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Equivalence treatment in homogenization via Monte Carlo method

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ABSTRACT

The multi-group constants generated via continuous energy Monte Carlo method do not satisfy the equivalence between heterogeneous and homogeneous calculation. To meet the requirement of equivalence, the general equivalence theory (GET) and the superhomogenization method (SPH) are applied to the Monte Carlo based group constants. Both of the methods improved accuracy. Inheriting the essences of GET and SPH, the super equivalence method (SPE) is developed in this paper to overcome the limitations of the two conventional equivalence techniques. The three methods have been implemented into the Monte Carlo based homogenization code MCMC. Test calculations were carried out in a simplified PWR reactor core and the C5G7 MOX fuel benchmark. The study has shown that the equivalence treatment is necessary in Monte Carlo homogenization calculations and the SPE method can meet the requirement.

1. Introduction

Currently, the reactor core calculation in the framework of deterministic method can be divided into two stages: an assembly-level transport calculation, followed by a core-level diffusion calculation. One of the most important issues in the two-stage analysis of reactor core is to generate of the accurate homogenized multi-group constants which directly influence the accuracy of the core results. The current state-of-the-art methodology has limited capabilities in providing highly accurate results for the new, more complex designs (e.g., arbitrary geometry, increased heterogeneity). On the other hand, the recent developments in computational technologies have led to a major decline in calculation cost. Consequently, dense studies have been made in recent years in Monte Carlo based homogenized cross sections and group parameters for the deterministic reactor simulation codes (Ilas and Rahnema, 2003; Tohjoh et al., 2005; Rahnema et al., 2006; Van der Marck et al., 2006; Fridman and Leppänen, 2011; Hart and Maldonado, 2014; Nelson, 2014).

One of the most attractive aspects of Monte Carlo method is its ability to deal with almost arbitrarily complex geometry. To generate the homogenized cross sections through point-wise energy Monte Carlo method provides an almost direct access to the evaluated nuclear data. There is no need for the multi-group condensation of the cross sections or treatments of resonance shielding, which has not yet been well solved in the complicated problems in deterministic methods. Another advantage of using Monte Carlo method for homogenization is its versatility. The same code and data bank can be used for a wide range of applications, almost any fuel or reactor configuration, without loosing the reliability of the calculation scheme. This is not always the case with deterministic lattice transport codes, which often rely on various application-specific methods and data libraries.

To generate homogenized group constants via Monte Carlo method in the framework of two-step reactor physics calculation, two main problems should be considered and solved, one of which is Monte Carlo based generation methods for multi-group constants, and the other is the equivalence treatment because the infinite lattice of identical symmetric motives assumption is still used.

A code, named "Monte Carlo Multi-group Constants Generation Code", or MCMC, as part of RMC Program, is being developed in Tsinghua University. To generate the homogenized group constants for reactor core analysis is the designated capability of the RMC Program. The Monte Carlo multi-group constants homogenization methods have been investigated and both assembly and core level validations have shown the encouraging agreements with the references. Meanwhile, the numerical results have also revealed that the equivalence treatment is necessary for Monte Carlo homogenization.

General equivalence theory (GET) and the superhomogenization method (SPH) have been applied to satisfy the equivalence requirement in deterministic methods. The paper has implemented GET

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and SPH into MCMC code and the improved accuracy is observed. However, both of the conventional methods have their limitations. The super equivalence method (SPE) is thus proposed to preserve the surface currents, the reaction rates and the eigenvalue. The methods are introduced in Sections 2 and 3. In Section 4, the numerical results are presented for different equivalence methods. Concluding remarks are given in Section 5.

2. MCMC homogenization methods

Brief description of MCMC homogenization methods is provided in this section to make this paper thorough.

2.1. General cross sections

We follow the work by Redmond (1997) to generate the general cross sections, i.e. the total, absorption, neutron generation cross sections.

The flux, ϕ_g, and the reaction rate, $\Sigma_g\phi_g$, are calculated by track length estimator

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

$$\Sigma_g\phi_g = \frac{\int_{E_g}^{E_{g-1}} dE \int_V dV \sum_{i=1}^N WTL_V^i(E)\Sigma(r,E)}{V\sum_{i=1}^N W_0^i} \tag{2}$$

where, $WTL_V^i(E)$: weight of ith particle times the track length of ith particle at energy E in volume region V; V: volume of region of interest; W_0^i: original weight of particle i; N: number of particle histories tracked; $\Sigma(r,E)$: cross section as a function of energy and position; Σ_g: then can be calculated by the following equation

$$\Sigma_g = \frac{\int_{E_g}^{E_{g-1}} dE \int_V dV \sum_{i=1}^N WTL_V^i(E)\Sigma(r,E)}{\int_{E_g}^{E_{g-1}} dE \int_V dV \sum_{i=1}^N WTL_V^i(E)} \tag{3}$$

2.2. Group transfer cross sections and Legendre components

The calculation of the group-to-group cross sections and Legendre components is not explicit because the differential scattering cross sections do not exist in point-wise interaction data. The scattering event method is proposed to calculate the group transfer cross sections and Legendre components, or P_n cross sections. In this method, the scattering event is simulated using an analog Monte Carlo estimator, the variations in angle or energy are tallied when the scattering event occurs.

For the scattering matrix, the fraction of neutrons scattering from group g to g' is estimated. The scattering fraction can be written as:

$$P_{g\to g'} = \frac{\int_{E_{g'}}^{E_{g'-1}} dE' \int_{E_g}^{E_{g-1}} dE \int_V dV \phi(r,E)\Sigma_s(r,E\to E')}{\int_{E_g}^{E_{g-1}} dE \int_V dV \phi(r,E)\Sigma_s(r,E)} \tag{4}$$

The group-to-group cross section is then calculated by multiplying the corresponding scattering fraction by the homogenized total scattering cross section:

$$\Sigma_{s,g\to g'} = P_{g\to g'}\Sigma_{s,g} \tag{5}$$

The P_n cross sections in one dimension is illustrated as an example. The P_n cross sections in one dimension are defined as follows:

$$\Sigma_{s,n,g\to g'} = \frac{\int_{E_g}^{E_{g'-1}} dE' \int_{E_g}^{E_{g-1}} dE \int_z \phi_n(z,E)\Sigma_{s,n}(z,E\to E')dz}{\int_{E_g}^{E_{g-1}} dE \int_z \phi_n(z,E)dz} \tag{6}$$

where $\Sigma_{s,n}$ is the nth Legendre component.

Assuming that the energy dependencies of the P_n fluxes are proportional to the energy dependence of the P_0 flux,

$$\phi_n(z,E) = C_n\phi_0(z,E) \tag{7}$$

Eq. (6) can be written as

$$\Sigma_{s,n,g\to g'} = \frac{\int_{-1}^{1}\left[\int_{E_{g'}}^{E_{g'-1}} dE' \int_{E_g}^{E_{g-1}} dE \int_z dz\phi(z,E)\Sigma_s(z,E)f(E\to E',\mu_0)\right]P_n(\mu_0)d\mu_0}{\int_{E_g}^{E_{g-1}} dE \int_z \phi(z,E)dz} \tag{8}$$

Set a number of cosine tally bins from −1 to 1. When a scattering event is simulated, the scattering angle is calculated and stored in the corresponding cosine bins. After the Monte Carlo simulation is finished, the numerical integral is calculated to obtain the P_n cross sections.

2.3. Diffusion coefficients

One of the main problems when trying to estimate the group constants via Monte Carlo method is how to define the homogenized diffusion coefficient. Various Monte Carlo methods have been used to define diffusion coefficients (Gast, 1981; Milgram, 1997; Ilas and Rahnema, 2003; Pounders, 2006; Keller, 2007; Gorodkov and Kalugin, 2009). The large number of approximately equivalent definitions indicates that the problem has not been completely solved.

In this paper, we use the most common practice, i.e. the transport cross section $\Sigma_{tr,g}$, to define the diffusion coefficient:

$$D_g = \frac{1}{3\Sigma_{tr,g}} \tag{9}$$

The first order Legendre moment of scattering $\Sigma_{s,1,g\to g}$, which presence accounts for linearly anisotropic scattering, is used in our study to define the transport cross section:

$$\Sigma_{tr,g} = \Sigma_{t,g} - \Sigma_{s,1,g\to g} \tag{10}$$

3. Equivalence treatment methods

3.1. General equivalence theory

This section and the following one briefly describe GET and SPH, since they are widely used in deterministic reactor physics analysis and the transplantation into Monte Carlo based homogenization is not much difficult.

Koebke and Henry set up the bases of GET, in which the heterogeneity factor is highlighted (Henry et al., 1978; Koebke, 1978). The detailed analysis of homogenization techniques for light water reactor has been performed by Smith (1986), with an emphasis on the discontinuity factor method.

In GET, the reference net neutron current of the heterogeneous system is preserved through the discontinuity factor at surface area of homogenized region. The discontinuity factor, $f_u^{\pm}$, is defined as follows:

$$f_u^{\pm} = \frac{\phi^{u\pm}}{\overline{\phi}^{u\pm}} \tag{11}$$

where $\phi^{u\pm}$ and $\overline{\phi}^{u\pm}$ represent the surface flux of a region obtained by heterogeneous and homogeneous calculation, respectively.

For the single assembly with zero net current boundary conditions, the homogenized fluxes are spatially flat. Since the assembly-averaged fluxes in the homogeneous and heterogeneous assembly calculation are equal, the discontinuity factors are simply