Development of random geometry capability in RMC code for stochastic media analysis

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ABSTRACT

Simulation of particle transport in random media poses a challenge for traditional deterministic transport methods, due to the significant effects of spatial and energy self-shielding. Monte Carlo method plays an important role in accurate simulation of random media, owing to its flexible geometry modeling and the use of continuous-energy nuclear cross sections. Three stochastic geometry modeling methods including Random Lattice Method, Chord Length Sampling and explicit modeling approach with mesh acceleration technique, have been developed in RMC to simulate the particle transport in the dispersed fuels. The verifications of the accuracy and the investigations of the calculation efficiency have been carried out. The stochastic effects of the randomly dispersed fuel particles are also analyzed. The results show that all three stochastic geometry modeling methods can account for the effects of the random dispersion of fuel particles, and the explicit modeling method can be regarded as the best choice.

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1. Introduction

The particle transport in random media has many applications, such as in the designs and analysis of Very High Temperature Gas-Cooled Reactors (VHTRs), light water reactors (LWRs) with Fully Ceramic Microencapsulated (FCM) fuel and some experimental research reactors.

The simplest approach to model such stochastic media is to homogenize the fuel particles and matrix. However, this kind of mixing approximation would lead to large errors in the calculations as it completely ignores the spatial self-shielding effects. In the previous researches, the particle distributions in stochastic media are assumed the regular lattice, which fails to account for the random distribution of the particles. The regular lattice also leads to an incorrect fuel-to-moderator ratio due to the inevitable truncation of the fuel particles at the outer boundary.

When using the traditional deterministic transport methods, approximate corrections have been developed to deal with the significant spatial and energy self-shielding effects of stochastic media. Taking the advantages of the flexible geometry modeling and the use of continuous-energy nuclear cross sections, Monte Carlo codes play an important role in the accurate simulation of

particle transport in random media, providing the benchmark for approximate deterministic codes.

However, if the random distributed fuel particles are defined cell by cell in the input file of a Monte Carlo code, the computational cost would be mainly consumed on calculating the distances to every surface of the fuel particles. In the previous researches, the particle distributions are described in regular lattice, which fails to account for the random distribution of the particles. Many Monte Carlo codes have the ability to treat the stochastic media, such as MCNP5 (Brown and Martin, 2004), SERPENT (Leppänen, 2007), MVP (Murata et al., 1997).

Among these codes, several approaches have been developed to deal with the stochastic effect, which can be divided into two categories: the approximate approach and explicit modeling approach. For the approximate approaches, there are Random Lattice Method, Chord Length Sampling and so on. For the explicit modeling approach, some researchers have focused on the fast algorithms for neutron tracking in stochastic media, such as Liang and Ji (2012) and SERPENT code (Leppänen, 2013).

In order to deal with the random microscopic particles, three stochastic geometry modeling methods have been developed in RMC code, which are Random Lattice Method, Chord Length Sampling and explicit modeling approach with mesh acceleration technique. The stochastic geometry modeling is based on ray tracking process, and applied to three dimensional continuous-energy Monte Carlo simulations. RMC is a continuous-energy Reactor Monte Carlo neutron and photon transport code being developed
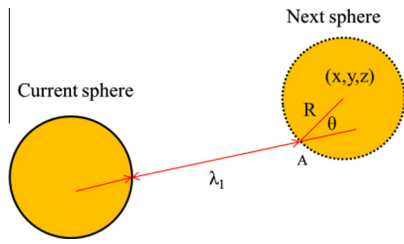
Fig. 1. On-the-fly sampling of sphere.

by Department of Engineering Physics at Tsinghua University, Beijing (Wang et al., 2015).

The remainder of this paper is organized as follows. Section 2 introduces the three stochastic geometry modeling methods and the implementations of these methods in RMC. The verifications of the accuracy and the investigations of the calculation efficiency are carried out in Section 3. The stochastic effects of the randomly dispersed fuel particles are also analyzed in this section. The comparisons between these three methods are discussed in Section 4, and the conclusions are presented in Section 5.

2. Computational method

2.1. Geometry modeling in RMC

RMC adopts constructive solid geometry technique represented by surfaces, cells, universes and lattices for flexible geometry modeling. The ray-tracking method is employed as main option for particle transport. A cell can be filled by a universe, while a universe consists of several cells. Lattice is a special kind of universe, which consists of cells with a certain regulation. Besides the current regular cubic and hexagonal lattices in RMC, a new chord-length-sampling lattice and a new dispersed-sphere lattice have been developed to describe the stochastic media in which a large number of spheres are distributed randomly in the matrices.

2.2. Random Lattice Method

The Random Lattice Method is firstly introduced by MCNP5 (Brown and Martin, 2004). Each time a particle encounters a cell filled by universe flagged as stochastic, a random translation (Eq. (1)) will be performed on the coordinates of the particle. Here, ξ_1, ξ_2 and ξ_3 are independent random numbers in (0,1). δ_x, δ_y and δ_z are independent maximum displacements in x, y and z directions. Special treatments are also needed to recover the fission sites for newborn neutrons in the eigenvalue calculation.
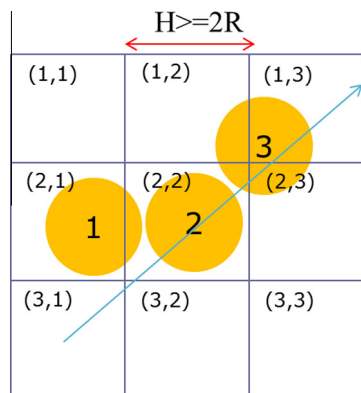

Fig. 2. Ray tracking with mesh acceleration.

$$\begin{aligned}
x &= x + (2\xi_1 - 1) \times \delta_x \\
y &= y + (2\xi_2 - 1) \times \delta_y \\
z &= z + (2\xi_3 - 1) \times \delta_z
\end{aligned} \quad (1)$$

Random Lattice Method can realize the randomness of geometry with little expense on memory and calculation time. The limitation of Random Lattice Method is that the randomness of geometry is restricted in the regular lattices. Moreover, the fuel particles are probably cut by the boundary of cells.

2.3. Chord Length Sampling

The Chord Length Sampling is firstly introduced by Zimmerman and Adams (1991). The core idea of Chord Length Sampling is to use probability distribution functions to describe the distance (i.e. the chord length) by which the particles will travel in the matric or in the fuel particles. By using the exponential distribution approximately, the positions of new fuel particles are sampled "on-the-fly" during the tracking process rather than being calculated explicitly. As shown in Fig. 1, the distance to the position A to enter the next sphere after leaving the current sphere is firstly sampled according to Eq. (2). Secondly, the angle θ in which the neutron enters the next sphere are sampled, and then the center (x, y, z) of the next sphere are determined.

The chord length in the matric is sampled by Eq. (2), while the particles are simulated explicitly in the fuel particles. Here, λ_1 denotes the chord length in matric, R denotes the radius of fuel particles, and PF denotes the packing fraction of particles fuel.

$$p(\lambda_1) = \frac{3}{4R} \cdot \frac{\text{PF}}{1 - \text{PF}} \cdot e^{-\lambda_1 \frac{3}{4R} \frac{\text{PF}}{1-\text{PF}}} \quad (2)$$

The Chord Length Sampling greatly reduces the memory and calculation time. Chord Length Sampling suffers from the drawbacks of the approximation of exponential distribution. This method cannot avoid the boundary cutting either.

In order to implement the Chord Length Sampling, a new chord-length-sampling lattice has been developed in RMC.

2.4. Explicit modeling with mesh acceleration

Different from the Random Lattice Method and Chord Length Sampling which use the approximations for realizing the random geometry, the explicit modeling treats the distributions of fuel particles or pebbles explicitly, without any approximations.

A new dispersed-sphere lattice has been developed in RMC. The spheres can be filled by universes with detailed structures such as multi-level spheres or sub-level dispersed-sphere lattice for double-heterogeneous reactors.

The explicit modeling of random geometry in RMC can either generate the random coordinates of fuel particles/pebbles inside the RMC code or read the coordinates from a separate file.

The mesh acceleration technique uses the virtual meshes which divide the domain of dispersed-sphere lattice to locate the positions of fuel particles. The sphere intersecting with the meshes are marked as belonging to these meshes. As in Fig. 2, sphere 1 belongs to meshes (2,1) and (2,2), sphere 2 belongs to (2,2), while sphere 3 belongs to (1,2), (1,3), (2,2) and (2,3).

This mesh acceleration technique is employed for both the generation of distributions of fuel particles or pebbles, and the geometry tracking process.

Random Sequential Addition (RSA) method (Widom, 1966) is usually used to generate the distributions of fuel particles, which cannot overlap with the boundary and other fuel particles. In the original RSA, the computational complexity is $O(N^2)$ due to the global overlap checking, where N is the total number of particles. In the mesh acceleration technique, the overlap checking of a new