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Original Article

A PROPOSAL ON ALTERNATIVE SAMPLING-BASED MODELING METHOD OF SPHERICAL PARTICLES IN STOCHASTIC MEDIA FOR MONTE CARLO SIMULATION

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ABSTRACT

Chord length sampling method in Monte Carlo simulations is a method used to model spherical particles with random sampling technique in a stochastic media. It has received attention due to the high calculation efficiency as well as user convenience; however, a technical issue regarding boundary effect has been noted. In this study, after analyzing the distribution characteristics of spherical particles using an explicit method, an alternative chord length sampling method is proposed. In addition, for modeling in finite media, a correction method of the boundary effect is proposed. Using the proposed method, sample probability distributions and relative errors were estimated and compared with those calculated by the explicit method. The results show that the reconstruction ability and modeling accuracy of the particle probability distribution with the proposed method were considerably high. Also, from the local packing fraction results, the proposed method can successfully solve the boundary effect problem. It is expected that the proposed method can contribute to the increasing of the modeling accuracy in stochastic media.

1. Introduction

Stochastic media with randomly distributed spherical particles have been utilized for very high temperature reactors (pebble bed and prismatic reactors), radiation shielding materials, and the blankets of fusion reactors. For spherical particle modeling in Monte Carlo (MC) simulations, three kinds of methods are known: repeated structure, explicit method, and chord length sampling (CLS) method. The CLS is a modeling method that randomly samples the chord lengths on the ongoing neutron track during the MC simulation. The CLS method has high calculation efficiency because the MC simulation can be pursued with few geometries as well as automatic modeling of stochastic geometries. The CLS method was first proposed by Zimmerman and Adams [1]. After that, Murata et al [2] and Donovan et al [3] proposed the

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sampling scheme for the calculation of multiplication factors. Recently, many works have attempted to increase or to confirm the accuracy of CLS [4–6]. A technical issue referred to as the *boundary effect* has been noted when trying to confirm the accuracy of the CLS method [7]. In finite stochastic media, spherical particles cannot be located outside of the medium boundaries; therefore, the volume packing fraction is gradually decreased at the region near the boundary of the stochastic media. Also, the number density in the center region (which is not affected by the wall boundaries) is changed. Fig. 1 is an example of the failure in treating the boundary effect using CLS in a previous study [7]. With resampling scheme in the CLS method, only the track lengths are simulated in the Monte Carlo simulation. Therefore, the spherical particle resampling with the method developed in the previous study was pursued near the boundary as the positions of the spherical particle cannot be properly considered.

In this study, an alternative CLS method based on the geometrical cross section of spheres was proposed to increase the sampling accuracy in finite stochastic media. First, the characteristics of stochastic particle distribution were analyzed, and then corrections were applied to the proposed method. Finally, the proposed method was verified.

2. Methods

The alternative CLS method proposed in this study is a sampling method of the center position for the spherical particle geometry modeling. The conventional CLS method samples the chord length from the current position to the surface of the sphere (Fig. 2A). As shown in Fig. 2B, the proposed method samples the center position of the sampled particle. Hence, it gives an advantage in treating the boundary effect of finite stochastic media because the sphere's location is known.

To develop the proposed sampling method with high accuracy, analysis of the center position distribution of the spherical particles is essential when sampling the spherical particle. In the next section, the distribution properties of the center positions in stochastic media were analyzed with the explicit method. Using the information from the following section, geometry sampling and modeling methods were proposed.

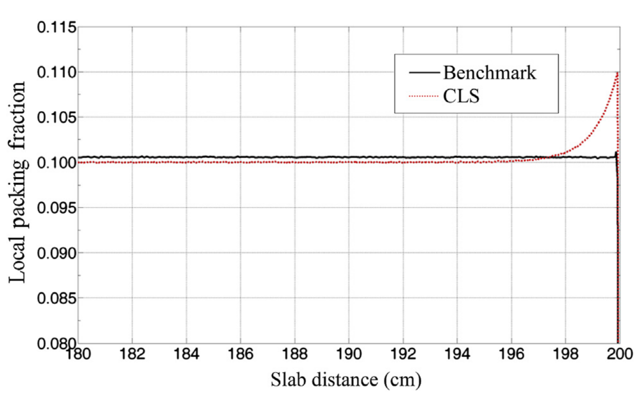

Fig. 1 – Spatial distribution of local packing fractions estimated in a previous study [7]. Source: http://www.tandfonline.com/doi/full/10.1080/00411450.2011.639432, copyright holder: Taylor & Francis Group, LLC, year of copyright: 2011.

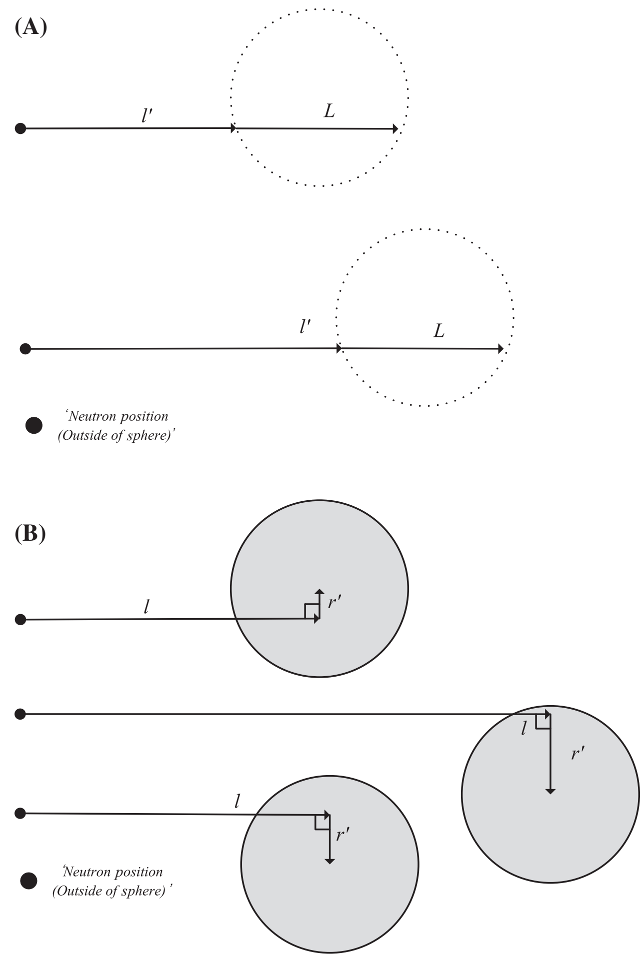

Fig. 2 – Introduction of schemes with the conventional chord length sampling (CLS) and proposed methods. (A) Sampling of chord lengths with conventional CLS method. (B) Sampling of particle position in the proposed method.

2.1. *Analysis of the random spherical particle distribution*

For the analysis of the distribution of the spherical particles, a benchmark problem was set. The medium is a 102 cm × 22 cm × 22 cm hexahedron, and the radius (r) of the spherical particles, which is filled in the medium, is 1 cm. For the 10%, 20%, 30%, and 40% volume packing fractions, the particle positions were randomly sampled with the modified random sequential addition method [8]. In the modified random sequential addition method, the particles are first sampled in the medium without considering the overlaps of the spherical particles. Then, the particles, which are overlapped with each other, are moved with $0.1r$ length as shown in Fig. 3. If the particles are moved to the out-of-boundary of the medium, they are removed and re-sampled in the medium. The movement process is repeated and stopped until