Monte Carlo Resonance Calculation for the Method of Characteristics

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To combine the advantages of the method of characteristic (MOC) in computing efficiency and the Monte Carlo (MC) method in continuous energy accuracy, we are investigating a hybrid method. It employs the MC method to simulate the resonance energy range, to make the MOC calculation more accurate. In contrast, it costs less computing time than the pure MC method. This summary introduces the theory of the hybrid method and preliminary numerical results.

I. METHODOLOGY

I.A. The MOC Method

In the Method of characteristic (MOC)[1] , neutron transport equation is written as an integral equation in a certain characteristic line:

$$\varphi_{i,k}(r_0+s\Omega_m,\Omega_m)=\varphi_{i,k}(r_0,\Omega_m)\exp(\int_0^s-\Sigma_{t,i}(r_0+s'\Omega_m)ds')+ \int_0^s Q_i(r_0+s'\Omega_m,\Omega_m)\exp(\int_{s'}^s-\Sigma_{t,i}(r_0+s''\Omega_m)ds'')ds' \quad (1)$$

where i is the number of flat source region, k is the number of line segment, m is the number of direction. s is the length of line segment (cm).

Assuming constant source and constant material property for each line segment, the equation above can be integrated along the characteristic line and the flux of ending point can be written as Eq. (2).

$$\varphi_{i,k}(r_0+s\Omega_m,\Omega_m)=\varphi_{i,k}(r_0,\Omega_m)\exp(-\Sigma_{t,i}s)+\frac{Q_i(\Omega_m)}{\Sigma_{t,i}}[1-\exp(-\Sigma_{t,i}s)] \quad (2)$$

The form above is analytical. The neutron flux of the ending point can be obtained then. Once obtained all the characteristic lines of the problem by sweeping the line segments one by one, the scalar flux of each flat source region can be obtained. This method can deal with complex geometry, but still use the multi-group cross sections. So the resonance calculation is necessary. And it has great impact on the accuracy of the results. The error in multi-group data is from the inexact assumptions made for the resonance self-shielding treatment such as Dancoff factor, rational approximations.

I.B. The MC Method

In the Monte Carlo (MC) method, sampling is used to solve the emission density equation which is another form of the neutron transport equation:

$$Q(r,\Omega,E)=S(r,\Omega,E)+\int_{4\pi}\int_0^{E_{\max}}\int_0^{\infty}K(r',\Omega',E'\to r,\Omega,E)Q(r',\Omega',E')drdE'd\Omega' \quad (3)$$

where $Q(r,\Omega,E)$ is the emission density ($cm^{-3}s^{-1}$), $S(r,\Omega,E)$ is external source ($cm^{-3}s^{-1}$).

Phase space point in energy, space and direction can be sampled according to the probability density function $K(r',\Omega',E'\to r,\Omega,E)$ as in Eq. (4), which is consist of two parts: the transport kernel in Eq. (5) and collision kernel in Eq. (6):

$$K(r',\Omega',E'\to r,\Omega,E)=T(\mathrm{r}'\to \mathrm{r}\,|\,\Omega',E')C(\Omega',E'\to\Omega,E\,|\,r) \quad (4)$$

$$T(\mathrm{r}'\to \mathrm{r}\,|\,\Omega',E')=\Sigma_t(r,E')e^{-\tau(r,r',E')} \quad (5)$$

$$C(\Omega',E'\to\Omega,E\,|\,r)=\frac{\Sigma_s(r,E')}{\Sigma_t(r,E')}f(r,\Omega',E'\to\Omega,E) \quad (6)$$

The simulation of neutrons is the sampling process of the transport and collision kernels. In sampling of the travelling distance and the collision reaction, micro cross section in a certain energy will be used. The cross section data is continues energy point-wise cross section. It is much more accurate than the multi-group cross section in deterministic method as MOC. And the Resonance phenomenon is implicitly considered in the MC simulation.

However, in solving the critical calculation, the MC method needs a lot of cycles to get the converged eigenvalue k_{eff} and the converged fission source. The computational cost is too large, and becomes the main disadvantage of MC method.

I.C. The Hybrid Method

Recent years, there are many researches on the hybrid of deterministic and Monte Carlo methods. WAGNER[2] raise a method called forward weighted consistent adjoint driven importance sampling (FW-CADIS) method by using the deterministic method to provide the source bias parameters for MC simulation to accelerate the convergence of fission source. LEE[3] used the CMFD method to accelerate the MC fission source convergence. Yang and Larsen[4] proposed the functional Monte Carlo (FMC). It firstly uses a low order equation to calculate the

Eddington factor that weakly depend on the solution of high order equation. Then the Eddington factor can be employed to accelerate the convergence of high order equation. Hyunsuk[5] proposed a hybrid method which uses MC to simulate the resonance and thermal energy range and uses MOC to sweep fast and thermal groups. It is tested in an 8-group problem, and has been proven to be capable of solving the problem faster than the pure MC and more accurate than the pure MOC.

In this paper, a hybrid strategy in energy space is investigated. It is based on a 69-group MOC, in which the 15 to 27 groups are regarded as resonance groups. Depend on different resonance method, this process introduce different degree of error.

In contrast, the MC simulation is used to simulate the resonance energy range and passes its flux to MOC. MOC sweeps only the fast and thermal energy groups. In one transport calculation, first sweep the fast group for enough inner iteration times, then start fixed source Monte Carlo simulation with fission source and tally the results in resonance group, after that, use the fast group flux from MOC and resonance group flux from MC to sweep over the thermal group with MOC solver, and get the thermal group flux.

In critical calculation in reactor physics. The flow of hybrid method is as follows:

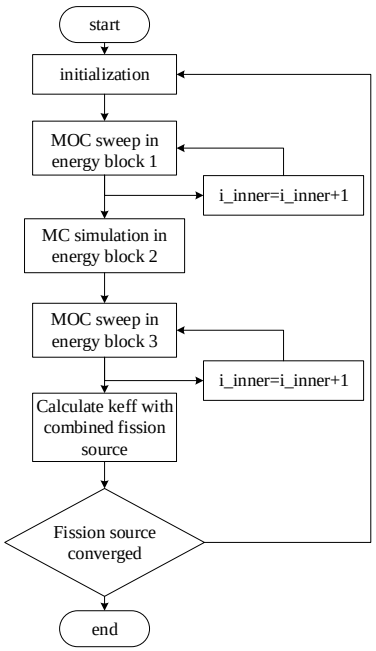

Fig. 1. Flow chart of hybrid method

For critical calculation of transport equation. power iteration is needed. In each power iteration, the form of updating flux is written as Eq. (7).

$$L\Phi^{n} - S\Phi^{n} = \frac{1}{k_{eff}^{\,n-1}} F\Phi^{n-1} \tag{7}$$

And update eigenvalue k_{eff} as Eq. (8).

$$k_{eff}^{\,n} = k_{eff}^{\,n-1} \frac{\sum_{g=1}^{G} \nu\Sigma_f \Phi^{n}}{\sum_{g=1}^{G} \nu\Sigma_f \Phi^{n-1}} \tag{8}$$

In the hybrid method, each power iteration is divided into three parts. The first and third parts are solved by MOC, and the second part (resonance part) is solved by MC. Eigenvalue can be obtained in the form in Eq. (9).

$$k_{eff}^{\,n} = k_{eff}^{\,n-1} \frac{\sum_{g\in G_1} \nu\Sigma_f \Phi^{n} + \sum_{g\in G_2} \nu\Sigma_f \Phi^{n} + \sum_{g\in G_3} \nu\Sigma_f \Phi^{n}}{\sum_{g\in G_1} \nu\Sigma_f \Phi^{n-1} + \sum_{g\in G_2} \nu\Sigma_f \Phi^{n-1} + \sum_{g\in G_3} \nu\Sigma_f \Phi^{n-1}} \tag{9}$$

Compared to the former research[4]. This method use fine group structure in MOC to ensure the accuracy. Solver in both parts use the data from ENDF/BVII.0. The source which given to MC for simulation is flat in each group and each flat source region, corresponding to the MOC.

II. NUMERICAL RESULTS

In the initial stage of the research, a 2D single pin problem is calculated to validate the hybrid transport solver. A traditional 69 group structure was chosen. 15 to 27 group was set as resonance range, which is solved by MC simulation. Actually, the energy range can be chosen freely. The 69 group cross section data is from ENDF/BVII.0 and is produced by code of NECP laboratory. The continuous energy point-wise cross section is in ACE format which is from ENDFB/VII.0. The MOC solver is from the high-fidelity neutronics code for reactor physics calculations, which is called NECP-X, developed independently by NECP laboratory. The resonance is calculated by global-local method in MOC solver, the method is developed by NECP laboratory and has been fully verified. The MC solver is from OpenMC[6] code. The results are compared with the directly MC calculation, and directly MOC calculation.

The MC calculation used 100000 particles with 50 inactive cycles and same number of active cycles with hybrid method. In order to keep the same tally time in both MC and hybrid method.

The hybrid calculation use 100000 particles for each fixed source simulation in once power iteration.

The eigenvalue of the test case is shown below, together with the calculation time, iteration times and error to MC.

TABLE I. Results of three kinds of methods

	keff	Calculation error	Time/s	Iteration times	Error to MC
MC	1.47620	0.00075	653.53	/	/
MOC	1.47451	0.00001	40.07	5	-0.114%
hybrid	1.47708	0.00001	442.70	7	0.059%

Compared to the pure MOC, hybrid method is more accurate. While the increase of speed is not too much compared with pure MC calculation. The further research will focus on it and make some improvements.

The flux of different groups has also been compared.

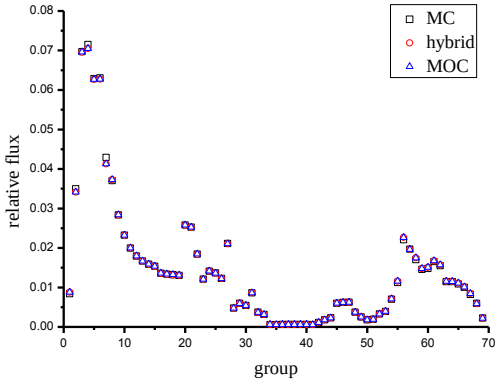

Fig. 2. Energy spectrum calculated by three kinds of methods

According to Fig. 2, the spectrum of three methods are in good agreement.

III. CONCLUSIONS

According to the present numerical results, the hybrid method can increase the accuracy of k_{eff} in transport compared with the pure MOC multi-group method. And the speed of hybrid method also increase compared with the traditional Monte Carlo method. There are still some improvements need to be made to speed up the calculation and make the hybrid method more efficient. We are still working on more numerical investigations. It is supposed to be added in the revised summary.

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