Development and Verification of FSMOC Code

YU Rui[a], ZHAO Qiang[b] and GU Long[a,*]
[a] *Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, 730000,China*
[b] *Fundamental Science on Nuclear Safety and Simulation Technology Laboratory, Harbin Engineering University, Harbin,150001,China*
[*]GU Long: gulong@impcas.ac.cn

1. Introduction

The increasing heterogeneity and complexity of the core design posts a challenge to the traditional power distribution calculations. Meanwhile, along with the proposition of high-fidelity computational requirements for reactor, the core physics calculation method transits from traditional three-step method to the two-step (pin-by-pin) method and the whole core direct transport calculation[1]. The method of characteristics (MOC) integrally solves the neutron transport equation along the neutron flight trajectory. Its transport solving process is not restricted by the boundary conditions and geometry, which makes it applicable to solve the neutron transport equation with high precision and easy popularization in arbitrary complex geometry theoretically[2]. Therefore, the MOC was chosen as the method to solve the steady state Boltzmann transport equation in the code of FSMOC (Fine Solver Based on Method of Characteristics).

FSMOC code is written in Fortran95/2003 language under Microsoft Visual Studio 2010. The code mainly consists of front geometry preprocessing module, AutoCAD interface module and transport calculating module. The front geometry preprocessing module is developed to describe the geometry of computational domain. In order to debug the program and facilitate users to intuitively observe the information of geometry and characteristic lines within the repetitive structure (such as cell), an interface module is developed to link to AutoCAD based on the DXF file of the AutoCAD software. Transport equation solving module is developed by using the source iteration method on the condition of flat source approximation assumption. These modules will be described in detail in the following sections.

2. Geometry Preprocessing

The front geometry preprocessing module in the FSMOC code is used to describe the geometry of computational domain and obtain the information of geometry and characteristic line.

2.1 Geometry construction and division

Transport calculation can be implemented only after obtain the geometrical features. Geometry construction in FSMOC code is realized by simultaneously solving equations. For example, mathematical equation can describe circular geometry, whose equation is as follows:

$$x^2 + y^2 = r^2 \qquad (1)$$

where r is the radius, which requires user's input, such as the radius of the fuel pellets, and clad diameter. In addition, the lattice can be divided in accordance with circular to get a fine mesh region while inputting the desired radius.

Straight line also can be described by its equation:

$$y = kx + b \qquad (2)$$

where k is the slope and b is intercept. Line building in FSMOC code is mainly used for the description of the cell length and width of each grid, and linear division of fine cell region.

Through the methods mentioned above, we can easily build and divide the geometry, which are illustrated in Fig. 1.

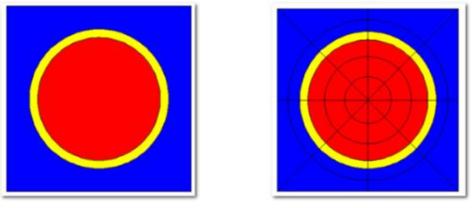

Fig. 1. Geometry construction and division of fuel cell.

2.2 Angular quadrature set

Angular quadrature set that allows modular ray tracing is provided as follows in FSMOC code. The azimuthal angles and polar angles can be chosen independently. The azimuthal quadrature set proposed by Filippone is used in FSMOC code, its detailed form is as follows[3]:

$$\tan(\varphi_r) = (\Delta y / \Delta x) \times \frac{r}{(N_\varphi + 1 - r)}, r = 1, 2, \cdots, N_\varphi \qquad (3)$$

$$\delta A_r = \frac{\Delta x}{r} \sin\varphi_r = \frac{\Delta y}{N_\varphi + 1 - r} \cos\varphi_r \qquad (4)$$

where Δx and Δy means the size of cell, N_φ represents the number of azimuthal angles, δA_r is the characteristic line density, $N_l = (N_\varphi + 1)$ rays for each of N_φ azimuthal angles, the weights given as:

$$\sum_r^{N_\varphi} \omega_r \cos(2s\varphi_r) = \begin{cases} \pi/2, if\,(s=0) \\ 0, if\,(s = 1, 2, \cdots, N_\varphi - 1) \end{cases} \qquad (5)$$

The Tabuchi and Yamamoto (TY) polar quadrature is used in FSMOC code to define the polar angles and its corresponding weights. The TY polar quadrature is listed in Table I[4].

Table I. TY Polar Angles and Corresponding Weights

Total number of polar angles	Tabuchi and Yamamoto (TY)	
	$\sin\theta$	ω
1	0.798184	1.000000
2	0.363900	0.212854
	0.899900	0.787146
3	0.166648	0.046233
	0.537707	0.283619
	0.932954	0.670148

3. AutoCAD Interface Module

As mentioned above, the correctness of the geometric information is the prerequisite and basis for subsequent transport calculation. The AutoCAD interface module is developed based on DXF file of AutoCAD, which will make the MOC tracks of fundamental cell (not all the whole domain) display in AutoCAD as the form of images. DXF (Drawing Exchange Format) is a CAD data file format developed by Autodesk for enabling data interoperability between AutoCAD and other programs[5]. The basic organization of a DXF file is HEADER section, CLASSED section, TABLES section, BLOCKS section, ENTITIES section, OBJECTS section and EOF section in order. A complete DXF file is more complex, not all of the section information needed to be provided at the time of application, but the ENTITIES section is necessary for DXF file structure[6].The process to convert user data in DXF file format and display in AutoCAD is illustrated in Fig. 2:

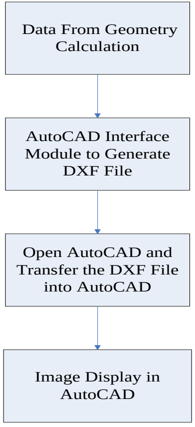
Data From Geometry Calculation
AutoCAD Interface Module to Generate DXF File
Open AutoCAD and Transfer the DXF File into AutoCAD
Image Display in AutoCAD

Fig. 2. Flow chart of user data into DXF file.

Fig. 3 is a 4x4 lattice geometry example using this method to achieve an image displaying in AutoCAD software:

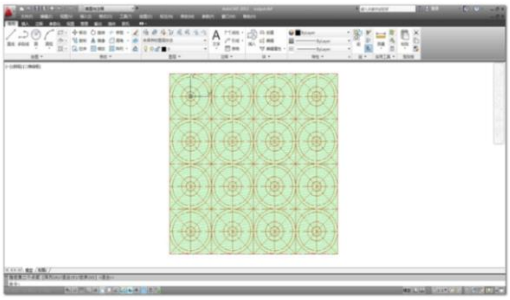

Fig. 3. Example of AutoCAD interface module application.

4. Method of Characteristics

MOC is one of the basic and commonly used methods to treat the linear hyperbolic partial differential equation, especially for the first-order partial differential equations. The fundamental idea is to transform the partial differential equation into the corresponding problem of ordinary differential equation. By solving the ordinary differential equation, we can obtain the solution of the former partial differential equation[7].

MOC is used to solve the Boltzmann transport equation in 2D by discretizing both polar and azimuthal angles and integrating the characteristic form of the equation for a particular azimuthal and polar quadrature [8].

The characteristics form of the Boltzmann transport equation in its discretized form[9] :

$$\frac{d\Phi^g_{m,i}}{ds_m} + \Sigma^g_{tr,i}\Phi^g_{m,i} = Q^g_{m,i} \qquad (6)$$

Where s_m represents the track length in the direction of neutron motion Ω_m, g is the energy group index, i is the mesh index. Φ represents the angular flux. This equation may be integrated along the streaming path s_m, traversing a mesh of constant material properties $\Sigma^g_{tr,i}$, assuming a spatially constant source $Q^g_{m,i}$, to produce an equation which relates the value of the angular flux at any point in the mesh along the path to the value of the angular flux entering the mesh as:

$$\begin{aligned}\Phi^g_{m,i.k}(s_{m,i,k}) &= \Phi^g_{m,i,k}(0)e^{-\Sigma^g_{tr,i}s_{m,i,k}} \\ &\quad + \frac{Q^g_{m,i}}{\Sigma^g_{tr,i}}(1-e^{-\Sigma^g_{tr,i}s_{m,i,k}})\end{aligned} \qquad (7)$$

The average value of the angular flux within mesh i in direction m along segment k is then given by:

$$\bar{\Phi}^g_{m,i,k} = \frac{Q^g_{m,i}}{\Sigma^g_{tr,i}} + \frac{\Phi^g_{m,i,k}(0)-\Phi^g_{m,i,k}(s_{m,i,k})}{\Sigma^g_{tr,i}\cdot s_{m,i,k}} \qquad (8)$$

A number of tracks may cross each mesh for each direction, and the average value of the angular flux must then be calculated as the volume-weighted average of all tracks crossing the mesh:

$$\bar{\Phi}^g_{m,i} = \frac{\sum_k \bar{\Phi}^g_{m,i,k} s_{m,i,k} \delta A_m}{\sum_k s_{m,i,k} \delta A_m} \qquad (9)$$

To compensate for this error in the estimation of the volume-weighting scheme of Eq. (9), the track lengths may be scaled such that they give the correct volume or area for each region through which they pass.

$$s'_{m,i,k} = s_{m,i,k} \frac{V_i}{\sum_k s_{m,i,k} \delta A_m} \qquad (10)$$

Where V_i is the true area (2D) or volume (3D) of the region i.

Then, according to the different weights of direction, the final expression for the scalar flux in mesh i can be given:

$$\phi_i^g = \sum_m \omega_m \bar{\Phi}^g_{m,i} \qquad (11)$$

Where ω_m is the weight of direction m, ϕ represents the scalar flux.

5. Benchmark verification

In order to ensure the validity of modeling and numerical methods, and able to meet accuracy requirements, it is necessary to verify the FSMOC code established in this article.

5.1BWR lattice benchmark with two gadolinium pins

This benchmark is 4×4 boiling water reactor lattice with adjacent gadolinium burnable poison pins. The geometry and pin layout in the assembly is shown in Fig. 4.

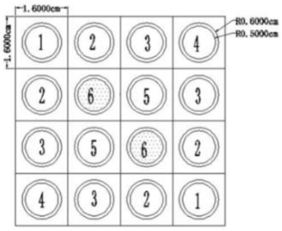

Fig. 4. Size and layout of BWR assembly benchmark.

Pins with number from one to five represent the regular fuel with 3% UO_2. The pin fuel numbered six is a burnable pin with 3% UO_2 and 3% Gd_2O_3. The clad material of pin is Zircaloy -2, and water is selected as the moderator. The cross section of the benchmark is not listed in here, and it is available in reference[10].

At the time of calculating this benchmark, every cell should be divided to a fine mesh. Its division style is illustrated in Fig.5.

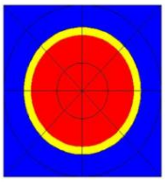

Fig. 5. Pin cell discretization of BWR lattice benchmark.

In the lattice calculation, 14 azimuthal and 3 polar angles are used to discretize the angular flux, and 43 characteristic lines are selected in each angle. The average line density of each direction is about 0.047cm. The reflective boundary is implemented and the convergence criteria of the effective multiplication factor and the neutron flux both are set to 10^{-6} in this benchmark. In order to compare with the results of DRAGON code in reference[10], the normalized pin power is computed according to Eq.（12）.

$$R_{fis} = \frac{\int_{pin}[\sum_g(\Sigma_g^f \Phi_g)]dA}{\int_{allpins}[\sum_g(\Sigma_g^f \Phi_g)]dA} \qquad (12)$$

The result of k_{eff} and the normalized pin power are listed in Table II and Table III respectively.

Table II. Result of k_{eff} in BWR Lattice Benchmark

Code	k_{eff}	error（pcm）
DRAGON[10]	0.986561	----
FSMOC	0.987282	72

Table III. Normalized Pin Power Calculation of BWR Lattice Benchmark

6.9391E-2 6.9513E-2 0.1755%	6.6246E-2 6.6272E-2 0.0388%	6.9398E-2 6.9401E-2 0.0041%	7.2549E-2 7.2547E-2 -0.0028%
6.6246E-2 6.6272E-2 0.0387%	2.4344E-2 2.4300E-2 -0.1788%	6.2429E-2 6.2421E-2 -0.0133%	6.9398E-2 6.9388E-2 -0.0144%
6.9398E-2 6.9401E-2 0.0041%	6.2429E-2 6.2421E-2 -0.0134%	2.4344E-2 2.4294E-2 -0.2044%	6.6246E-2 6.6227E-2 -0.0285%
7.2549E-2 7.2547E-2 -0.0028%	6.9398E-2 6.9388E-2 -0.0144%	6.6246E-2 6.6227E-2 -0.0285%	6.9391E-2 6.9382E-2 -0.0130%

DRAGON[10] FSMOC Error

As is showed in Table II and Table III, FSMOC code can give excellent accuracy for both effective multiplication factor and relative flux distribution for neutron transport problem.

5.2 C5G7 MOX benchmark problem

2D C5G7 MOX benchmark problem was proposed by OECD/NEA to test the ability of modern deterministic transport methods and codes to such reactor core problem without spatial homogenization[11]. It has the feature of strong leakage, large energy spectrum variation and strong non-uniformity, which makes the C5G7 MOX benchmark problem a harsh example for code validation and widely used in the testing of a new generation of reactor physics calculation software. The core configurations are shown in Fig.6.

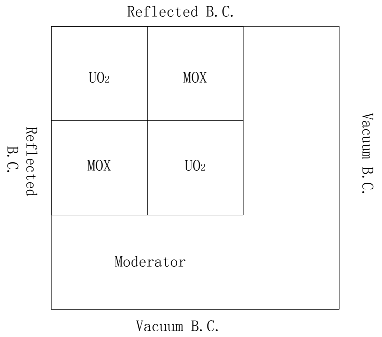

Fig.6. 1/4 Core configuration of 2D C5G7-MOX benchmark.

As indicated in Fig.6, reflected boundary conditions are applied to the top and left of the geometry while vacuum boundary conditions are applied to the right and bottom of the geometry. The overall dimensions of the 1/4 core are 64.26 × 64.26 cm, and the size of each assembly are 21.42 × 21.42 cm. In addition, the width of the water reflector is also 21.42 cm. Reactor core consists of UO_2 fuel assemblies and MOX fuel assemblies. Each fuel assembly is made up of 17 × 17 lattice of square pin cells. The length of pin cell is 1.26 cm and all of the fuel pins and guide tube have a 0.54 cm radius .When calculating this problem, each cell of the core is divided into 24 sub- regions. Four azimuthal angles and two polar angles are selected when calculating, line density of each direction of is about 0.044cm, the convergence criteria of the effective multiplication factor and the neutron flux both are set to 10^{-6}.Under such calculating condition, the results are shown in Table IV-Table VI.

Table IV. Result Contrast of k_{eff}

code	k_{eff}	error（pcm）
MCNP	1.186550	----
FSMOC	1.185835	-72

Table V. Result for Specific Pin Power

Pin power	MCNP	FSMOC	Error.%
Maximum pin power	2.498	2.492741	-0.2105
Minimum pin power	0.232	0.237594	2.4112

Table VI. Assembly Power Percent Errors

Assembly style	MCNP	FSMOC	Error.%
Inner UO_2 Assembly	492.8	491.98422	-0.1655
Outer UO_2 Assembly	139.8	140.29313	0.3527
MOX Assembly	211.7	211.86068	-0.0759

As shown from Table IV to Table VI, the error of the effective multiplication factor between MCNP reference solutions and FSMOC code is approximate 72 pcm. Assembly power and pin power both can meet the requirement.

6. Conclusions

A transport theory code called FSMOC based on MOC has been developed. The interface module based on the DXF file is developed for easily debugging code and intuitively observing information of geometry and characteristic line. The DXF file is simple but able to improve work efficiency. And the code is verified and validated by various benchmarks.

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