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An Adjoint p-CMFD Scheme for Monte Carlo k-Eigenvalue Calculations

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ABSTRACT

Although the Monte Carlo method is very powerful for complicated problems, it requires huge computation time. Thus there exists a strong demand for a methodology to decrease the computation time.

The partial current-based Coarse Mesh Finite Difference (p-CMFD) rebalance method was applied for this purpose. In this paper, coupling of forward and adjoint solutions in p-CMFD rebalance method is presented to reduce the computational load more efficiently in Monte Carlo criticality calculation. Here, the adjoint flux in the adjoint p-CMFD/MCNP method is used as the weights in Monte Carlo calculation.

The numerical results of the original MCNP method, p-CMFD/MCNP method, and p-CMFD with adjoint/MCNP method are presented for comparison.

I. INTRODUCTION

The Monte Carlo method is widely used in particle transport calculations, especially in complex geometry. The Monte Carlo method gives very accurate solution if we use enough particle histories. The MCNP code [1] is one of the most popular Monte Carlo computer codes and it is applied to the various problems in nuclear engineering. To solve eigenvalue problems with MCNP, however, we need tremendous amount of computation time even with computers of nowadays due to the large number of particle

histories and generations required for acceptably small standard deviation. Reducing the computational burden in Monte Carlo calculations is thus a great challenge.

It is easily predicted that computation time will be much reduced if we can reduce the required number of generations in the k-code calculation in MCNP. The p-CMFD/MCNP scheme was developed to reduce the computation time and it provided good performance for the reduction of computation time. [8] In this p-CMFD/MCNP scheme, the partial current-based Coarse Mesh Finite Difference (p-CMFD) method [3] was chosen as the deterministic component to make good estimation of eigenvalue and fission source.

However due to the stochastic errors in MCNP calculation, the p-CMFD method provides solutions with some bias. Thus, in this paper, an adjoint p-CMFD method is proposed to reduce the bias due to the stochastic errors in Monte Carlo calculation and we tested the scheme on a test problem. A comparison with the reference MCNP/p-CMFD scheme is presented. The results are encouraging.

II. MCNP/ P-CMFD METHOD

Here, the Monte Carlo k-eigenvalue problem is decomposed into a fixed-source Monte Carlo problem (in whole core) and an eigenvalue coarse-mesh deterministic problem. In a particular generation of the Monte Carlo calculation, the problem is posed as a fixed-source problem in which the source is provided by the fission neutron distribution given by the Monte Carlo solution at the end of the previous generation, combined with the k_{eff} and coarse-mesh flux distribution obtained by the p-CMFD solution. That is,

$$S(\vec{r}, E) = \frac{1}{k_{eff}} \nu\Sigma_f(\vec{r}, E)\phi(\vec{r}, E), \quad (1)$$

where

$$\phi(\vec{r}, E) = \phi_m(\vec{r}, E) \cdot f_M(\vec{r}, E), \quad (2)$$

and $\phi_m(\vec{r}, E)$ is obtained from Monte Carlo calculation in fine meshes, k_{eff} and $f_M(\vec{r}, E)$ are obtained from p-CMFD deterministic calculation to be described below.

$f_M(\vec{r}, E)$ is the ratio of p-CMFD to Monte Carlo scalar fluxes in coarse mesh M.

The coefficient parameters in the p-CMFD equation are in turn obtained using the results of the Monte Carlo calculation in the previous generation.

In the p-CMFD acceleration in an eigenvalue problem, the equations for coarse-mesh scalar fluxes are for each coarse mesh (dropping group index g),

$$\sum_{M'} \int_{MM'} d\Gamma \hat{n} \cdot \vec{J}^{l+1} + \int_{V_M} dV \sigma_a \phi^{l+1} = \frac{1}{k_{eff}} \int_{V_M} dV \nu\sigma_f \phi^{l+1}, \tag{3}$$

where M is coarse mesh index and the current at interface $M+1/2$ is given as follows:

$$J_{M+1/2}^{l+1} = J_{M+1/2}^{+,l+1} - J_{M+1/2}^{-,l+1}, \tag{4}$$

$$J_{M+1/2}^{+,l+1} = \frac{-\tilde{D}_{M+1/2}(\phi_{M+1}^{l+1} - \phi_M^{l+1}) + 2\hat{D}_{M+1/2}^{+}\phi_M^{l+1}}{2}, \tag{5}$$

$$J_{M+1/2}^{-,l+1} = \frac{\tilde{D}_{M+1/2}(\phi_{M+1}^{l+1} - \phi_M^{l+1}) + 2\hat{D}_{M+1/2}^{-}\phi_{M+1}^{l+1}}{2}, \tag{6}$$

where $\tilde{D}_{M+1/2}$ is the usual coupling coefficient determined by the finite difference method and $\hat{D}_{M+1/2}^{\pm}$ are correction coefficients of partial currents, which are obtained from high order (i.e., Monte Carlo) results. The coefficients parameters in Eq. (3) are homogenized cross sections in each coarse mesh, that are given as,

$$\sigma_{x,M} = \frac{\sum_{m \in M} \sigma_{x,m} \phi_m^{l+1/2} V_m}{\sum_{m \in M} \phi_m^{l+1/2} V_m}. \tag{7}$$

The system of equations (3) for the whole problem provides k_{eff} and coarse-mesh average scalar fluxes. The scalar flux distributions are then updated as,

$$\phi_m^{l+1} = \phi_m^{l+1/2} \frac{\phi_M^{l+1}}{\phi_M^{l+1/2}}, \tag{8}$$

for fine mesh m that is in coarse mesh M.

In summary, the speedup scheme consists of a fixed-source Monte Carlo calculation in which the fission source distribution (including k_{eff}) is provided by the p-CMFD equation which in turn requires Monte Carlo solution for its coefficient parameters. This coupled procedure continues until the solution converges. Fig. 1 shows a schematic computational flow.

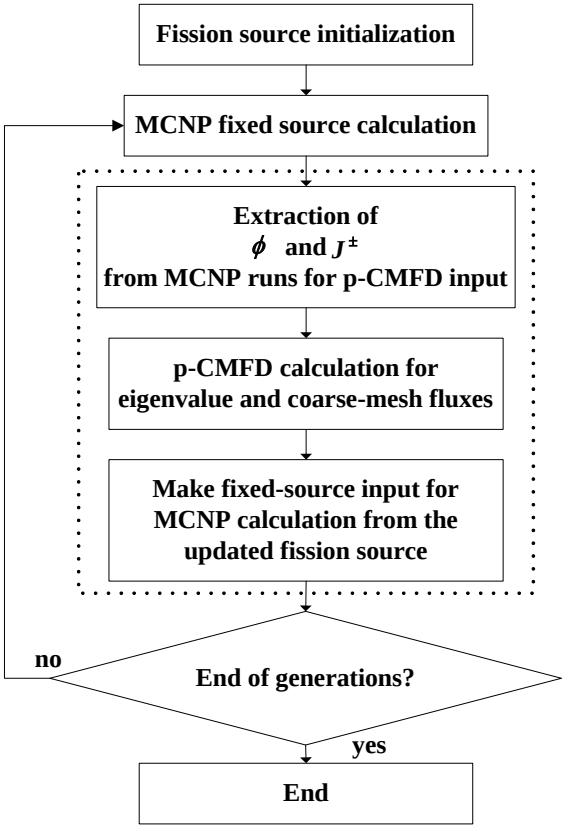


Fig. 1: Computational flow of MCNP/p-CMFD scheme

III. ADJOINT MCNP/ P-CMFD METHOD

Since there exist fluctuations in flux $\phi_m(\vec{r}, E)$ due to the stochastic errors in MCNP calculation, the coarse-mesh average scalar fluxes given by p-CMFD calculation will have certain errors. We in addition perform an adjoint p-CMFD calculation with adjoint source of fission cross section. The adjoint flux is then used as weight in the MCNP calculation. The adjoint p-CMFD equation is given as follows (dropping group index g):

$$\left[H - S\right]^T \phi^* = q_{ex}^*, \tag{9}$$

where ϕ^* is adjoint flux of ϕ,

$$H^T = \begin{bmatrix} & & & & & \vdots & & & & & \\ 0 & \cdots & 0 & B_{I-1} & A_{I-1} & C_{I-1} & 0 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & B_I & A_I & C_I & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & 0 & B_{I+1} & A_{I+1} & C_{I+1} & 0 & \cdots & 0 \\ & & & & & \vdots & & & & & \end{bmatrix}, \tag{10}$$

$$A_I = \tilde{D}_{I-1/2} + \hat{D}^-_{I-1/2} + \tilde{D}_{I+1/2} + \hat{D}^+_{I+1/2} + \sigma_{aI}, \tag{10a}$$

$$B_I = -\tilde{D}_{I-1/2} - \hat{D}^-_{I-1/2}, \tag{10b}$$

$$C_I = -\tilde{D}_{I+1/2} - \hat{D}^+_{I+1/2}, \tag{10c}$$

and if we drop mesh index I,

$$S^T = \begin{bmatrix} 0 & \sigma_{s12} & \sigma_{s13} & \cdots & \sigma_{s1G} \\ \sigma_{s21} & 0 & \sigma_{s23} & \cdots & \sigma_{s2G} \\ \sigma_{s31} & \sigma_{s32} & 0 & \cdots & \sigma_{s3G} \\ \vdots & & \vdots & & \vdots \\ \sigma_{sG1} & \sigma_{sG2} & \sigma_{sG3} & \cdots & 0 \end{bmatrix}. \tag{11}$$

In this adjoint equation, the adjoint flux ϕ^* will have the meaning of “fission importance”, if we choose

$$q^{ex*} = \frac{1}{k_{eff}} \begin{bmatrix} \nu\sigma_{f1} \\ \nu\sigma_{f2} \\ \vdots \\ \vdots \\ \nu\sigma_{fG} \end{bmatrix}. \quad (12)$$

The eigenvalue used in the adjoint p-CMFD calculation is obtained by the p-CMFD calculation above, Eq. (3). The adjoint fluxes of adjoint p-CMFD calculation are then used in MCNP/ p-CMFD calculation as the weights of fission source:

$$w_{I,g} = \sum_{g'} \phi^*_{g',I}, \quad \text{for all group } g, \quad (13)$$

where $w_{I,g}$ is the weight in MCNP calculation. Fig. 2 shows a schematic computational flow.

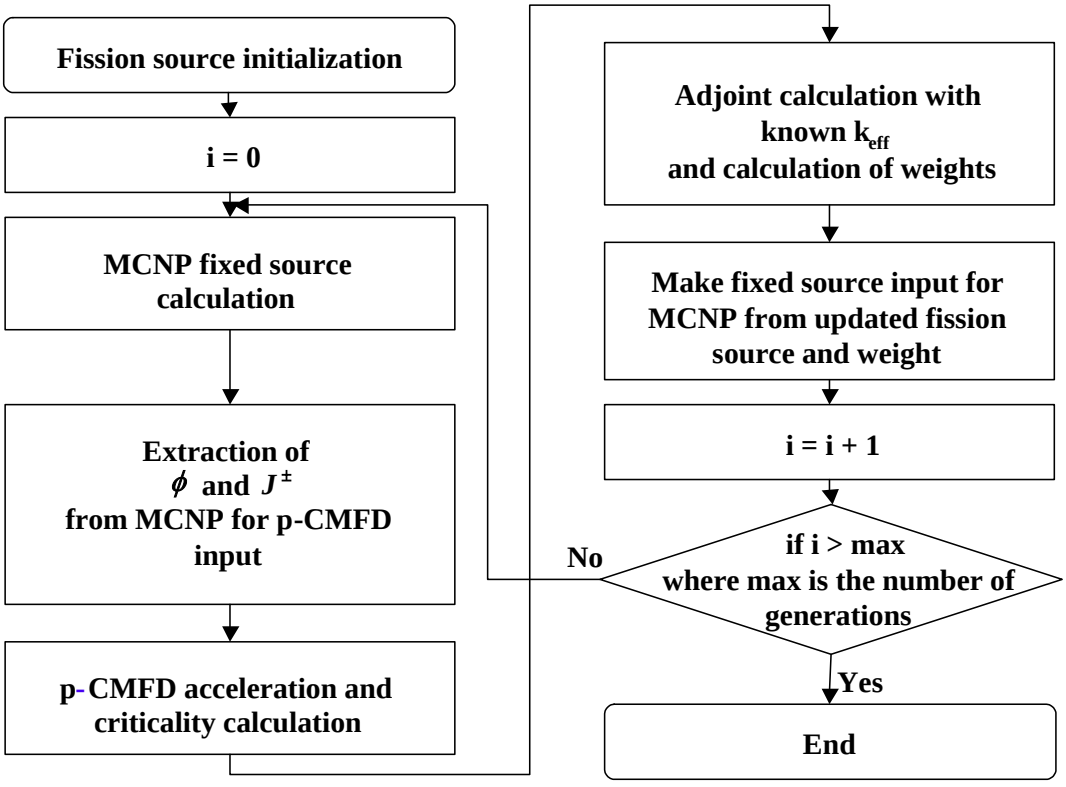


Fig. 2: Computational flow of adjoint MCNP/p-CMFD scheme

IV. NUMERICAL RESULTS

We applied the MCNP/p-CMFD scheme and the adjoint MCNP/p-CMFD scheme to a test problem which consists of 18x18 fuel pins. Boundary conditions are all reflective and 7 energy group cross sections in Ref. [5] are used. The detailed configuration of the problem is described in Fig. 3. A comparison of the results of MCNP/p-CMFD and original MCNP method are already presented in Ref. [8] and showed good performance. Thus in this paper, we focus on the comparison of the MCNP/p-CMFD method with the adjoint MCNP/p-CMFD method.

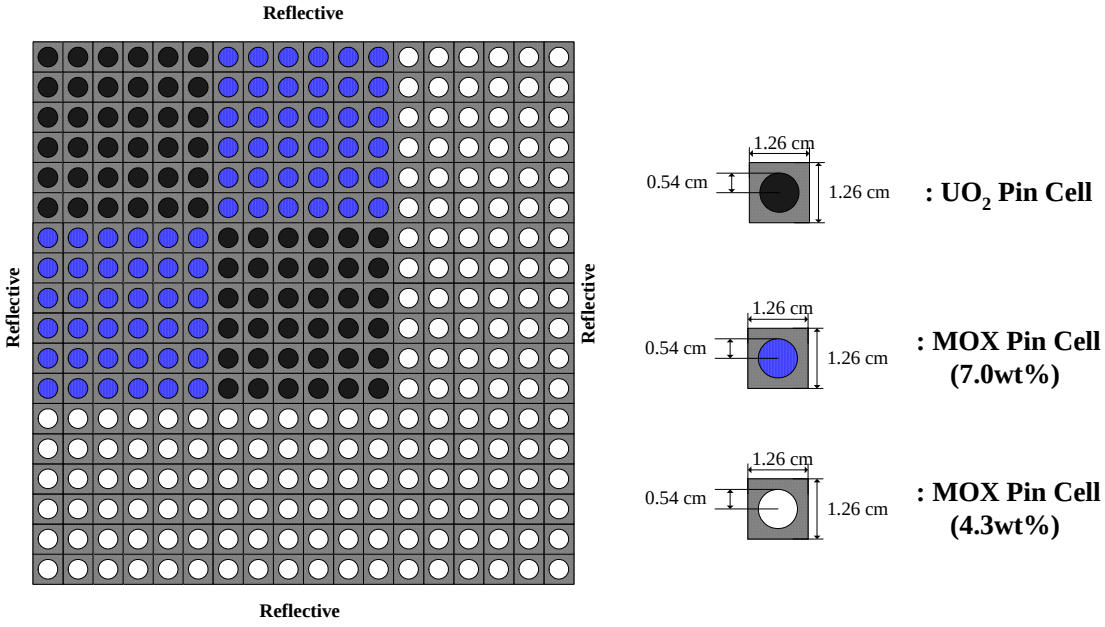
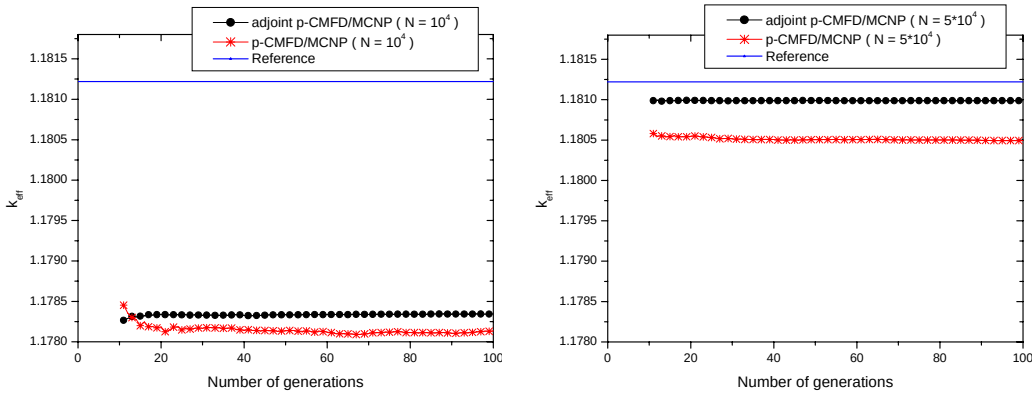


Fig. 3: Configuration of a test problem

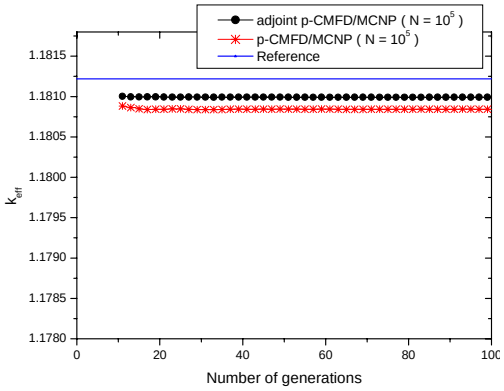
The results are presented in Fig. 4 and Fig. 5 and in Table I. From Fig. 4, we observe that k_{eff} in the adjoint MCNP/p-CMFD scheme exhibits very small bias as the number of generation increases while k_{eff} in the MCNP/p-CMFD still has some bias. This may be due to more accurate fission source distribution resulting from the use of adjoint fluxes as weights provided by the adjoint MCNP/p-CMFD scheme.

As an alternative use of the two schemes, Fig. 5 shows the results of a switching calculation in which the first 20 generations are done by the adjoint MCNP/p-CMFD scheme or the MCNP/p-CMFD scheme, and then switched to the conventional MCNP

calculation up to 300 generations. The results show good performance of the adjoint MCNP/p-CMFD scheme. Thus it is expected that the adjoint MCNP/p-CMFD gives more exact initial guess rather than that of MCNP/p-CMFD scheme for the same computational burden.



(a) 10^4 histories/generation **(b) 5×10^4 histories/generation**



(c) 10^5 histories/generation

Fig. 4: k_{eff} as functions of generation and number of histories (N) per generation (first 10 generations skipped)

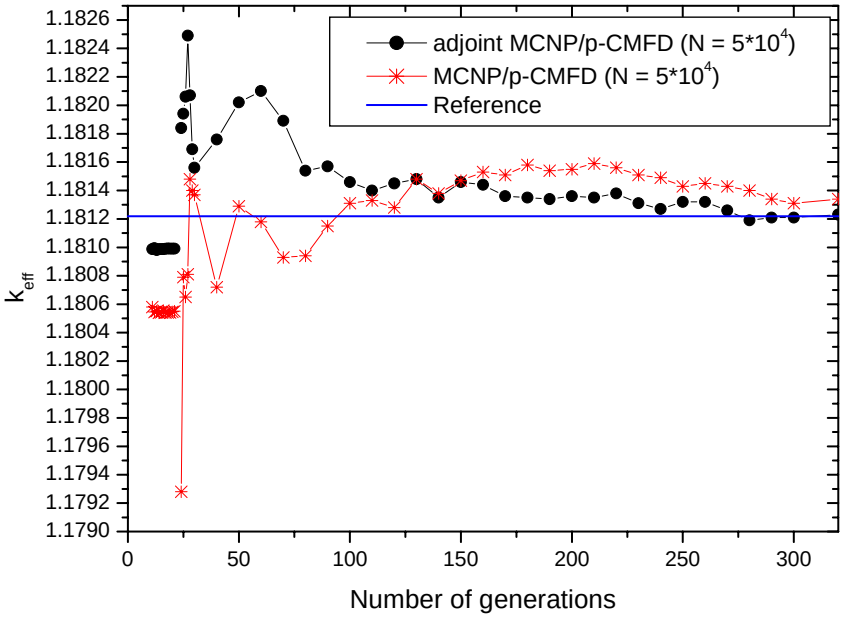


Fig. 5: Initialization by MCNP/p-CMFD and adjoint MCNP/p-CMFD (First MCNP/p-CMFD or adjoint MCNP/p-CMFD 20 generations and then MCNP 300 generations)

Table I shows the sensitivity of k_{eff} on the number of particle histories per generation. We calculated k_{eff} by averaging the results of every p-CMFD calculation in both of the MCNP/p-CMFD scheme and the adjoint MCNP/p-CMFD scheme. We skipped k_{eff} of the first 10 generations. From Table I, we note that the adjoint MCNP/p-CMFD scheme provides more accurate eigenvalues than MCNP/p-CMFD for all particle histories tested.

In comparison with the conventional MCNP, the adjoint MCNP/p-CMFD is more efficient by a factor of about 6.6 while the MCNP/p-CMFD by a factor of 3.

Table I: Sensitivity of k_{eff} on particle histories and generations[a]

	Total number of particles	k_{eff}	% error[e]		Total number of particles	k_{eff}	% error[e]
Ref MCNP	**$1.5*10^8$ ($500^b/3*10^{5c}$)**	**1.18122 (0.00006)[d]**	**-**	**MCNP**	**10^7 ($500/2*10^4$)[f]**	**1.18095 (0.00024)**	**0.0229**
MCNP / p-CMFD	**10^6 ($100/10^4$)**	**1.17814 (0.00030)**	**0.2607**	**Adjoint MCNP / p-CMFD**	**10^6 ($100/10^4$)**	**1.17834 (0.00005)**	**0.2438**
	$5*10^6$ ($100/5*10^4$)	**1.18049 (0.00006)**	**0.0618**		**$5*10^6$ ($100/5*10^4$)**	**1.18099 (0.000015)**	**0.0195**
	10^7 ($100/10^5$)	**1.18084 (0.00003)**	**0.0322**		**10^7 ($100/10^5$)**	**1.18099 (0.000008)**	**0.0195**
	$3*10^6$ ($30/10^5$)	**1.18084 (0.00003)**	**0.0322**		**$3*10^6$ ($30/10^5$)**	**1.18099 (0.000008)**	**0.0195**
	$1.5*10^6$ ($30/5*10^4$)	**1.18051 (0.00007)**	**0.0602**		**$1.5*10^6$ ($30/5*10^4$)**	**1.18099 (0.000019)**	**0.0195**

[a] : First 200 generations skipped in conventional MCNP and first 10 generations skipped in MCNP/p-CMFD and the adjoint MCNP/p-CMFD

[b] : Number of generations

[c] : number of histories per generation

[d] : standard deviation

[e] : % error of k_{eff}

[f] : 200 generation skip

IV. CONCLUSIONS AND FUTURE WORK

For the test problem, the eigenvalue in the adjoint MCNP/p-CMFD has less bias than that of the MCNP/p-CMFD. The adjoint MCNP/p-CMFD is more efficient by a factor of two than the MCNP/p-CMFD. The results may indicate that the adjoint-weight process helps the fission source to reach equilibrium distribution faster.

Although the adjoint MCNP/p-CMFD scheme presented better performance, there still exist rooms for improvement such as the application of group-wise weighting, the extension to the continuous-energy Monte Carlo problem, and the further reduction of bias in k_{eff} [8].

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