A CMFD Acceleration with SP₃ Approximation for the Monte Carlo Neutron Transport

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1. Introduction

The stochastic Monte Carlo (MC) method is one of many ways to solve the neutron transport equation in order to analyze nuclear reactors. This method makes it possible to describe the actual environment precisely in any complex geometry; hence it is considered the most accurate method. However, the computational time involved in tracking every single particle and recording physical quantities is usually unacceptably long for practical reactor analysis. In order to reduce the computing time and statistical uncertainty in MC calculations, a coarse mesh finite difference (CMFD) method was introduced by Lee et al. [1] and many related researches [2-4] were done. The diffusion-based CMFD acceleration has become a popular scheme to accelerate the source convergence in MC eigenvalue problems. In this paper, we tried to evaluate the feasibility of a new SP3-based CMFD acceleration of the MC method.

2. Methods and Results

In this section, mathematical background is presented for the CMFD application with SP₃ approximation in the MC calculation. The SP₃ equations are briefly derived [5], and the theory of the CMFD for the MC application is described.

2.1 SP₃ approximation

The derivation of the SP_3 approximation starts from $1D P_3$ equations:

$$\frac{d\phi_{1,g}}{dx} + \Sigma_{tg}\phi_{0,g} = \sum_{g'=1}^{G} \Sigma_{s0g' \to g}\phi_{0,g'} + \frac{1}{k}\chi_{g}\sum_{g'=1}^{G} \nu \Sigma_{fg'}\phi_{0,g'} \\
\frac{2}{3}\frac{d\phi_{2,g}}{dx} + \frac{1}{3}\frac{d\phi_{0,g}}{dx} + \Sigma_{tg}\phi_{1,g} = 0 \\
\frac{3}{5}\frac{d\phi_{3,g}}{dx} + \frac{2}{5}\frac{d\phi_{1,g}}{dx} + \Sigma_{tg}\phi_{2,g} = 0 \\
\frac{3}{7}\frac{d\phi_{2,g}}{dx} + \Sigma_{tg}\phi_{3,g} = 0$$
(2.1)

These four equations can be compressed into the two double differential equations. By substituting the derivative with the gradient operator in the two equations, the SP₃ equations can be obtained as follows:

$$-D_{0,g}\nabla^{2}\hat{\phi}_{0,g} + \Sigma_{tg}\hat{\phi}_{0,g} = Q + 2\Sigma_{tg}\phi_{2,g}$$

$$-D_{2,g}\nabla^{2}\phi_{2,g} + \Sigma_{tg}\phi_{2,g} = \frac{2}{5}(\Sigma_{tg}\phi_{0,g} - Q)$$
 (2.2)

where $D_{0,g}$ and $D_{2,g}$ are the diffusion coefficient of group g, defined by

$$D_{0,g} \cong \frac{1}{3\Sigma_t},$$
$$D_{2,g} \cong \frac{9}{35\Sigma_{tg}} = \frac{27}{35} D_{0.5}$$

Q is the neutron source

and

C

$$Q = \sum_{g'=1}^{O} \Sigma_{s0g' \to g} \phi_{0,g'} + \frac{1}{k} \chi_g \sum_{g'=1}^{O} \nu \Sigma_{fg'} \phi_{0,g'},$$
$$\hat{\phi}_{0,g} = \phi_{0,g} + 2\phi_{2,g}$$
(2.3)

2.2 CMFD application in the MC method

The CMFD method is based on the finite difference method with a correction factor which is obtained from the high-fidelity solutions. For example, in the onedimension, the one-group balance equation for SP_3 approximation is expressed as

$$\frac{1}{\Delta x} \left(J_0^{i,r} - J_0^{i,l} \right) + \Sigma_t^i \hat{\phi}_0^i = Q + 2\Sigma_t^i \phi_2^i$$
(2.4)

$$\frac{1}{\Delta x} \left(J_2^{i,r} - J_2^{i,l} \right) + \Sigma_t^i \phi_2^i = \frac{2}{5} \left(\Sigma_t^i \phi_2^i - Q \right)$$
(2.5)

where $J_0^{i,r}$ is the net current at the right surface of cell *i* such as

$$\begin{aligned} & \overset{r_{i,r}}{}_{0} = -D_0 \nabla_x \hat{\phi}_0 = -D_0 \nabla_x (\phi_0 + 2\phi_2) \\ & = -\tilde{D}_0 (\hat{\phi}_0^{i+1} - \hat{\phi}_0^i) + \hat{D}_0 (\hat{\phi}_0^{i+1} + \hat{\phi}_0^i) \end{aligned}$$
(2.6)

and

$$J_{2}^{i,r} = -D_{2}\nabla_{x}\phi_{2}$$

= $-\tilde{D}_{2}(\phi_{2}^{i+1} - \phi_{2}^{i})$ (2.7)

The net current, J_0 , is readily calculated from the MC calculation. However, it would require substantial numerical cost to calculate the reference second-moment neutron flow in the MC calculation. Therefore, the leakage correction is only applied to the zeroth moment equation, and the second moment equation is just solved in a conventional way without the correction.

The correction factor, \hat{D}_0 , is calculated as follows:

$$\hat{D}_{0} = \frac{J_{0}^{ref} + \tilde{D}_{0}(\hat{\phi}_{0}^{i+1} - \hat{\phi}_{0}^{i})}{\hat{\phi}_{0}^{i+1} + \hat{\phi}_{0}^{i}}$$
(2.8)

where \tilde{D}_n (n = 0 or 2) is the effective diffusion coefficient at the interface of the two neighboring cells, defined by

$$\tilde{D}_0 = \frac{2d_0^{i+1}d_0^i}{d_0^{i+1} + d_0^i} \tag{2.9}$$

$$d_0^i = D_0 / \Delta x_i \tag{2.10}$$

and

$$\tilde{D}_2 = \frac{2d_2^{i+1}d_2^i}{d_2^{i+1} + d_2^i}$$
(2.11)

$$d_2^i = D_2 / \Delta x_i \tag{2.12}$$

 $\hat{\phi}_0$ is the sum of the zeroth moment and two times of the second moment as defined in Eq. (2.3). The reference net current and the node average zeroth moment are obtained from the high-fidelity MC calculation. However, the second moment involved in the $\hat{\phi}_0$ is not evaluated by the MC calculation. Thus, the second moment is directly obtained by the CMFD calculation such that

$$\hat{\phi}_0 = \phi_0^{MC} + 2\phi_2^{CMFD} \tag{2.13}$$

Unlike the MC method simulating any arbitrary geometry, the finite difference method requires standardized mesh grid system to establish the balance equation. As a consequence, the energy condensation and cross-section homogenization in a coarse mesh should be implemented. The one-group constant can be calculated as follows:

$$\Sigma_{\alpha}^{i} = \frac{\int_{0}^{\infty} dE \int_{V_{i}} d\vec{r} \Sigma_{\alpha}(\vec{r}, E) \phi(\vec{r}, E, t)}{\int_{0}^{\infty} dE \int_{V_{i}} d\vec{r} \phi(\vec{r}, E, t)}$$
(2.14)

where V_i is the coarse mesh cell i.

The flux distribution from the CMFD calculation is used to improve the fission source distribution for the MC calculation. The neutron flux distribution adjusts the weight of the fission neutrons in the following way:

$$w_r^{i\prime} = w_r^i \cdot p_r \tag{2.15}$$

where p_r is the probability density function of the neutron flux distribution at region r such that

$$p_r = \frac{v \Sigma_f^r \phi^r V^r}{\sum_r v \Sigma_f^r \phi^r V^r}$$
(2.16)

3. Numerical Results

Numerical tests were performed with the unrodded C5G7 benchmark problem depicted in Figs. 1 and 2 [6]. The MC simulation was done with 25 inactive cycles, 1,000 active cycles, and 200,000 histories in a single cycle. The CMFD module was activated after the first 2 and 5 inactive cycles for the comparison, and parameters such as net current, neutron flux, and group constants were accumulated over the active cycles to generate CMFD factors.



Fig. 1 Configuration of C5G7 unrodded core



Fig. 2 Vertical section of C5G7 unrodded core

The Shannon entropy was compared to characterize the convergence rate of the fission source distribution in Figs. 3 and 4 for each case; (1) stand-alone MC, (2) MC-CMFD with diffusion equation, and (3) MC-CMFD with SP₃ equation. The entropy asymptotically decreases, and reaches a plateau region. The entropy with a CMFD feedback showed a very different behavior from the standard MC calculation. The SP₃ approximation usually provides more accurate flux distribution than the diffusion approximation. Therefore, it was expected that the SP₃ equation also stabilizes the fission source distribution, and thus the fission source will quickly approach the converged distribution. However, no big difference on the convergence rate was observed as shown in Figs. 3 and 4.



Fig. 3 Comparison of the Shannon entropy for three cases (CMFD coupling from the 2nd inactive cycle)



Fig. 4 Comparison of the Shannon entropy for three cases (CMFD coupling from the 5th inactive cycle)

In Fig. 5, all the cumulative multiplication factors for each case are plotted together with the reference value. One can see that both CMFD multiplication factors converge to the reference one and the SP₃-based multiplication factor is in general closer to the standard MC value throughout the simulation. Regarding the CMFD coupling in the active MC cycle, there is a controversial issue on potential bias of the solution. In this preliminary study, we observed that no bias is introduced by SP₃-based CMFD.



Fig. 5 Comparison of the accumulated multiplication factor for three cases

3. Conclusions

A CMFD acceleration with the SP₃ approximation is applied to the MC calculation. The new SP₃-based CMFD method quickly stabilizes the fission source distribution as fast as the conventional diffusion-based CMFD method, and thereby also decreases the number of inactive cycles. In the future, feasibility of the SP₃ CMFD acceleration of the active Monte Carlo cycle will be investigated in a systematic way.

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