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One-step Monte Carlo global homogenization based on RMC code

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ABSTRACT

Due to the limitation of the computers, the conventional homogenization method is based on many assumptions and approximations, and some tough problems such as energy spectrum and boundary condition are faced. To deal with those problems, the Monte Carlo global homogenization is adopted. The Reactor Monte Carlo code RMC is used to study the global homogenization method, and the one-step global homogenization method is proposed. The superimposed mesh geometry is also used to divide the physical models, leading to better geometric flexibility. A set of multigroup homogenization cross sections is online generated for each mesh under the real neutron energy spectrum and boundary condition, the cross sections are adjusted by the superhomogenization method, and no leakage correction is required. During the process of superhomogenization, the author-developed reactor core program NLSP3 is used for global calculation, so the global flux distribution and equivalent homogenization cross sections could be solved simultaneously. Meanwhile, the calculated homogenization cross section could accurately reconstruct the non-homogenization flux distribution and could also be used for fine calculation. This one-step global homogenization method was tested by a PWR assembly and a small reactor model, and the results show the validity.

1. Introduction

The conventional two-step physical calculation method uses the microscopic cross sections of the nuclides to generate the homogenization cross sections of various assemblies, and then uses those homogenization cross sections to carry out the global diffusion calculation. Therefore, the calculated homogenization cross sections are very important for the accuracy of reactor physical analysis. At the same time, a series of problems such as resonance effect [1], leakage correction [2] and equivalent homogenization [3] need to be considered in the homogenization calculation.

For the deterministic physical analysis, the above problems would be solved with approximations and assumptions, and some local correction is made to ensure the balance between computational efficiency and accuracy. Therefore, it is inevitable to reduce the flexibility of the deterministic methods.

Compared with the deterministic methods, the continuous energy Monte Carlo method (MC) could accurately describe all kinds of geometric lattice configurations, avoid the complicated resonance self-shielded calculation, retain more energy information, have higher calculation accuracy [4] and wider adaptability. Therefore, the Monte Carlo Homogenization (MCH) is a development tendency of the reactor physics analysis.

In recent years, the Monte Carlo Homogenization (MCH) has developed a lot. Dr. Zhang [6] from Tsinghua University studied the calculation method of multigroup cross sections with MC, modified the multigroup cross sections with superhomogenization theory (SPH). Dr. Li [7] developed a MCH code named MCMC, and proposed the Super Equivalent method (SPE) based on the generalized equivalence theory (GET) and SPH [8]. At the same time, SERPENT [5] and McCARD [9] also have done a lot of work on this topic, especially about the *BN* leakage correction and diffusion coefficient.

During the calculation of the assemblies, because it is a nonlinear calculation process, the real energy spectrum can hardly be given in advance. At the same time, the real boundary conditions are approximated by the reflective boundary conditions, leading to a large deviation of the generated cross sections. Therefore the *BN* leakage correction is required to modify the cross sections. For this

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problem, the global homogenization [10] is put forward. This method hope to solve all the homogenization problems at once, so that the global calculation accuracy could be in line with the continuous energy MC calculation.

In this paper, the Reactor Monte Carlo Code (RMC) [11] is used to study the global homogenization method. To achieve better geometric flexibility, the superimposed mesh geometry [12] is adopted to do the geometric division, and the homogenization cross sections of each mesh are online generated. Since each assembly or mesh has the real boundary condition and energy spectrum, the leakage correction is not required. The author-developed reactor core program NLSP3 are coupled with RMC code, to verify the generated cross section and to conduct the SPH correction. In each iterative step of SPH equivalent correction, the NLSP3 [13] carries out the global calculation, so the global flux distribution and equivalent homogenization cross sections could be worked out at the same time once iterative convergence, realizing the one-step global homogenization calculation.

The one-step homogenization method was tested by a self-built example, a pressurized water reactor (PWR) assembly and a small reactor model. The results prove the validity of the method. In this paper, the Section 2 describes the homogenization calculation based on the Monte Carlo method, especially about the equivalent homogenization for the superimposed mesh geometry, as well as the introduction of the author-developed reactor core program NLSP3. The calculation flowchart is given in the Section 3. In the end, the numerical verification and conclusion are given.

2. Theory

This section mainly introduces the theoretical model and computational characteristics of the Monte Carlo homogenization method. It gives a brief description of the MC method, and analyzes the relevant formulas of the Monte Carlo homogenization method. At the same time, to highlight the geometric feature of the one-step homogenization method, the superimposed mesh geometry is also introduced, as well as the mesh-divided figures of the calculation examples in the subsequent numerical verification. Finally, the author-developed core program NLSP3 is also given.

2.1. Monte Carlo method

Monte Carlo method, also called stochastic simulation method, infers the solution of the estimated values through computer simulation of particle transport process, observation and analysis of a large number of particle behaviors. The basic idea of MC is to approximate the integral with the mathematical expectation of the random variable g(x) which is under the probability density function f(x),

$$\langle g \rangle = \int g(r) \cdot f(r) dr \tag{1}$$

The MC calculation is based on the continuous energy library and high performance computer, to obtain the expectation and standard deviation of the quantities concerned. The continuous energy cross sections could be used for accurate geometric and energy modeling without any approximation. Since each neutron is independent in the simulation, MC calculation has obvious advantage in parallelism.

When it is difficult to deal with some new types of fuel or reactor systems by traditional deterministic method, it is considered an ideal choice to conduct continuous energy MC simulation to generate multigroup cross sections for the global diffusion calculation. The advantages are mainly reflected in the following aspects:

(1) For the MC method, there is no limitation in geometry modeling, and almost no approximation in the transport process;
(2) With the continuous energy cross section, there is no need to deal with resonance problem;

The RMC code is a continuous energy Monte Carlo code developed by REAL team at Tsinghua University, it can carry out reactor physical calculation efficiently. The jobs of global homogenization in this paper is achieved in the RMC code.

2.2. Global homogenization

The reactor is composed of different assemblies, and the most accurate calculation method is to do the global fine calculation. However, due to the limitation of computer, it is still unable to cope with the huge cost of the global fine calculation, so the two-step calculation is the main calculation method now, and the key point of the two-step calculation method is the assembly homogenization.

The global diffusion calculation usually adopts nodal method or finite difference method. In both the nodal method and the finite difference method, the two-step calculation has to do the assembly homogenization, and the generated multigroup cross sections will be used for the following global diffusion calculation. Therefore, how to correctly obtain the homogenization cross sections and keep the results of homogenization calculation and non-homogenization calculation consistent is very important.

Compared with the results of non-homogenization calculation, a lot of information is lost in homogenization calculation. So the homogenization cross sections must be able to guarantee the conservation of some important parameters. The conservation means the integral of some physical quantities obtained on each homogenization region remain equal between the global diffusion calculation after homogenization and the non-homogenization transport calculation. Generally, the following three physical quantities are selected:

The reaction rate of all energy groups is conserved:

$$\int_{V_i} \overline{\Sigma}_{x,g} \overline{\phi}_g(r) dV = \int_{V_i} \Sigma_{x,g} \phi_g(r) dV \qquad x = a, f, s, \cdots \qquad g = 1, \cdots, G \tag{2}$$

The interface current of all energy groups is conserved:

$$-\int_{S_{ik}} \overline{D}_g(r) \frac{\partial}{\partial u} \overline{\phi}_g(r) \cdot dS = \int_{S_{ik}} J_g^u(r) \cdot dS \quad g = 1, \cdots, G \quad k = 1, 2, \cdots, K \tag{3}$$

The eigenvalue of reactor is conserved:

$$-\sum_{k=1}^{K}\int_{S_{ik}}\overline{D}_g(r)\nabla\overline{\phi}_g(r)\cdot dS+\int_{V_i}\overline{\Sigma}_{t,g}\overline{\phi}_g(r)dV$$
$$=\sum_{g'=1}^{G}\left(\int_{V_i}\overline{\Sigma}_{g'\to g}\overline{\phi}_g(r)dV+\frac{1}{k}\int_{V_i}\chi_g\nu\overline{\Sigma}_{f,g'}\overline{\phi}_{g'}(r)dV\right)\quad g=1,\cdots,G\quad i=1,2,\cdots,I \tag{4}$$

where, $\overline{\Sigma}_{x,g}$ is the homogenization cross section of a reaction type, $\overline{\phi}_g(r)$ is the flux distribution after homogenization. $\Sigma_{x,g}$ is the non-homogenization cross section of a reaction type, $\phi_g(r)$ is the global flux distribution before homogenization. $\overline{D}_g$ is the diffusion coefficient. J_g^u is the net current on a surface. χ_g is the fission neutron spectrum.

Normally, the homogenization cross section satisfying the above three conservation conditions could be called the equivalent homogenization constant. Assuming that all the homogenization parameters are constant within the region, then the "ideal" homogenization cross section could be strictly defined:

$$\overline{\Sigma}^i_{x,g}\equiv\frac{\int_{V_i}\Sigma_{x,g}\phi_g(r)dV}{\int_{V_i}\overline{\phi}_g(r)dV}\qquad x=a,f,s,\cdots\qquad g=1,\cdots,G \tag{5}$$

However, it is difficult to calculate the strictly defined homogenization cross section. It is commonly to use the traditional volume weight method, and the boundary condition choose the reflective boundary condition. At the same time, the global homogenization flux distribution is approximated by the flux distribution of the assembly transport calculation. So, the calculated homogenization cross section is redefined:

$$\overline{\Sigma}^i_{x,g}\equiv\frac{\int_{V_i}\Sigma_{x,g}\phi_{A,g}(r)dV}{\int_{V_i}\phi_{A,g}(r)dV}\qquad x=a,f,s,\cdots\qquad g=1,\cdots,G \tag{6}$$

where, $\phi_{A,g}(r)$ is the flux distribution of the assembly transport calculation.

Using the Monte Carlo method to calculate the neutron flux and reaction rate, according to the relationship between the neutron flux ϕ, reaction rate R and macroscopic cross section Σ, we can have the following formula to calculate the total cross section, absorption cross section, scattering cross section and fission cross section,

$$\Sigma=\frac{R}{\phi} \tag{7}$$

The RMC code choose the track length to calculate the neutron flux and various reaction rates. The generation of the homogenization cross section is derived below.

The definition of volume weight group flux is

$$\phi_g=\frac{\iiint_{V\,t}\int_{E_g}^{E_{g-1}}\phi(r,E,t)dEdtdV}{V} \tag{8}$$

Monte Carlo calculation is a static calculation process, the time t in the above formula and the following formula means the time from the generation to the disappearance of the neutron. According to the definition of flux

$$\phi(r,E,t)=\nu N(r,E,t) \tag{9}$$

We can have the following formula,

$$\phi_g=\frac{\iiint_{V\,t}\int_{E_g}^{E_{g-1}}\nu N(r,E,t)dEdtdV}{V} \tag{10}$$

If we change the integral of time to the integral of length, then,

$$\phi_g=\frac{\iiint_{V\,s}\int_{E_g}^{E_{g-1}}N(r,E,t)dEdsdV}{V} \tag{11}$$

where, $\boldsymbol{s}$ is the distance from the generation to disappearance of the neutron, v is the velocity of neutrons. In Monte Carlo method, the neutron density is equivalent to the sum of neutron weight W per volume, and the distance is equivalent to the track length TL, so the above formula could be rewritten as

$$\phi_g=\frac{\int_{E_g}^{E_{g-1}}dE\int_V dV\sum_{i=1}^{N}W\cdot TL_V^i(E)}{V\sum_{i=1}^{N}W_0^i} \tag{12}$$

when, $W.\ TL^i$ is the product of weight and track length of the ith neutron at energy E and volume V; W is the neutron's weight; N the total number of neutrons.

For reaction rate, we could have the similar formula,

$$\Sigma_g\phi_g=\frac{\int_{E_g}^{E_{g-1}}dE\int_V dV\sum_{i=1}^{N}W\cdot TL_V^i(E)\cdot\Sigma(r,E)}{V\sum_{i=1}^{N}W_0^i} \tag{13}$$

The integral of energy in the above formula could be obtained by summing in Monte Carlo method. According to the above formula, the calculation formula of the homogenization cross section could be written as,

$$\Sigma_g=\frac{\int_{E_g}^{E_{g-1}}dE\int_V dV\sum_{i=1}^{N}W\cdot TL_V^i(E)\cdot\Sigma(r,E)}{\int_{E_g}^{E_{g-1}}dE\int_V dV\sum_{i=1}^{N}W\cdot TL_V^i(E)} \tag{14}$$

For calculation within each energy interval, we have to know the distribution of fission neutrons in each energy interval, i. e$\chi(E)$, the

fission energy spectrum. The fission energy spectrum of different fission isotopes are not the same, but there is little difference. Therefore, the approximated energy spectrum could be calculated by experimental simulation. For Monte Carlo method, we could get the fission energy spectrum by counting the fission neutrons' energy.

$$\chi(E) = p(E) \tag{15}$$

where, $p(E)$ the probability of neutron production in each energy interval.

For the scattering cross section, the neutron energy before and after scattering were recorded, and the energy interval was determined and statistically analyzed to obtain the scattering probability,

$$P_{g\to g'} = \frac{\int_{E_{g'}}^{E_{g'-1}} dE' \int_{E_g}^{E_{g-1}} dE \int_V \phi(r,E)\Sigma_s(r,E\to E')dV}{\int_{E_g}^{E_{g-1}} dE \int_V \phi(r,E)\Sigma_s(r,E)dV} \tag{16}$$

The inter-group transfer cross section is the product of the scattering fraction and scattering cross section

$$\Sigma_{s,g\to g'} = P_{g\to g'} \bullet \Sigma_{s,g} \tag{17}$$

The homogenization cross section generated from the above formulas can't guarantee the conservation of the integral reaction rates in all homogenization regions, and the continuity of the interface current is also neglected. Therefore, it is necessary to modify the homogenization cross section calculated by the traditional method, and try to maintain the conservation of reaction rate, interface current and eigenvalue before and after homogenization, that is the equivalent homogenization.

In this research, the superhomogenization theory is chosen for the equivalent homogenization. The basic idea is to adjust the homogenization cross section and flux to make sure that the reaction rates are conserved before and after homogenization.

At present, the superhomogenization theory requires only one equivalent factor named *SPH* in each region and each energy interval. As shown in the equation, we want the reaction rate to be conservative

$$\overline{R} = \overline{\Sigma}_g \overline{\phi}_g = \Sigma_g \phi_g = R \tag{18}$$

$$\textit{Let } \mu_g \textit{ means the SPH factoe, } \mu_g^k = \frac{\overline{\phi}_g^k}{\phi_g^k} \tag{19}$$

$$\textit{Then we will have } \Sigma_g^{k+1} = \mu_g^k \overline{\Sigma}_g^k \tag{20}$$

where, the superscript k here is the iterative time. As can be seen from the above equations, the solution of *SPH* requires an iterative process. During the iterative process, we have to continuously calculate the new flux distribution and update the *SPH* factors by using the reactor core program. This iterative process could be done by MC or deterministic program, for efficiency, we choose a deterministic program – the author-developed reactor core program NLSP3.

2.3. Superimposed mesh geometry

Monte Carlo method could describe some very complex physical models, and a large number of statistical particle histories are required to converge to an acceptable solution. The superimposed mesh geometry was proposed [13] to achieve variance reduction. The superimposed mesh eliminates the need to specify the geometry in many superfluous finely divided geometric regions. Particles are transported in the physical geometry, but their variance reduction weight window parameters are taken from the superimposed mesh. Therefore, the superimposed mesh is very favorable in visualization and simplify.

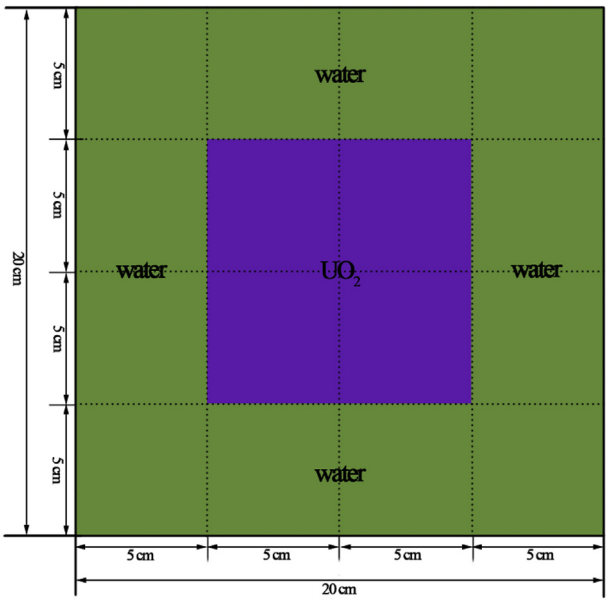

Fig. 1. The superimposed mesh geometric division of the first example.

To improve the geometric flexibility of the global homogenization method and make it possible to more effectively use the superimposed mesh capability, this global homogenization method is based on the superimposed mesh geometry.

There are three problems calculated in this paper, the first one is a self-built model, it consists of pure water with a density of 1.0 g/cm3 and uranium dioxide with a density of 9.8 g/cm3, the superimposed mesh geometric division for the first model shows in Fig. 1.

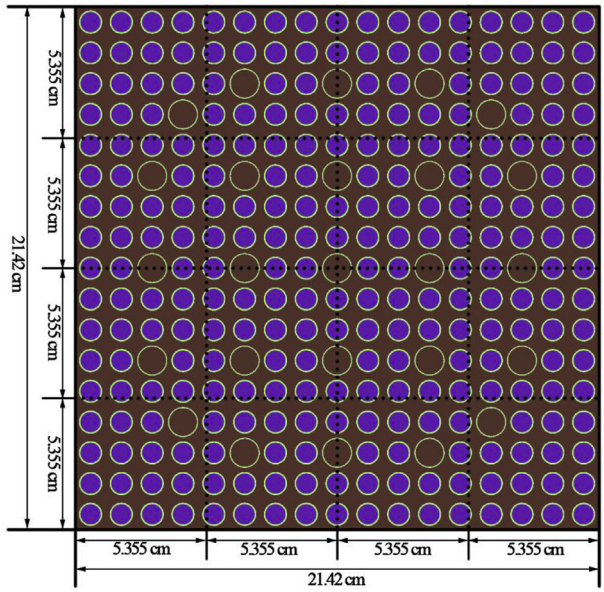

Fig. 2. The superimposed mesh geometric division of the second example.

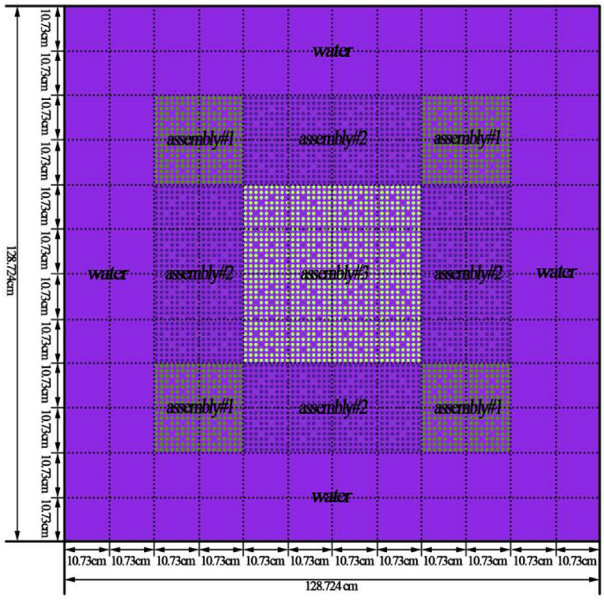

Fig. 3. The superimposed mesh geometric division of the third model.

There are a total of 4*4 = 64 meshes, and each one has its own homogenization cross section generated from the volume weight method. Because each mesh is at a different spatial position, even though its material composition is the same, its cross section may be different. Meanwhile, due to the random fluctuation of MC, the scattering probability and fission neutron energy spectrum obtained is also different. The size of each mesh is 5 cm*5 cm, which could be directly set as the size of nodes of the reactor core program NLSP3, without further geometric division.

The second example is a standard PWR assembly divided into 4*4 = 16 meshes. Each mesh contains fuel rods and control rod guidance. Fig. 2 shows the mesh geometric division. We will also generate a set of homogenization cross section for each mesh, and use the NLSP3 code to do the SPH equivalent homogenization correction.

The third example is a calculation model of a small reactor. Inside the core is a 4*4 assembly layout, and outside the core is water reflection layer. There are 12*12 = 144 meshes, each of which is 10.727 cm*10.727 cm. See Fig. 3 for specific geometric division. The RMC code will calculate a set of homogenization cross section for each mesh, then the NLSP3 code will do the SPH correction iteration to modify the section data of each mesh. When the SPH correction iteration is completed, the global calculation is finished at the same time.

2.4. The NLSP3 code

The NLSP3 code (see Fig. 4) was independently developed by the author, and it could be used for global reactor core calculation. This code is based on the SPN theory and nonlinear iterative method.

The SPN theory is the simplified spherical harmonics method for solving the neutron transport equation. It was widely studied and it shows a great potential in the Next Generation Reactor Physics Calculation because of its better accuracy than diffusion method. The following equation shows the SP_N equation,

$$-\frac{n(n-1)}{(2n+1)(2n-1)\Sigma_t}\nabla^2\phi_{n-2}(r)-\frac{2n^2+2n-1}{(2n+3)(2n-1)\Sigma_t}\nabla^2\phi_n(r) -\frac{(n+1)(n+2)}{(2n+1)(2n+3)\Sigma_t}\nabla^2\phi_{n+2}(r)+\Sigma_t\phi_n(r) =S\delta_{n0} \tag{21}$$

where, $\delta_{n,0}$ is the Dirichlet function, and S is the source term.

The SP3 equation can be get when N is equal to three. After deformation, a similar form to the diffusion equation could be obtained and the some traditional nodal method could be used to solve the SP3 equation, such as the nonlinear iterative method. Assuming that the neutron scattering and the source term are

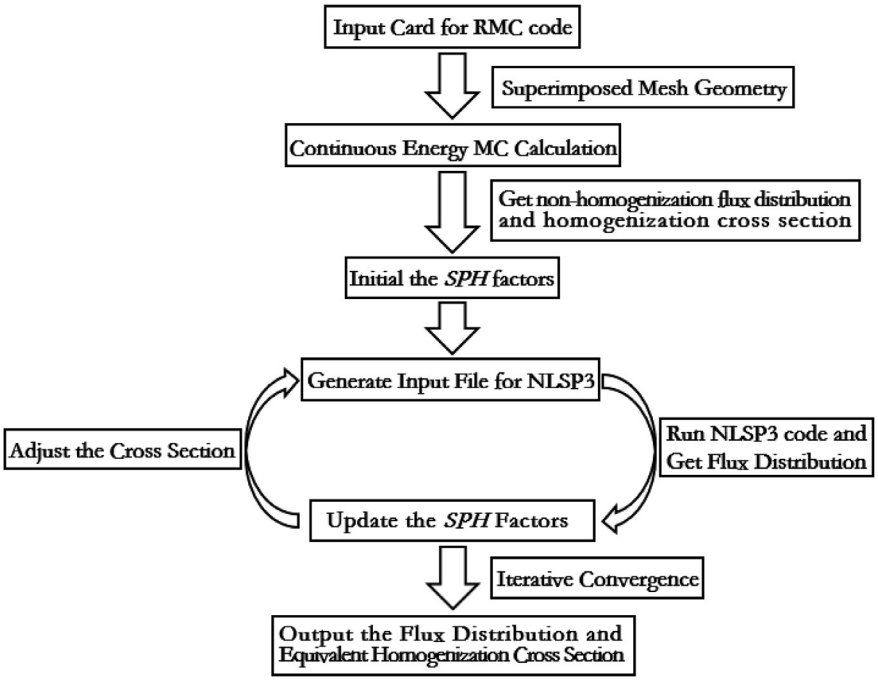

Fig. 4. The flowchart of the one-step homogenization method.

isotropic, and the *nth* high order scattering is zero, then the specific form of the SP3 equation and the boundary conditions shows as follow,

$$-D^k_{0,g}\nabla^2\phi^k_{0,g}(r)+\Sigma^k_{r0,g}\phi^k_{0,g}(r)-2\Sigma^k_{r0,g}\phi^k_{2,g}(r)=S^k_{0,g}(r) \tag{22.a}$$

$$-D^k_{2,g}\nabla^2\phi^k_{2,g}(r)+\Sigma^k_{r2,g}\phi^k_{0,g}(r)-\frac{2}{5}\Sigma^k_{r0,g}\phi^k_{0,g}(r)=-\frac{2}{5}S^k_{0,g}(r) \tag{22.b}$$

$$\begin{aligned}J^k_{0,gu+}=&-D^{k,FDM}_{1,gu+}\left(f^{k+1}_{0,gu-}\overline{\phi}^{k+1}_{0,g}-f^k_{0,gu+}\overline{\phi}^k_{0,g}\right)-D^{k,NOD}_{1,gu+}\left(f^{k+1}_{0,gu-}\overline{\phi}^{k+1}_{0,g}+f^k_{0,gu+}\overline{\phi}^k_{0,g}\right)\\&-D^{k,FDM}_{3,gu+}\left(f^{k+1}_{2,gu-}\overline{\phi}^{k+1}_{2,g}-f^k_{2,gu+}\overline{\phi}^k_{2,g}\right)-D^{k,NOD}_{3,gu+}\left(f^{k+1}_{2,gu-}\overline{\phi}^{k+1}_{2,g}+f^k_{2,gu+}\overline{\phi}^k_{2,g}\right)\end{aligned} \tag{24.a}$$

$$\begin{aligned}J^k_{2,gu+}=&-D^{k,FDM}_{2,gu+}\left(f^{k+1}_{2,gu-}\overline{\phi}^{k+1}_{2,g}-f^k_{2,gu+}\overline{\phi}^k_{2,g}\right)-D^{k,NOD}_{2,gu+}\left(f^{k+1}_{2,gu-}\overline{\phi}^{k+1}_{2,g}+f^k_{2,gu+}\overline{\phi}^k_{2,g}\right)\\&-D^{k,FDM}_{4,gu+}\left(f^{k+1}_{0,gu-}\overline{\phi}^{k+1}_{0,g}-f^k_{0,gu+}\overline{\phi}^k_{0,g}\right)-D^{k,NOD}_{4,gu+}\left(f^{k+1}_{0,gu-}\overline{\phi}^{k+1}_{0,g}+f^k_{0,gu+}\overline{\phi}^k_{0,g}\right)\end{aligned} \tag{24.b}$$

where,

$$\begin{aligned}D^k_{0,g}=&\frac{1}{3\Sigma^k_{t,g}}D^k_{2,g}=\frac{9}{35\Sigma^k_{t,g}}\Sigma^k_{r0,g}=\Sigma^k_{t,g}-\Sigma^k_{s,gg'}\Sigma^k_{r2,g}\\=&\frac{9}{5}\Sigma^k_{t,g}-\frac{4}{5}\Sigma^k_{s,gg'},D^k_{2,g}=\frac{9}{35\Sigma^k_{t,g}},\Sigma^k_{r0,g}=\Sigma^k_{t,g}-\Sigma^k_{s,gg'},\Sigma^k_{r2,g}\\=&\frac{9}{5}\Sigma^k_{t,g}-\frac{4}{5}\Sigma^k_{s,gg'}\end{aligned} \tag{22.c}$$

The source term expression,

$$\begin{aligned}S^k_{0,g}(r)=&\Sigma^G_{\substack{g'=1\\g'\neq g}}\Sigma^k_{0,g'g}\left[\phi^k_{0,g}(r)-2\phi^k_{2,g}(r)\right]\\&+\frac{1}{K_{eff}}\chi^k_g\Sigma^G_{g'=1}\nu\Sigma^k_{f,g'}\left[\phi^k_{0,g'}(r)-2\phi^k_{2,g'}(r)\right]\end{aligned} \tag{22.d}$$

At the boundary, we have the neutron flux and current under the Marshak boundary condition as follow, where, the superscript "*M*" represents the quantities at the node boundary.

$$J^{\pm}_0(r)=\frac{1}{4}\phi^M_0(r)\pm\frac{1}{2}\vec{\mathbf{n}}\cdot J^M_0(r)-\frac{3}{16}\phi^M_2(r) \tag{23.a}$$

$$J^{\pm}_2(r)=\frac{21}{80}\phi^M_2(r)\pm\frac{1}{2}\vec{\mathbf{n}}\cdot J^M_2(r)-\frac{3}{80}\phi^M_0(r) \tag{23.b}$$

The conventional nonlinear iterative method is based on the nodal method and nonlinear iterative strategy, which is characterized by the use of the simplified CMFD formula of the neutron diffusion equation containing the nodal coupling corrective coefficients in global calculation. Adopting the conventional nonlinear iterative method to solve the SP3 equation, the numerical instability problem is found during the coupling correction of the high-order flux. Even though in other nodal approaches, the numerical instability problem is still existing when CMFD formula is used to speed up the calculation on the SPN equation. So, a new nonlinear iterative method is proposed with the using of a new coupling corrective relationship.

The new coupling corrective relationship focuses on the coupling at the angle, and seems a bit more complicated than the conventional one. Except for the calculation at the vacuum boundary, the coupling corrective coefficients have many ways to calculate, which brings in more margin to deal with the numerical instability.

The core program NLSP3 is developed to achieve the new nonlinear iterative method for solving SP3 equation. And it had been verified by some benchmarks, such as 2D-IAEA and 3D-TAKEDA. The flowchart of the NLSP3 code is shown in the figure below.

3. Flowchart of one-step global homogenization

This section mainly introduces the process of the one-step homogenization method, and gives the corresponding calculation flowchart. The one-step global homogenization method is based on RMC code and NLSP3 program, and it focuses on the global homogenization. The SPH method is chose to do the equivalent homogenization, and the global calculation is also finished while the iteration is converged. The detailed calculation process of the one-step global homogenization method is as follows, shown in Fig. 4.

1. Write RMC input card for the calculation examples, as well as the superimposed mesh geometric division;
2. Perform continuous energy MC calculation to get the non-homogenization flux distribution and the homogenization cross section;
3. Initialize the SPH factors, the initial SPH factors are set to be 1;
4. Generate the input file for the reactor core program NLSP3, and run NLSP3;

Table 1
The calculation results of the self-built example.

Data types	result
Relative standard deviation of non-homogenization flux	1.0000E-02
Flux maximum deviation compared with non-homogenization flux	0.0025%
Relative standard deviation of fine calculation flux	4.4775E-04
Flux maximum deviation compared with fine calculation flux	2.4198%
Total calculation time (mins)	0.5580
Calculation time for SPH iterative (mins)	0.0823

Table 2
The calculation results of the standard PWR assembly.

Data types	result
Relative standard deviation of non-homogenization flux	1.7490E-02
Flux maximum deviation compared with non-homogenization flux	0.0023%
Relative standard deviation of fine calculation flux	1.1389E-03
Flux maximum deviation compared with fine calculation flux	1.4119%
Total calculation time (mins)	4.2597
Calculation time for SPH iterative (mins)	0.0788

Table 3
The calculation results of the small reactor model.

Data types	result
Relative standard deviation of non-homogenization flux	5.3096E-03
Flux maximum deviation compared with non-homogenization flux	0.0042%
Relative standard deviation of fine calculation flux	5.2126E-04
Flux maximum deviation compared with fine calculation flux	1.8291%
Total calculation time (mins)	33.0032
Calculation time for SPH iterative (mins)	0.2515

5. Update the SPH factors with the new homogenization flux distribution, determine whether the values of SPH factors converges;
6. Use the updated SPH factors to adjust the cross sections;
7. If converged, output the flux distribution and the equivalent homogenization cross section, or go back to the step 4;

4. Calculation results

To verify the one-step global homogenization method, a self-built example, a standard PWR assembly and a small reactor model are calculated. The calculations focus on the numerical accuracy of the one-step global homogenization method for reconstructing global flux distribution with the generated homogenization cross section. The reconstructed flux distribution is compared with the non-homogenization flux distribution and the fine-mesh calculated flux distribution.

The three calculation examples are all based on superimposed mesh geometry, the details are shown in Figs. 1–3. During the one-step global homogenization calculation, the RMC code firstly works out the non-homogenization flux distribution and homogenization cross section, then the NLSP3 code carries out the SPH iterative calculation with the homogenization cross section.

The NLSP3 code has four iterative convergence criterions to control the calculation, among them, the nonlinear convergence criterion is used to determine whether the coupling correction factors have been stable, the Keff convergence criterion is used to guarantee the value of Keff convergence, the outer convergence criterion and inner convergence criterion are used to achieve the source iterative calculation.

In the calculation process of the three examples in this paper, the same iterative convergence criterion is used, in which the nonlinear convergence criterion is 1.0E-04, the Keff convergence criterion is 1.0E-04, the outer convergence criterion is 1.0E-04, and the inner convergence criterion is 1.0E-05. Meanwhile, the convergence criterion of SPH is 1.0E-03.

For the self-built example, shown in Fig. 1. RMC performs the non-homogenization calculation with 200 cycles, 20 of them are inactive cycles, and each cycle has 500 particles. While for the fine calculation, there are 500 cycles, 50 of them are inactive cycles, and each cycle has 100,000 particles. The details are shown in Table 1.

For the standard PWR assembly, shown in Fig. 2, RMC performs non-homogenization calculation with 200 cycles, 20 of them are inactive cycles, and each cycle has 5000 particles. While for the fine calculation, there are 500 cycles, 50 of them are inactive cycles, and each cycle has 500,000 particles. The details are shown in Table 2.

For the small reactor model, shown in Fig. 3, RMC performs non-homogenization calculation with a total of 500 cycles, 100 of them are inactive cycles, and each cycle has 10,000 particles. While for the fine calculation, there are 500 cycles, 100 of them are inactive cycles, and each cycle has 1000,000 particles. The details are shown in Table 3.

It could be seen from the calculation results that the one-step global homogenization method could reconstruct the non-homogenization flux distribution with very high accuracy, and the generated homogenization cross section could also be used for fine-mesh calculation.

The one-step global homogenization method can simultaneously work out the homogenization cross sections and global flux distribution. For global variance reduction, if the global flux distribution is available, we can set the weight windows parameters with the following formula,

$$W_{th} = \frac{2}{\beta + 1} \cdot \frac{\phi_i}{\max(\phi_i)} \tag{25}$$

where, W_{th} is the lower weight windows, $\beta$is the ratio of upper

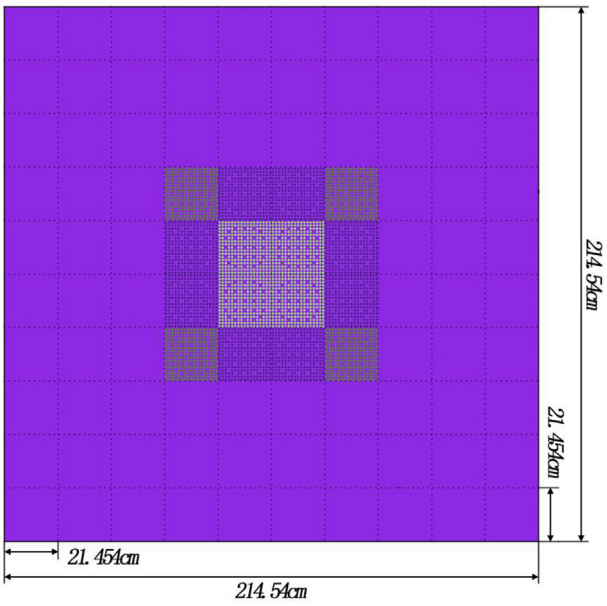

Fig. 5. The deep penetrating mode of the small reactor.

Table 4
The results of self-built small reactor mode.

Quantities	RMC direct simulation	RMC simulation after one-step method
AV.Re	5.1544E-03	1.2260E-03
AV.FOM	4.9475E+01	1.2295E+03
σ.Re	5.1543E-03	1.2260E-03
$\sigma_{max}/\sigma_{min}$	383.66	13.74
Time (mins)	760.7848	541.1342

weight windows to the lower weight windows, normally 5. ϕ_i is the flux in the *ith* mesh, max(ϕ_i)is the maximum flux within all the mesh.

The one-step global homogenization method is based on the superimposed mesh geometry, so the mesh weight windows technique in RMC is used for variance reduction. A deep penetrating mode (Fig. 5) is built based on the mode of small reactor, this example is similar to the mode of small reactor, except that there are two additional reflecting layers around the reactor core. Use the one-step global homogenization method to work out the homogenization cross sections, and then to get the global flux distribution with fine-mesh calculation. Eq. (25) is used to find out the weight windows parameters, and the global calculation is performed.

The one-step global homogenization method makes sense for global variance reduction. In order to better quantify the global variance reduction, there are three kinds of reference quantity [14]:

Average relative deviation:

$$AV.\mathrm{Re} = \sqrt{\frac{\sum_{i=1}^{N}\mathrm{Re}_i^2}{N}} \tag{26}$$

Average figure of merit.

$$AV.FOM = \frac{N}{T\cdot\sum_{i=1}^{N}\mathrm{Re}_i^2} \tag{27}$$

Standard Deviation of Relative Deviation:

$$\sigma_{\mathrm{Re}} = \sqrt{\frac{1}{N}\cdot\sum_{i=1}^{N}\mathrm{Re}_i^2 - \frac{1}{N^2}\cdot\left(\sum_{i=1}^{N}\mathrm{Re}_i^2\right)^2} \tag{28}$$

To demonstrate the value of global variance reduction, the results calculated by RMC directly and the results after one-step global homogenization method are compared, and the calculated results show in Table 4. Where, $\sigma_{max}/\sigma_{min}$ is the ratio of the biggest variance to the lowest variance, it is used to measure the effect of flattening the variance.

As can be seen from Table 4, the Average Figure of Merit was increased by 25 times. Meanwhile, to more intuitively view the effect of one-step global homogenization method on flattening variance, a map (Fig. 6) is made to show the variance distribution of the whole reactor. It is obvious that the one-step global homogenization method can flatten variance, and can greatly achieve variance reduction. Therefore, it is proved from the above numerical verifications that the one-step global homogenization method can make sense for global variance reduction.

In conclusion, the RMC code and NLSP3 code are coupled to achieve superhomogenization correction. Since the NLSP3 code is a deterministic program, even though dozens or hundreds of iterations are required in the calculation, the NLSP3 code takes much

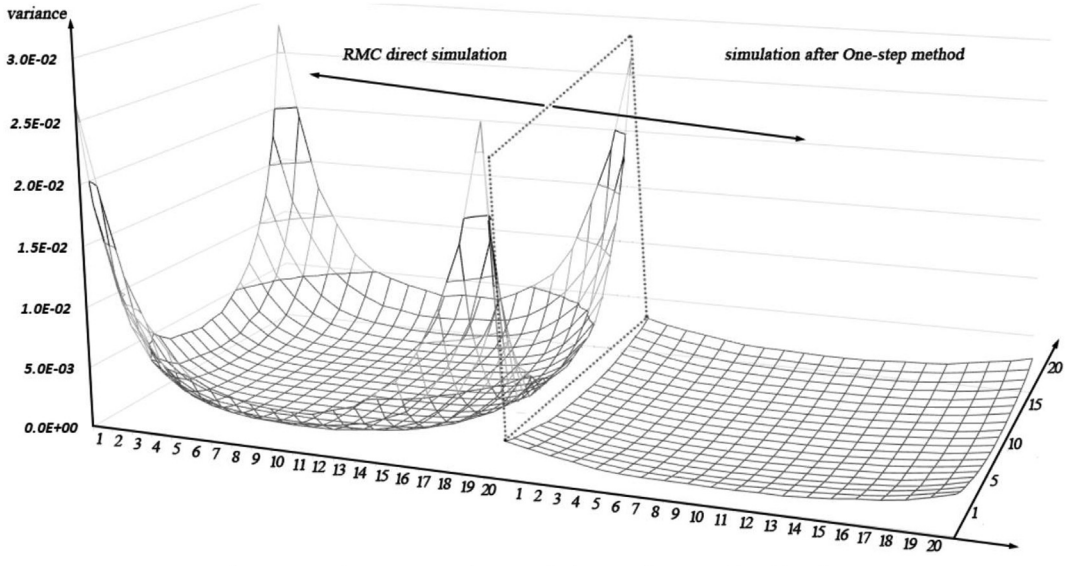

Fig. 6. The comparison of the variance distribution.

less time than RMC, significantly lower than the RMC non-homogenization calculation, so the SPH iterative correction calculation is very fast. Meanwhile, the numerical verifications shows that the one-step global homogenization method has great value in global homogenization and global variance reduction.

5. Conclusion

The conventional two-step physical calculation method consists of the assembly calculation and the global diffusion calculation, and the homogenization cross section is very important for reactor physics calculation. However, due to the limitation of the computer, the conventional homogenization method is based on many assumptions and approximations, and some tough problems are faced. In order to solve these problems, the global homogenization method based on Monte Carlo was proposed. This method hope to solve all the homogenization problems at once, so that the calculation accuracy could be in line with the continuous energy MC calculation. Meanwhile, since the calculation example is under the real boundary condition and energy spectrum, there is no need to do the *BN* leakage correction.

The global homogenization method was studied with the RMC code and NLSP3 code, among which the RMC code is a Monte Carlo code developed at Tsinghua University and the NLSP3 code is reactor core program independently developed by the author. The one-step global homogenization method is put forward after coupling the RMC and NLSP3, and it could work out the equivalent homogenization cross section and the flux distribution at the same time, which has higher efficiency and flexibility. In order to improve the geometric flexibility, the homogenization calculation could be based on the superimposed mesh geometry, and the cross section of each mesh could be used directly by the NLSP3 code, no more geometric division is needed.

The one-step global homogenization method chooses the superhomogenization theory to do the equivalent correction, and the cross section after equivalent correction has high accuracy. Even though only few particles are used in the non-homogenization Monte Carlo calculation, the accuracy of the global calculation with the generated cross section is still very high. There are three examples were calculated, the results show that the homogenization cross section generated by the one-step global homogenization method could be used to reconstruct non-homogenization flux distribution with high accuracy.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.net.2019.04.001.

References

[1] T. Hideki, M. Yasushi, Accuracy of interpolation methods for resonance self-shielding factors, Nucl. Sci. Technol. 18 (2) (1981) 152–161.
[2] I. Petrovic, P. Benoist, BN Theory: Advances and New Models for Neutron Leakage Calculation, Plenum Press, New York, 1996, pp. 223–281.
[3] J.H. Won, N.Z. Cho, Discrete ordinates method-like transport computation with equivalent group condensation and angle-collapsing for local/global iteration, Ann. Nucl. Energy 38 (4) (2011) 846–852.
[4] S. Liu, J. Liang, Q. Wu, et al., BEAVRS full core burnup calculation in hot full power condition by RMC code, Ann. Nucl. Energy 101 (2017) 434–446.
[5] J. Leppanen, M. Pusa, E. Fridman, Overview of the methodology for spatial homogenization in the Serpent 2 Monte Carlo code, Ann. Nucl. Energy 96 (2016) 126–136.
[6] P. Zhang, Research on the Reactor Physics Analysis Methods and Characteristics of Supercritical Water-Cooled reactor, PhD Thesis, Tsinghua University, 2012.
[7] M.C. Li, Research on Lattice Homogenization via Continuous-Energy Monte Carlo Method, PhD Thesis, Tsinghua University, 2012.
[8] A. Yamamoto, Improvement of SPH method for pin-by-pin core calculations, Nucl. Sci. Technol. 41 (12) (2004) 1155–1165.
[9] H.J. Shim, McCARD: Monte Carlo code for advanced reactor design and analysis, Nucl. Eng. Technol. 44 (2) (2012) 161–176.
[10] W. Boyd, Reactor multi-group cross sction generation for fine-mesh deterministic neutron transport simulations, PhD Thesis, Institute of Technology, Massachusetts, 2017.
[11] K. Wang, Z.G. Li, et al., RMC – a Monte Carlo code for reactor core analysis, Ann. Nucl. Energy 82 (2015) 121–129.
[12] J.S. Hendricks, Superimposed Mesh Plotting in MCNP. LA-UR-01-1003, 2001.
[13] Q.Q. Pan, H.L. Lu, D.S. Li, K. Wang, A new nonlinear iterative method for SPN theory, Ann. Nucl. Energy 110C (2017) 920–927.
[14] Q.Q. Pan, J.J. Rao, K. Wang, The optimal source bias method based on RMC code, Ann. Nucl. Energy 121 (2018) 525–530.