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Multi-Group Neutron Cross Sections and Scattering Matrix Calculations Via Monte Carlo Method

Ahmad Pirouzmand, Fatemeh Mohammadhasani

Department of Nuclear Engineering, School of Mechanical Engineering, Shiraz University, Shiraz, Iran.
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ABSTRACT

This study describes a new methodology to estimate multi-group neutron cross sections and scattering matrix elements from a Monte Carlo simulation, particularly from MCNPX 2.7 code. The geometric flexibility associated with the Monte Carlo method makes it very suitable for the generation of highly accurate multi-group constants. While the deterministic lattice codes are not capable of dealing with energy as a continuous variable the Monte Carlo codes such as MCNPX make use of a continuous energy cross sections data for neutron transport calculations. To determine the scattering matrix, an output file of a MCNPX run (so-called PTRAC file) with all relevant source, collision and terminal events of the simulation is used. First, by a separately special program in MATLAB, the PTRAC file is read and tracks are selected in the geometrical region for which one wants to calculate the multi-group constants. Then, information such as coordinates of the particle position, particle direction with coordinates axes, energy and weight of the particle are extracted. The multi-group scattering matrix elements are generated via the weight-to-flux ratio method using the above data available in the PTRAC file. The proposed method is validated using three benchmark problems involve a slab, a pin cell, and a fuel assembly of Tehran research reactor (TRR). The generated multi-group constants via presented method and multiplication factor calculation presents a good comparison to the reference values.

Keywords: Multi-group cross sections generation, Monte Carlo method, PTRAC file, weight to flux ratio

1. INTRODUCTION

Multi-group neutron cross sections have many applications in the reactor physics. They are the foundation of discrete ordinates and diffusion theory codes as well as nodal diffusion theory codes [1]. Multi-group cross sections also can be used in Monte Carlo codes to decrease the running time of the calculation. In addition, in some Monte Carlo codes, multi-group cross sections are essential for performing adjoint calculations [2]. The derivation of multi-group cross sections is a complicated, multi-stage procedure, as cross section can vary strongly with energy, especially in the resonance region. Normally the continuous-energy cross section data is processed to obtain fine-group cross sections, without taking into account the geometry of the system. In a cell or lattice calculation the geometry is taken into account, often in an approximate way, to condense the fine-group cross sections to few-group cross sections homogenized over a certain region, mostly (part of) a fuel assembly [1]. Apart from approximating the geometry, a lattice code inherently applies approximations to the neutron transport model. Therefore, there is an interest in obtaining multi-group cross sections without major approximations. This can be accomplished with a general purpose Monte Carlo code. However, not all Monte Carlo codes have the required options for that and no general purpose Monte Carlo code will be able to estimate the elements of the scattering matrix belonging to the multi-group set[3]. As mentioned, the generation of multi-group neutron cross sections is usually the first step in the solution of reactor physics problems. This typically includes generating condensed cross section sets, collapsing the scattering kernel, and within the context of diffusion theory, computing diffusion coefficients that capture transport effects as accurately possible [4].

Cross section generation with deterministic method using lattice codes such as CASMO, TRITON and WIMSD5 has been done so far for many calculations [5,6,7]. Although the calculation of multi-group constants has historically been done via deterministic methods, it is natural to think of using the Monte Carlo method due to its gettometric flexibility and robust computational capabilities such as continuous energy transport calculations [4]. There are some studies in background which have investigated the cross sections generation with probabilistic approach. For example the MCNP source code was modified for generation of multi-group cross sections by E. L. Redmon [8]. The continuous energy cross section data was directly manipulated to obtain as much information as possible about the desired multi-group cross sections [8]. In an another similar work, first, the scattering matrix was evaluated from output file of a MCNP5 run, then with a developed program MgXsect (that is a complex analysis program) the event file is read and group cross sections were calculated[3]. Yoshioka et al. have generated multi-group scattering matrix using weight-to-flux ratio based on a continuous energy Monte Carlo technique. In their proposed method a multi-group constant generation system with MCNP4C has been developed by preparing an additional function on the MCNP4C code that calculates the weight-to-flux ratio [8].

* *Sorumlu Yazar (Corresponding Author)*
e-posta: pirouzm@shirazu.ac.ir
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In this paper a cross section generation method has been implemented using the MCNPX 2.7 Monte Carlo code results which is capable of computing macroscopic cross sections and scattering matrix for transport or diffusion applications. To determine the scattering matrix, an output file of MCNPX run (PTRAC file) with all relevant events of the simulation is used. Using a MATLAB program the PTRAC file is read and tracks are selected in the geometrical region of interest to calculate the multi-group constants. Information such as coordinates of the particle position, particle direction with coordinates axes, energy and weight of the particle are extracted from the read–event file. This data are then used to obtain the average cosine of scattering angle, the multi-group scattering matrix via weight-to-flux ratio method and the diffusion coefficient for the selected region.

2. THE METHODOLOGY

In this study the multi-group diffusion constants based on the Monte Carlo method are generated using a new methodology as shown in Figure 1. First, fission, absorption, and total reaction rates are computed for each energy group by tallying in MCNPX 2.7 code, directly. Then, group cross sections are calculated by dividing the calculated reaction rates by the estimated flux for energy group g (Eqs. 1-3). On the other hand, it is not possible to process the scattering cross section from the energy group g' to the energy group g in the same way (Eq. 4). As shown in Figure 1, an MCNPX output file (PTRAC) is generated with all relevant events of the simulation. In order to obtain an estimate of the scattering matrix elements, the event file is read into the MATLAB and tracks are selected in the chosen geometrical region for which one wants to calculate the scattering matrix elements. This region can be a cell with only one material or a combination of cells with different materials for which multi-group constants are calculated. The data related to energy, position and direction of particle for each history from the mentioned file are extracted. Also, an important parameter from the read–event file, namely the particle weight during particle transport from an event to another event is calculated. Then, using extracted weights for different energy groups, the scattering matrix elements using the weight to flux ratio method are computed [9]. Herein, the weight is tallied according to the in-scattering and out-scattering groups when particle experiences a scattering reaction at the volume V. The scattering matrix elements are then written as equations (8) to (10) as an example for two-group problem [9]. Note that, the up-scattering in the scattering matrix calculations is ignored. It is notable that the mean scattering cosine $\bar{\mu}$ is needed to deduce the diffusion constants. Therefore, μ_g is tallied when the neutrons experience scattering in group g. By averaging from the tallied μ_g values, $\bar{\mu}_g$ is computed. The diffusion coefficient D is consequently deduced through Eq. (7).

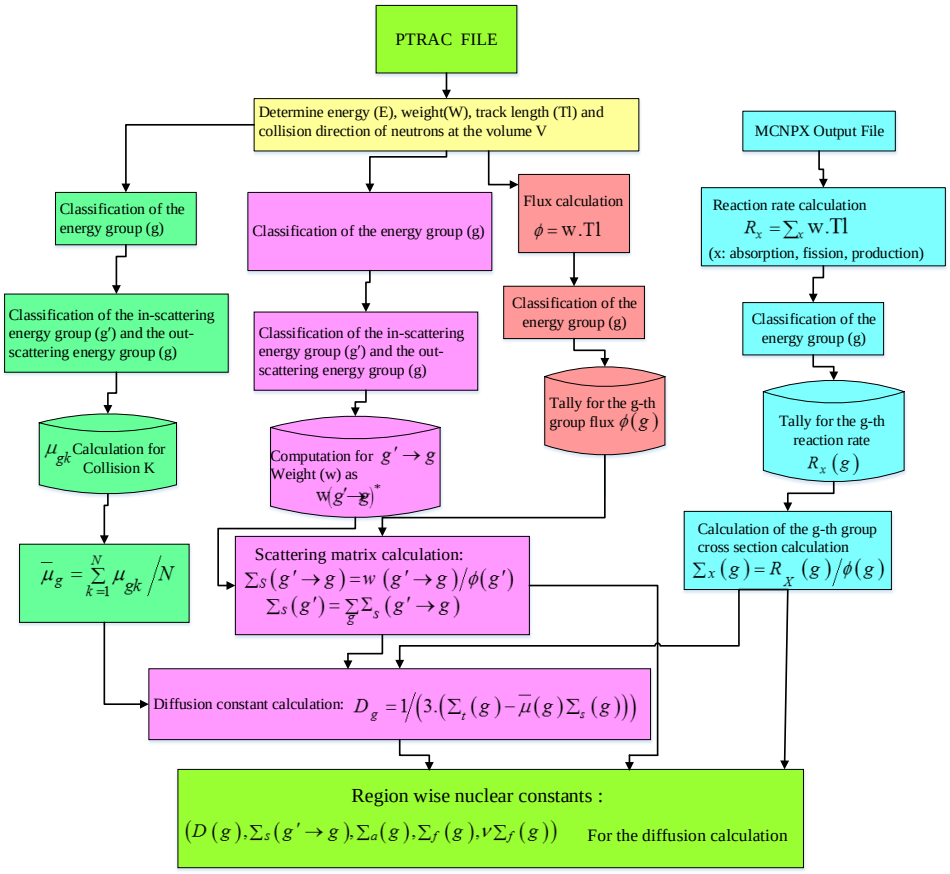

Figure 1. Block diagram of the methodology used in this study for multi-group constants generation.

The definitions of multi-group constants are given by [10]:

$$\Sigma_{ag} \equiv \frac{\int_{E_g}^{E_{g-1}} \Sigma_a(E)\varphi(E)dE}{\int_{E_g}^{E_{g-1}} \varphi(E)dE} \quad (1)$$

$$\Sigma_{tg} \equiv \frac{1}{\varphi_g}\int_{E_g}^{E_{g-1}} \Sigma_t(E)\varphi(E)dE \quad (2)$$

$$\nu_g \Sigma_{fg} \equiv \frac{1}{\varphi_g}\int_{E_g}^{E_{g-1}} \nu(E)\Sigma_f(E)\varphi(E)dE \quad (3)$$

$$\Sigma_{sg'g} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma_S(E'\to E)\varphi(E')}{\int_{E_g}^{E_{g-1}} \varphi(E)dE} \quad (4)$$

$$\Sigma_{sg'} \equiv \sum_{g'=1}^{G} \Sigma_{sg'g} \quad (5)$$

$$D_g \equiv \frac{\int_{E_g}^{E_{g-1}} D(E)\nabla\varphi(E)dE}{\int_{E_g}^{E_{g-1}} \nabla\varphi(E)dE} \quad (6)$$

We also know that the diffusion coefficient given in Eq. (5) can be expressed with Eq. (6) as:

$$D = \frac{1}{3\Sigma_{tr}} \quad (7)$$

where $\Sigma_{tr} \equiv \Sigma_t - \bar{\mu}\Sigma_s$ and $\bar{\mu}$ is the average cosine of scattering angle.

$$\Sigma_{s1\to1} = \Sigma_{s11} = \frac{W_1(1\to1)}{\varphi_1} \quad (8)$$

$$\Sigma_{s1\to2} = \Sigma_{s12} = \frac{W_2(1\to2)}{\varphi_1} \quad (9)$$

$$\boldsymbol{\Sigma_{s2\to2} = \Sigma_{s22} = \frac{W_2(2\to2)}{\varphi_2}} \quad (10)$$

3. RESULTS

In this section the results of the presented method implementation for the group constants generation is presented. First, a third-region slab and a BWR pin cell benchmark problems are studied to validate the present method [9, 11]. Then, the proposed method is applied for a more practical problem which is a standard fuel box of Tehran research reactor (TRR) [12].

3.1. The Slab Problem

This problem consisting of two slabs of fissionable material (Uranyl solution with 10 % enriched ^{235}U) separated by a water zone [11]. Each zone has a 20 cm width (Fig. 2) with region-wise number densities of nuclide given in Table 1. An MCNPX run is done with 50 cycles from which the first 10 cycles are skipped to let the fission source distribution convergence. For each cycle nominally 10000 neutrons are simulated. The multi-group effective cross sections for the fissionable zones are calculated for four energy groups with inner boundaries at 0.82 MeV, 748.52 eV and 0.625 eV and are compared with the results computed by SCALE5 code tabulated in Table 2. Also, an event file is generated for the last 40 cycles. Then the MATLAB script is run to obtain the scattering matrix elements as given in Table 3. The results are comparable with the results given in the reference [3].

3.2. Pin-Cell Analysis

Three-group pin-cell analysis without neutron leakage is performed in this section. Table 4 presents the calculation conditions of the pin-cell model shown in Fig. 3. Table 5 gives the three-group constants for the BWR UO_2 lattice under cold conditions at 300K [9]. This table also displays the calculated results using MCNP4C source code modification by Yoshioka et al., for comparison. The discrepancy in the results is mainly due to different data library used. While we use the ENDF/VII data library, they have utilized the JENDL-3.2 nuclear data library.

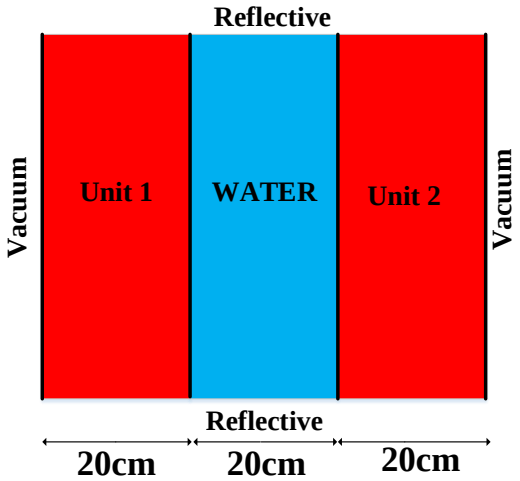

Figure 2. Geometry of slab benchmark problem[11]

Table 1. Number density of nuclide for slab problem[atoms/barn.cm][11]

Uranyl Solution	
H	5.9347E-02
N	2.1220E-03
O	3.7258E-02
U-235	7.6864E-05
U-238	6.8303E-04
Water	
H	6.6658E-02
O	3.3329E-02

Table 2. Comparison of the effective cross sections computed by MCNPX with SCALE5 code results

	MCNPX results in this study				**SCALE5/172 group master's results [3]**			
Group (g)	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**
Upper energy[ev]	1.00E+7	8.20E+5	7.48E+2	6.25E-1	1.00E+7	8.20E+5	7.48E+2	6.25E-1
Lower energy[ev]	8.20E+5	7.48E+2	6.25E-1	0.00	8.20E+5	7.48E+2	6.25E-1	0.00
σ_t [barn]	2.68E+0 ±0.7%	9.28E+0 ±0.5%	1.42E+01 ±0.5%	1.92E+1 ±0.6%	2.68E+0	9.25E+0	1.43E+01	2.90E+1
σ_c[barn]	7.59E-3 ±1.1%	4.54E-3 ±0.7%	1.30E-1 ±1.1%	2.73E-1 ±0.6%	9.67E-3	4.46E-3	1.27E-1	2.64E-1
σ_s[barn]	2.65E+0 ±0.7%	9.26E+0 ±0.5%	1.41E+1 ±0.5%	1.85E+1 ±0.6%	2.67E+0	9.24E+0	1.41E+1	2.84E+1
$\nu\sigma_f$[#.barn]	1.02E-2 ±0.8%	4.58E-3 ±0.5	6.14E-2 ±0.6%	8.75E-1 ±0.6%	1.02E-2	4.60E-3	6.21E-2	8.42E-1
ν	2.78E+00	2.44E+00	2.44E+00	2.44E+0	2.78E+00	2.45E+00	2.43E+00	2.44E+00

Table 3. Scattering matrix calculated by MCNPX for the slab benchmark [barn]

Group	**1**	**2**	**3**	**4**
1	1.65E+00	-	-	-
2	1.01E+00	8.31E+00	-	-
3	8.73E-04	1.10E+00	1.26E+01	-
4	0.0	9.52E-04	1.73E+00	1.98E+01

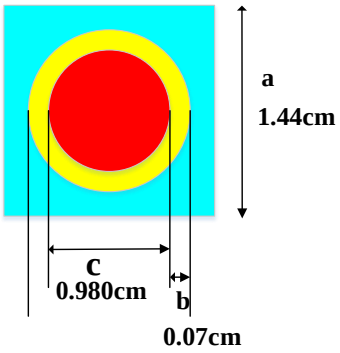

Figure 3. Configuration of the pin-cell benchmark [9]

Table 4. Calculation conditions for the pin-cell model [9]

Case	BWR 9×9 UO_2
Fuel rod pitch (a) [cm]	1.440
Clad thickness(b) [cm]	0.07
Pellet diameter (c) [cm]	0.980
Isotope composition in fuel [/barn/cm]	
U-234	9.776E-06
U-235	1.058E-03
U-236	6.513E-06
U-238	2.116E-02
O-16	4.447E-02
Cladding	Natural Zr

Table 5. Comparison of group constants computed in this study with Yoshioka's results

	This study			**Yoshioka's results[9]**		
Group (g)	1	2	3	1	2	3
Upper energy[ev]	1.00E+07	5.53E+03	3.93E+00	1.00E+07	5.53E+03	3.93E+00
Lower energy[ev]	5.53E+03	3.93E+00	1.00E-04	5.53E+03	3.93E+00	1.00E-04
D(g) [cm]	1.16E+00	5.82E-01	2.91E-01	1.23E+00	6.30E-01	2.38E-01
$\nu\sum_f$(g)[#/cm]	5.35E-03	1.92E-02	2.01E-01	5.20E-03	1.90E-02	1.94E-01
$\sum_f$(g)[cm^{-1}]	1.97E-03	7.90E-03	8.26E-02	1.92E-03	7.82E-03	7.96E-02
ν(g)	2.72E+00	2.44E+00	2.44E+00	2.71E+00	2.43E+00	2.44E+00
$\sum_a$(g)[cm^{-1}]	3.50E-03	3.19E-02	1.14E-01	3.49E-03	3.16E-02	1.09E-01
$\sum_{sl}$(g) [cm^{-1}]	4.78E-02	9.83E-02	0.00E+00	4.41E-02	8.66E-02	0.00E+00
$\sum_{g\to1}$[cm^{-1}]	4.46E-01	-	-	4.31E-01	3.02E-05	0.00E+00
$\sum_{g\to2}$[cm^{-1}]	4.78E-02	9.78E-01	-	4.40E-02	9.01E-01	2.57E-05
$\sum_{g\to3}$[cm^{-1}]	3.54E-05	9.83E-02	1.72E+00	3.03E-05	8.66E-02	1.48E+00

3.3. TRR Fuel Box Calculation

Herein, the proposed method is applied for a more practical situation which is the multi-group constants and scattering matrix calculations for a standard fuel box of Tehran research reactor (TRR). TRR fuel box specifications are listed in Table 6 [12]. Fig. 4 illustrates a two dimensional schematic of TRR fuel box [12]. Table 7 shows calculated multi-group cross sections and scattering matrix elements for four- energy group. These constants are then used in CITATION diffusion calculation code to compute the effective multiplication factor (k_{eff}) to compare with MCNPX direct calculation. The difference between the two codes results is less than 1% as shown in Table 8. These results illustrate that our proposed method has high accuracy in multi-group constants estimation for criticality calculations.

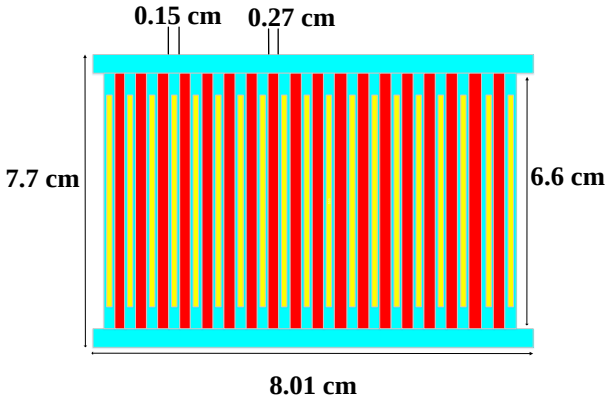

Figure 4. 2D TRR fuel box schematic [12]

Table 6. TRR standard fuel box specifications [12]

Number of Fuel Plates	19
Plate Thickness [cm]	0.15
Clad Thickness [cm]	0.04
Water Channel [cm]	0.27
Fuel Meat Thickness [cm]	0.07
Fuel Meat Width [cm]	6.0
Fuel Meat Length [cm]	61.5
FE external size [cm]	8.01×7.7×89.7

4. CONCLUSIONS

In this study a group constants generation method based on the calculation results of a continuous energy Monte Carlo (MCNPX 2.7 code) simulation was developed. This method features with no need for MCNPX source code modification and high accuracy in multi-group constants and scattering matrix calculations with relatively low number of history run. The proposed method was validated using several benchmark problems. First, the proposed method was applied to the slab benchmark and four-group effective cross sections were calculated and compared with the results of SCALE5 code (Table 2). This comparison revealed that the thermal fine-group cross sections in the SCALE5 master library were not properly treated for thermal scattering. The next problem was a pin-cell problem which we calculated the three-group constants and compared the results of MCNPX with a modified version of MCNP4C code. In this case the maximum discrepancy between two approaches was observed in

Table 7. Calculated 4-group cross sections and scattering matrix elements for TRR fuel box

Group	**1**	**2**	**3**	**4**
Upper energy[ev]	1.00E+07	8.21E+05	9.07E+02	6.25E-01
Lower energy[ev]	8.21E+05	9.07E+02	6.25E-01	0.00
D(g) [cm]	1.92E+00	8.85E-01	6.80E-01	2.68E-01
$\sum_c(g)[cm^{-1}]$	2.31E-04	5.30E-04	9.93E-03	2.25E-02
$\nu\sum_f(g)[\#/cm]$	1.43E-03	1.04E-03	1.34E-02	1.16E-01
$\sum_f(g)[cm^{-1}]$	5.22E-04	4.25E-04	5.49E-03	4.78E-02
$\sum_a(g)[cm^{-1}]$	7.53E-04	9.55E-04	1.54E-02	7.03E-02
$\nu(g)$	2.75E+00	2.44E+00	2.43E+00	2.43E+00
$\sum_{g\to1}[cm^{-1}]$	1.60E-01	-	-	-
$\sum_{g\to2}[cm^{-1}]$	7.28E-02	5.80E-01	-	-
$\sum_{g\to3}[cm^{-1}]$	7.26E-05	7.03E-02	8.04E-01	-
$\sum_{g\to4}[cm^{-1}]$	0.00E+00	3.45E-05	9.67E-02	1.43E+00

Table 8. Comparison of the multiplication factor calculated by MCNPX & CITATION codes

Multiplication factor	**MCNPX**	**CITATION**	**Error %**
k_{eff}	1.536	1.540	0.2

the scattering cross section of third energy group and subsequently in the corresponding diffusion coefficient (Table 5). The reason of detected deviations is basically due to different data libraries used. The proposed method in this study used the ENDF/VII data library whereas the JENDL-3.2 nuclear data library was used by Yoshioka et al. In the last stage the computation of four-group diffusion constants for a TRR's fuel assembly was performed. To validate the calculated cross sections, this fuel assembly was also simulated in CITATION code using the calculated four-group constants for the k_{eff} calculation which showed a difference about 0.2% compared to the MCNPX 2.7 results.

Finally, further evaluation of differences with deterministically generated multi-group cross sections will be needed for varying systems with different neutron flux spectra. The generated multi-group cross sections via mentioned methodology is under further investigation for using in nodal diffusion codes such as PARCS code for the steady state calculations and reactivity transient simulations.

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