoli-4® Monte Carlo code, and discuss how mixing statistics affects ensemble-averaged observables. Conclusions will be finally drawn in Section 5.

2. Description of the mixing statistics

In this section, we introduce three mixing statistics leading to random media with distinct features. The subscript or superscript m will denote the class of the stochastic mixing: $m = \mathcal{P}$ for Poisson tessellations, $m = \mathcal{V}$ for Voronoi tessellations, and $m = \mathcal{B}$ for Box tessellations. For each stochastic model, we describe the strategy for the construction of three-dimensional tessellations, spatially restricted to a cubic box of side L. Without loss of generality, we assume that the cubes are centered at the origin.

2.1. Isotropic Poisson tessellations

Markovian mixing is generated by using isotropic Poisson geometries, which form a prototype process of stochastic tessellations: a domain included in a d-dimensional space is partitioned by randomly generated $(d-1)$-dimensional hyper-planes drawn from an underlying Poisson process [4]. In order to construct three-dimensional homogeneous and isotropic Poisson tessellations restricted to a cubic box, we use an algorithm recently proposed for finite d-dimensional geometries [31,32]. For the sake of completeness, here we briefly recall the algorithm for the construction of these geometries (further details are provided in [33]).

We start by sampling a random number of hyper-planes N_H from a Poisson distribution of parameter $4\rho_{\mathcal{P}}R$, where R is the radius of the sphere circumscribed in the cube and $\rho_{\mathcal{P}}$ is the (arbitrary) density of the tessellation, carrying the units of an inverse length. This normalization of the density $\rho_{\mathcal{P}}$ corresponds to the convention used in [4], and is such that $\rho_{\mathcal{P}}$ yields the mean number of $(d-1)$-hyperplanes intersected by an arbitrary segment of unit length. Then, we generate the planes that will cut the cube. We choose a radius r uniformly in the interval $[0, R]$ and then sample two additional parameters, namely, ξ_1 and ξ_2, from two independent uniform distributions in the interval $[0, 1]$. A unit vector $\mathbf{n} = (n_1, n_2, n_3)^T$ with components

$$n_1 = 1 - 2\xi_1$$
$$n_2 = \sqrt{1 - n_1^2}\cos(2\pi\xi_2)$$
$$n_3 = \sqrt{1 - n_1^2}\sin(2\pi\xi_2)$$

is generated. Denoting by $\mathbf{M}$ the point such that $\mathbf{OM} = r\mathbf{n}$, the random plane will finally obey $n_1x + n_2y + n_3z = r$, passing trough $\mathbf{M}$ and having normal vector $\mathbf{n}$. By construction, this plane does intersect the circumscribed sphere of radius R but not necessarily the cube. The procedure is iterated until N_H random planes have been generated. The polyhedra defined by the intersection of such random planes are convex. Some examples of homogeneous isotropic Poisson tessellations are provided in Fig. 1.

2.2. Poisson-Voronoi tessellations

Voronoi tessellations refer to another prototype process for isotropic random division of space [4]. A portion of a space is decomposed into polyhedral cells by a partitioning process based on a set of random points, called 'seeds'. From this set of seeds, the Voronoi decomposition is obtained by applying the following deterministic procedure: each seed is associated with a Voronoi cell, defined as the set of points which are nearer to this seed than to any other seed. Such a cell is convex, because it is obtained from the intersection of half-spaces.

In this paper, we will exclusively focus on Poisson-Voronoi tessellations, which form a subclass of Voronoi geometries [34–36]. The specificity of Poisson-Voronoi tessellations concerns the sampling of the seeds. In order to construct Poisson-Voronoi tessellations restricted to a cubic box of side L, we use the algorithm proposed in [36]. First, we choose the random number of seeds N_S from a Poisson distribution of parameter $(\rho_{\mathcal{V}}L)^3$, where $\rho_{\mathcal{V}}$ characterizes the density of the tessellation. Then, N_S seeds are uniformly sampled in the box $[-L/2, L/2]^3$. For each seed, we compute the corresponding Voronoi cell as the intersection of half-spaces bounded by the mid-planes between the selected seed and any other seed. In order to avoid confusion with the Poisson tessellations described above, we will mostly refer to Poisson-Voronoi geometries simply as Voronoi tessellations in the following. Some examples of Voronoi tessellations are provided in Fig. 2.