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# Multigroup Monte Carlo Reactor Calculation with Coarse Mesh Finite Difference Formulation for Real Variance Reduction

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The coarse mesh finite difference (CMFD) formulation has been applied to Monte Carlo (MC) simulations in order to mitigate the issue of large real variances of pin power tallies in full-core problems. In this work, a parallelized multigroup (MG) two-dimensional (2-D) MC code named PRIDE (Probabilistic Reactor Investigation with Discretized Energy), which is capable of handling lattices of square pin cells within which circular substructures can be modeled, has been developed as a tool for the investigations of the new method. In this code, a scheme to construct a CMFD linear system is based on the MC tallies of coarse mesh average fluxes and the net currents at coarse mesh interfaces. These tallies are accumulated over the MC cycles to get more stable CMFD solutions which are used for feedback to MC fission source distribution (FSD). The feedback scheme in this code employs a weight adjustment of fission source neutrons for the next MC cycle that is to reflect the global CMFD FSD into the MC FSD. The performance of CMFD feedback has been investigated in terms of the number of inactive cycles required for the convergence of FSD and also the reduction of real variances of local property tallies in active cycles. The applications to 2-D multigroup full-core pressurized water reactor problems have demonstrated that the MC FSD converges considerably faster and the real variances of pin powers are smaller by a factor of 4 with CMFD FSD feedback. It is also noted that the large real variances of pin powers are caused mainly by the global assembly-wise fluctuations of power distributions in a large core rather than local fluctuations.

***KEYWORDS: Monte Carlo, CMFD, high dominance ratio problems, real variance***

## I. Introduction

As Brown[1)] indicated in a presentation at the M&C 2009 meeting in Saratoga, NY, the real variance of local properties, such as pinwise fission rates, can be significantly higher (by a factor of 5 or more) than the sample variance. The real error of local properties determined from an MC simulation can be considered a few times greater than the apparent error represented by the sample standard deviation. An early work of Ueki[2)] introduced the term *real variance*, which refers to the variance of mean values, and the term *apparent variance*, which refers to the expected value of sample variance. The uncertainty of a single MC calculation is expected to be close to the square root of the apparent variance or the apparent standard deviation. Ueki showed that the real variance could be much larger than the apparent variance according to the lag covariance[2)] and also showed that the bias in the sample variance could be significant in a high dominance ratio problem.[3)] Shim and Kim suggested some practical ways to estimate real variance in a single MC simulation.[4,5)] However, the best way to obtain a real variance is to calculate the variance of mean values through multiple MC runs with different random number sequences.

Meanwhile, a new kind of MC simulation, the functional Monte Carlo (FMC) method was developed by Larsen and Yang.[6–8)] The essential functionals for the FMC linear system are integrated during an MC simulation, and the solution is obtained by solving the FMC linear system. The final solution is, however, obtained from a statistical treatment on many FMC solutions so that it can be called a *hybrid MC* method. The FMC hybrid method gave better statistical error, which is smaller and more reliable than that of the analogue MC; however, only the 1-D FMC formulation is available at this time.

In this work we will reduce the real variance by employing the coarse mesh finite difference (CMFD) acceleration.[9)] CMFD has been widely used with deterministic methods such as the Method of Characteristics (MOC) and the nodal diffusion methods to achieve fast convergence. Similarly, CMFD can be applied to the MC eigenvalue calculation, and an improved global fission source distribution can be obtained by solving the CMFD linear system. Through the MC simulation utilizing CMFD updated fission source distribution, the variance of local properties can be reduced since the fluctuation of the fission source distribution can be smaller with this approach. This forms the basis for this work.

In order to assess the performance of CMFD acceleration on MC reactor calculation, a multigroup two-dimensional (2-D) MC code named PRIDE (Probabilistic Reactor Investigation with Discretized Energy), which is capable of handling a lattice of square pin cells within which circular

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substructures can be modeled, was developed as the basic tool for investigation. PRIDE is faster than other general-purpose MC codes such as MCNP and McCARD because of its significantly simplified geometry-handling routine. Thus, PRIDE is well suited for extensive MC trial runs.

In this paper, the details of real variance and apparent variances are explained first in Section II. It is followed by a description of the CMFD formulation and the weight adjustment scheme. The performance examination is presented in Section III. Conclusions are given in Section IV.

## II. Real Variance and CMFD on MC

### 1. Real and Apparent Variances

As mentioned before, the real variance refers to the variance of mean values. From its definition, the real variance of a tally $Q$ can be obtained as follows:

$$\sigma_R^2[Q_k] = E[Q_k^2] - E[Q_k]^2 \quad \text{where } Q_k = \frac{1}{N}\sum_{i=1}^{N} Q_{i,k} \tag{1}$$

The apparent variance is defined as

$$\sigma_A^2[Q_k] = E[\sigma_s^2[Q_k]] \quad \text{where } \sigma_s^2[Q_k] = \frac{1}{N(N-1)}\sum_{i=1}^{k}(Q_k - Q_{i,k})^2 \tag{2}$$

In Eq. (1), $k$ is the index of independent MC run. Those two values can be estimated from a statistical treatment on multiple MC run results. In this work, we determine the real variance after 25 independent MC runs performed with a different random number sequence and use the real standard deviation as an estimate of the mean value error.

The sample variance obtained from a single MC simulation reflects the uncertainty of the sample mean. Therefore, the mean of the sample variance, which is the apparent variance, should be the same as the real variance for the ideal MC simulation as long as there is no correlation in MC samples. However, in a practical MC reactor core calculation, a real variance appears much larger than an apparent variance. This is particularly noted in the local properties estimated in eigenvalue calculations. This underestimation of variance is related to the power iteration performed in analogue MC eigenvalue calculations.

Power iteration is carried out during an MC simulation to obtain a converged fission source distribution. In this process, the fission sources are generated from the fission events in the previous cycle so that each MC cycle starts from a previous fission source distribution. The consequence of this power iteration is that the tally $Q$ in an MC simulation is highly correlated with the one in the previous cycle. This is called *inter-cycle correlation*. The inter-cycle correlation appears to be strong for the local properties of MC tallies in a high dominance ratio problem. Pin power distribution calculations for large three-dimensional (3-D) full-core problems suffer from such strong inter-cycle correlation. The main objective of this work is to reduce the correlation between cycles to obtain better statistics, namely smaller real standard deviations by CMFD acceleration.

### 2. CMFD Formulation

The CMFD formulation can be illustrated using a simple diffusion equation as follows:

$$\frac{dJ(x)}{dx} + \Sigma_a(x)\phi(x) = \frac{1}{k}\nu\Sigma_f(x)\phi(x) \tag{3}$$

By applying Fick's law and performing discretization, the current term on the right-hand side of coarse mesh $m$ can be written as

$$J_m = -\frac{2D_m D_{m+1}}{h_m D_{m+1} + h_{m+1} D_m}(\bar{\phi}_{m+1} - \bar{\phi}_m) \equiv -\tilde{D}_{m+1}(\bar{\phi}_{m+1} - \bar{\phi}_m) \tag{4}$$

The neutron current represented by this finite difference approximation involves nontrivial truncation errors for large meshes. In order to correct the error, we introduce an additional correction factor $\hat{D}$ to conserve the current of a higher order system as

$$J_m = -\tilde{D}_{m+1}(\bar{\phi}_{m+1} - \bar{\phi}_m) + \hat{D}_{m+1}(\bar{\phi}_{m+1} + \bar{\phi}_m) \tag{5}$$

$\hat{D}$ will be determined by solving a higher order problem. After integrating the balance equation over the coarse mesh $m$, we can obtain the CMFD balance equation as

$$\begin{aligned}&(-\tilde{D}_{m+1} + \hat{D}_{m+1})\bar{\phi}_{m+1} + (-\tilde{D}_m - \hat{D}_m)\bar{\phi}_{m-1} \\ &+ (\tilde{D}_{m+1} + \tilde{D}_m + \hat{D}_{m+1} - \hat{D}_m + \Sigma_{a,m}h_m)\bar{\phi}_m = \frac{1}{k}\nu\Sigma_{f,m}\bar{\phi}_m h_m\end{aligned} \tag{6}$$

To construct a CMFD linear system by taking MC simulation as a higher order solution, the CMFD parameters such as diffusion coefficients, homogenized cross sections, node average fluxes and $\hat{D}$ need to be calculated from various MC tallies as follows:

$$D_m = \frac{1}{3\Sigma_{t,m}},\ \Sigma_{\alpha,m} = \left[\frac{\sum_{i\in m}\Sigma_{\alpha,i}\phi_i V_i}{\sum_{i\in m}\phi_i V_i}\right]_{MC},\ \text{and } \bar{\phi}_m = \left[\frac{\sum_{i\in m}\phi_i V_i}{\sum_{i\in m} V_i}\right]_{MC}. \tag{7}$$

$$\hat{D}_{m+1} = \left[\frac{J_m^+ + \tilde{D}(\bar{\phi}_{m+1} - \bar{\phi}_m)}{(\bar{\phi}_{m+1} + \bar{\phi}_m)}\right]_{MC} \tag{8}$$

Since the above definitions preserve the interface currents and the nodal reaction rates, the MC solution can be reproduced by solving the CMFD linear system.

In practical calculations, MC simulation tends to converge very slowly when the dominance ratio is high. In this case, the nodal balance of MC itself breaks down significantly; therefore, the CMFD solution cannot be the same as that for

MC. Even though the MC information is not exact, the CMFD linear system tends to converge faster than the MC system since the perturbation in the local area can propagate simultaneously across the whole domain in the CMFD linear system. This means that the CMFD solution can be more accurate than that of the MC, even with inaccurate information.

The primary reason for the underestimation of sample variances is the inter-cycle correlation. Analog MC cannot break the strong correlation between samples in adjacent cycles since the neutrons are generated from the fission sites of the previous cycle. However, if the exact fission source distribution is known and thus it is possible to generate the fission neutrons corresponding to the distribution, not preserving the fission sites of the previous cycle, the inter-cycle correlation would disappear. On the other hand, if the fission sites are preserved, but the weights of the fission sources are adjusted instead according to the exact fission source distribution, the correlation between samples can be weakened. In this work, the weights of fission source neutrons are adjusted according to the CMFD fission source distribution. The CMFD solution is not exact, but it is still reliable and does not fluctuate much so that the real variance can be reduced close to the level of the apparent variance. It should be noted that the accuracy of a CMFD solution is the key in successful real variance reduction. Therefore, the CMFD parameters should be evaluated from accumulated MC tallies.

### 3. Weight Adjustment

In the CMFD acceleration of MC, the obtained CMFD solutions can be fed back to the MC system by a weight adjustment scheme similar to the prolongation scheme in the deterministic approach. The weight adjustment scheme ensures that the global fission source distribution of the MC system can be the same as that of the CMFD system. For the weight adjustment, the fission fraction of node $m$ can be defined as

$$p_m = \frac{\psi_m}{\sum_{m=1}^{N_{coarse}} \psi_m} \tag{9}$$

where $\psi_m$ is the CMFD fission source in coarse mesh $m$. Assuming that total $N_{history}$ neutrons are generated in a cycle, then the expected fission source neutron in coarse mesh $m$ can be calculated simply as

$$E[n_m] = N_{history} \times p_m \tag{10}$$

This implies that if the weight sum of all the neutrons that are born in coarse mesh $m$ is the same as $E[n_m]$, the MC fission source distribution will be the same as CMFD. Thus, the next step is to adjust the weight of each fission neutron. Assuming that a fission neutron in coarse mesh $m$ has weight $\omega_i$, then the proper weight for this neutron is

$$\tilde{\omega}_i = \omega_i \times f_w \quad \text{where } f_w = \frac{E[n_m]}{\sum_{i \in m} \omega_i}. \tag{11}$$

This weight adjustment only modifies the weight of fission source neutrons in a coarse mesh with the same correction factor $f_w$. Since only the coarse mesh-wise global fission source distribution is modified, the local fission source distribution can be preserved in a coarse mesh. The overall procedure for CMFD acceleration is shown in Fig. 1. After the MC simulation, group constants are generated by homogenization routines. After that, the correction factor $\hat{D}$ is calculated to construct the CMFD linear system. Then the CMFD fission source distribution is generated and the weights of fission source neutrons are adjusted.

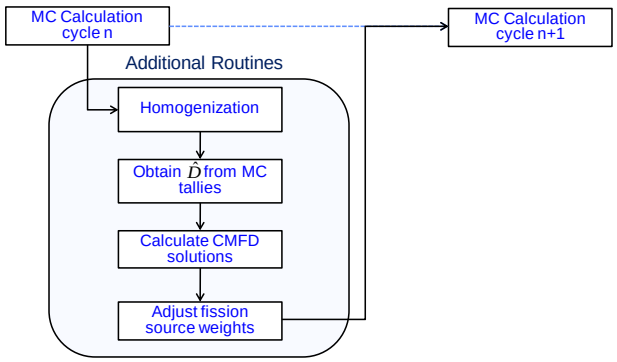


**Fig. 1** The MC-CMFD procedure.

## III. Performance Examination

In our previous work,[10] CMFD acceleration proved to be beneficial in simple 1-D and 2-D high dominance problems. It can reduce the number of inactive cycles significantly and reduce the real variance of local tallies as well. In this work, we assess the performance of CMFD acceleration in 2-D multigroup full core problems.

### 1. Test Problem 1: Simplified Hoogenboom–Martin MC benchmark

The Hoogenboom–Martin MC benchmark problem[10] is actually a 3-D full-core problem, but we simplified it to a 2-D two-group problem as Test Problem 1. The group constants are generated by DeCART[11] calculation, and the core configuration is simplified as shown in Fig. 2. Other geometries such as fuel pins and guide tubes are fully represented as the original problem.

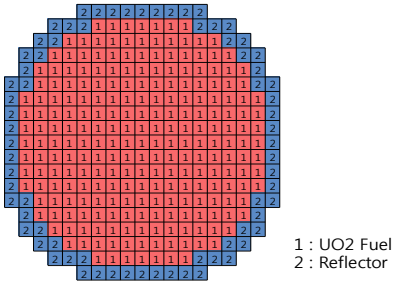


**Fig. 2** Simplified core configuration of Hoogenboom–Martin MC benchmark problem as Test Problem 1

At first, the convergence of MC fission source distribution was examined by monitoring the Shannon entropy, which is defined as

$$H_{src} = -\sum_{i=1}^{N_{FP}} p_i \cdot \log_2(p_i) \tag{12}$$

where $N_{FP}$ is the number of fuel pins in the problem domain and $p_i$ is the source fraction in the fuel pin $i$. The Shannon entropy behavior, which is plotted in Fig. 3, is evaluated from a single MC simulation with 100,000 histories per cycle. The blue line shows the Shannon Entropy in the conventional MC simulation from a flat initial source distribution. At a glance the fission source distribution of the conventional MC seems to converge beyond Cycle 150. However, if CMFD acceleration is applied after Cycle 10, the fission source distribution seems to converge rapidly, as the Shannon entropy drops suddenly and shows a very stable behavior.

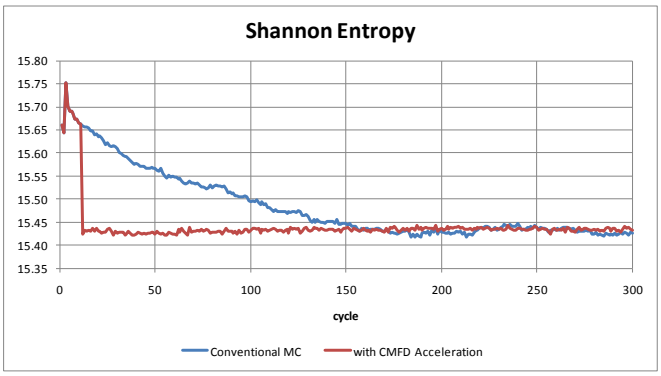


**Fig. 3** Shannon entropy behavior of Test Problem 1

Actual fission source distributions at Cycles 10, 11, 12, and 300 are plotted in Fig. 4. The fission source distribution of MC simulation is exact from the initial cycle to Cycle 10 since the weight adjustment was performed at Cycle 10. At Cycle 11 the fission source distribution in the conventional MC changes slightly compared with the previous one. However, the accelerated one changes to a different shape. At Cycle 12, minor changes are still noted in the conventional MC fission source distribution and the accelerated one sustains its shape. At Cycle 300, both distributions seem to be the same since the fission source distribution has already converged. Nevertheless, it is important that the converged fission source distribution is much like the accelerated one at Cycle 12. This indicates that the CMFD acceleration maintains the MC fission source distribution as a converged shape during the entire MC simulation, thus preventing the global fluctuation, which will be further explained later. This pattern shows how CMFD acceleration can improve MC simulation.

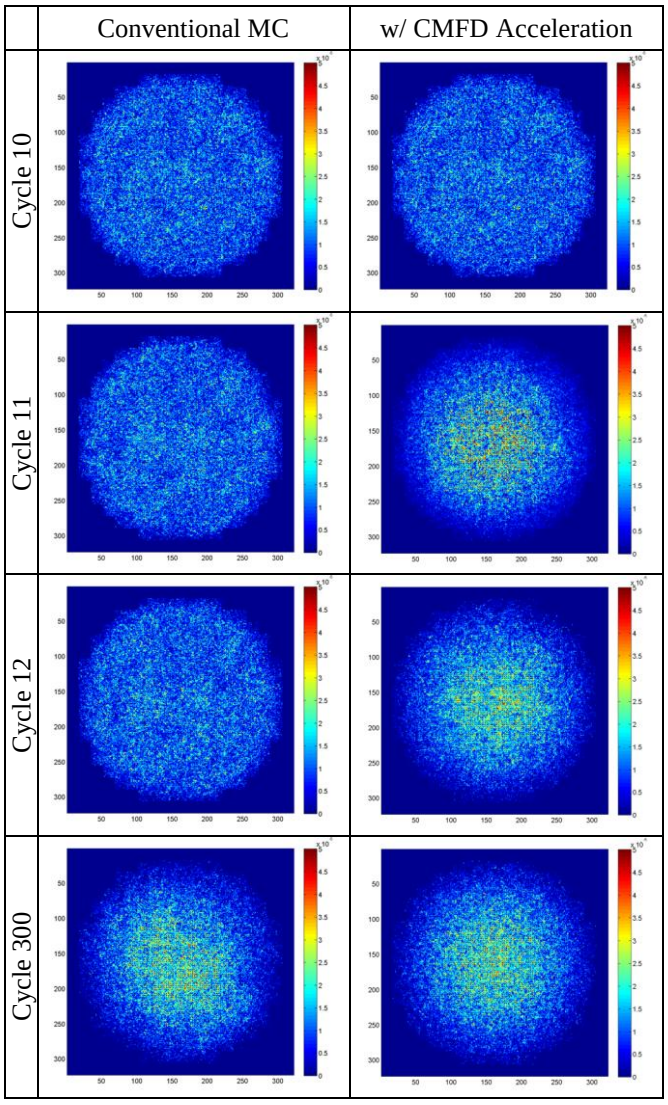


**Fig. 4** Fission source distribution at Cycles 10, 11, 12, and 300

The powers of fuel pins are obtained from multiple MC simulations using the following formulas for real statistics, which are a conventional statistical treatment on tally $Q_k$:

$$Q_k = \frac{1}{N_{ac}} \sum_{i=1}^{N_{ac}} Q_{i,k} \tag{13}$$

$$\overline{Q} = \frac{1}{N_r} \sum_{k=1}^{N_r} Q_k$$

$$\sigma_R^2[\overline{Q}] = \frac{1}{N_r(N_r-1)}\sum_{k=1}^{N_r}(\overline{Q}-Q_k)^2 = \frac{1}{N_r}\sigma_R^2[Q_k] \quad (14)$$

$$\sigma_A^2[\overline{Q}] \equiv \frac{1}{N_r}\sigma_A^2[Q_k] \quad (15)$$

where $N_{ac}$ is the number of active cycles, and $k$ and $N_r$ stand for the index and the total number of independent MC runs, respectively. The real standard deviation $\sigma_R[\overline{Q}]$ in Eq. (14) refers to the uncertainty of the mean value $\overline{Q}$. And the apparent standard deviation $\sigma_A[\overline{Q}]$ is defined as Eq. (15) for the fair comparisons of real and apparent standard deviations.

The MC results are obtained from 25 independent MC runs with 100,000 histories per cycle. Conservatively, 300 cycles are skipped as inactive cycles, and 1000 active cycles are performed. Each assembly is taken as a coarse mesh for CMFD formulation, and the CMFD linear system has the two-group energy structure as well.

As shown in Fig. 5, both pin power distributions are almost the same and well overlapped within their real standard deviations. However, the real standard deviation, which reflects the uncertainties of estimated pin powers, appears to be different. The first observation is that the real standard deviation is much larger than the apparent standard deviation in the conventional MC cases. For some fuel pins in the periphery regions, the real standard deviations are 3 or more times larger than those for the accelerated ones and the overall improvement in the real standard deviation is about a factor of 2. Another observation regarding this plot is that the distribution of real standard deviations in conventional MC reveals an asymmetric shape and its magnitude is much more amplified for periphery fuel pins than for center-core fuel pins. Therefore, the pin powers of periphery fuel pins from a single MC run can potentially have much larger uncertainties than would appear to be the case, and this will cause an asymmetric global pin power distribution.

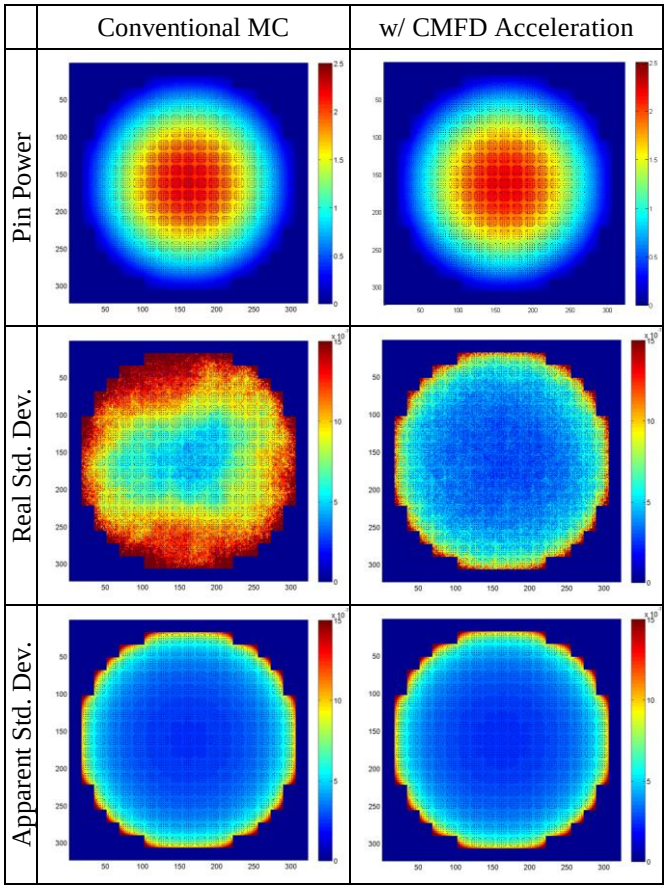


**Fig. 5** Estimated pin power and its error for Test Problem 1

On the other hand, the real standard deviation from the accelerated MC has a fairly symmetric distribution and is very close to that for the apparent standard deviation. This demonstrates that the MC solution can be improved even in a single MC-CMFD simulation.

## 2. Test Problem 2: Out–In Fuel Loading Core with 47-Group Cross Sections

Test Problem 2 is a variation of Test Problem 1 made to achieve a more realistic, flatter power distribution with 47-group cross sections. Three different types of fuel assemblies are loaded in the core as shown in Fig. 6: two types of low-enrichment fuel assemblies are loaded in the interior in a checkerboard pattern, and the highest enriched fuel assemblies are placed at the periphery to simulate an out–in fuel-loading pattern. The self-shielded 47-group microscopic cross sections were generated by the DeCART code. All other calculation conditions are the same as in Test Problem 1.

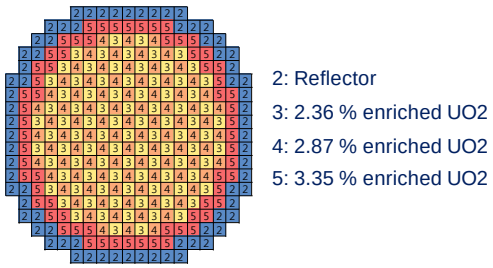


**Fig. 6** Core specification of Test Problem 2

The real and apparent standard deviation for the MC results, which consist of estimated pin power distributions, are plotted in Fig. 7 for conventional MC and the CMFD accelerated MC. At a glance, the apparent standard deviation and the pin power have very similar distributions for the two cases. Therefore, if the pin power distribution is obtained from a single MC simulation, the two solutions can be considered as the same solution with almost the same accuracy. In the aspect of real standard deviation, however, the solution with CMFD acceleration has actually much less uncertainty than the conventional MC. Also the real standard deviation of the MC-CMFD is much more similar to the apparent standard deviation than that of the conventional

MC is. It should be noted that the real standard deviation is slightly larger than the apparent standard deviation even if the CMFD acceleration is applied. This implies that the inter-cycle correlation is not perfectly eliminated. Therefore, to obtain a reliable MC solution consisting of real means and real standard deviations, a statistical treatment on the samples generated from multiple MC runs is still required.

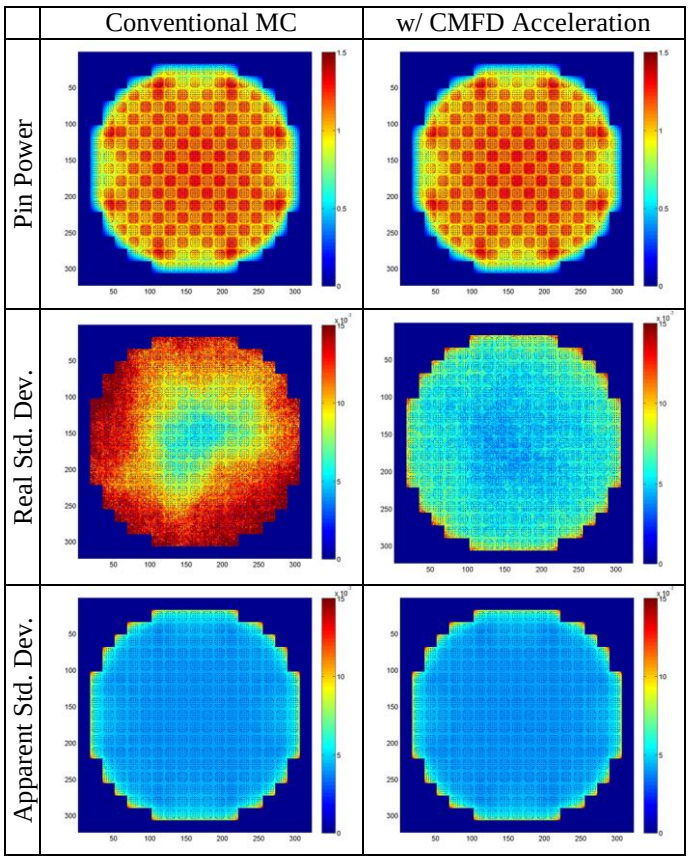


**Fig. 7** Estimated pin power and its error for Test Problem 2

It would be worthwhile to assess the magnitude of bias in standard deviation. The ratio of real standard deviation to apparent standard deviation for each fuel pin can be defined as

$$\left(r_{R/A}\right)_i = \left(\frac{\sigma_R}{\sigma_A}\right)_i \tag{16}$$

where $i$ is the fuel pin index. This ratio is plotted in Fig. 8. For the conventional MC case, the ratio varies from 1.5 to 3.5 and is larger for periphery fuel pins. However, the fuel pins at the boundary have smaller ratios than the other fuel pins. On the other hand, the ratio is almost flat over the whole core with CMFD acceleration.

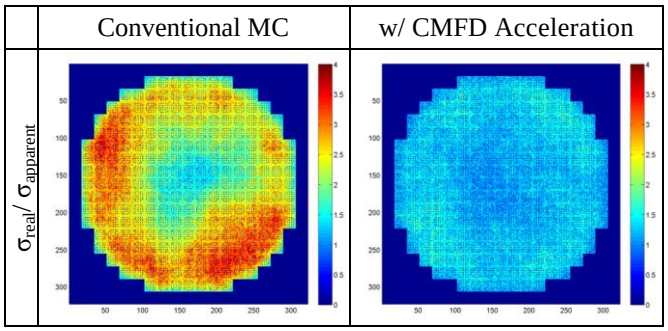


**Fig. 8** $\sigma_{real}/\sigma_{apparent}$ of pin power distribution for Test Problem 2

The maximum ratio—as well as the pin power weighted average ratio, which is defined by the following equation—is given in Table 1. In this table, the improvement of CMFD is about a factor of 2 for both average and maximum ratios.

$$\bar{r}_{R/A} = \frac{\sum_{i=1}^{N_{FP}} \left(\frac{\sigma_R}{\sigma_A}\right)_i \cdot \psi_i}{\sum_{i=1}^{N_{FP}} \psi_i} \tag{17}$$

**Table 1** The ratio of real to apparent standard deviations

| | Conventional MC | w/ CMFD Acceleration |
|---|---|---|
| $\bar{r}_{R/A}$ | 2.42 | 1.31 |
| $\max(r_{R/A})_i$ | 4.13 | 2.27 |

However, the benefit of CMFD acceleration should be considered greater than simply this factor of 2, because it yields the flat distribution of real standard deviation.

When the assembly power is considered, more obvious improvement can be observed as shown in Figs. 9 and 10.

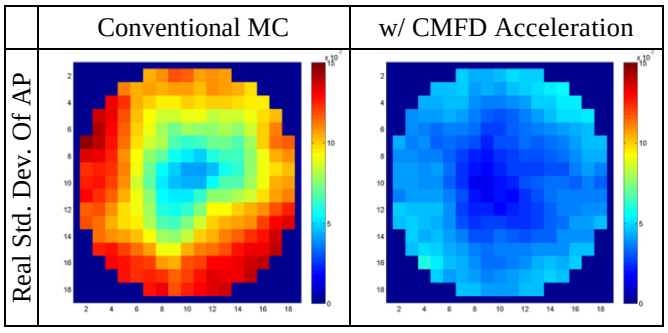


**Fig. 9** Real standard deviation of assembly power distribution for Test Problem 2

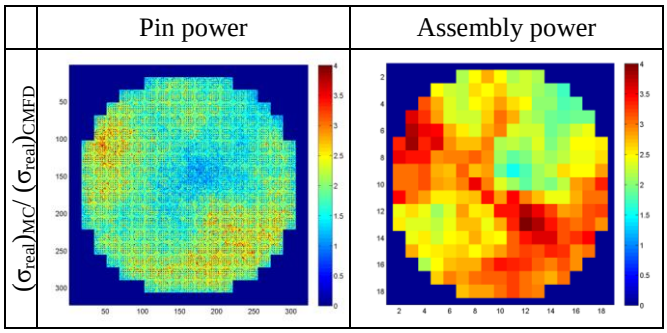


**Fig. 10** $(\sigma_{real})_{MC}/(\sigma_{real})_{CMFD}$ of pin power and assembly power for Test Problem 2

The improvement in MC solution by CMFD acceleration can be observed in a single MC simulation as well. For the examination of the improvement, a very accurate converged pin power distribution was obtained from 100 independent MC runs. This solution is set as the reference, and the accumulated pin power distribution of each MC cycle is compared with the reference. In Fig. 11, which shows the RMS error defined as

$$\varepsilon_{\psi} = \frac{\sqrt{\frac{1}{N_{FP}}\sum_{i=1}^{N}\left(\psi_i^{REF} - \psi_i^{MC}\right)^2}}{\frac{1}{N_{FP}}\sum_{i=1}^{N}\psi_i^{REF}} \tag{18}$$

The pin power error of the conventional MC fluctuates greatly, and it sometimes increases even though the value represents an accumulated one. Compared with the ideal error, which follows $1/\sqrt{n}$ and has the slope of 1/2 in a log–log scale, the observed error is much larger, and using more cycles does not guarantee a smaller error. In fact, the solution depends on when the MC simulation is stopped. On the other hand, this situation is well mitigated with the aid of CMFD acceleration. However, the pin power error reduction behavior still shows slightly larger errors than the ideal ones.

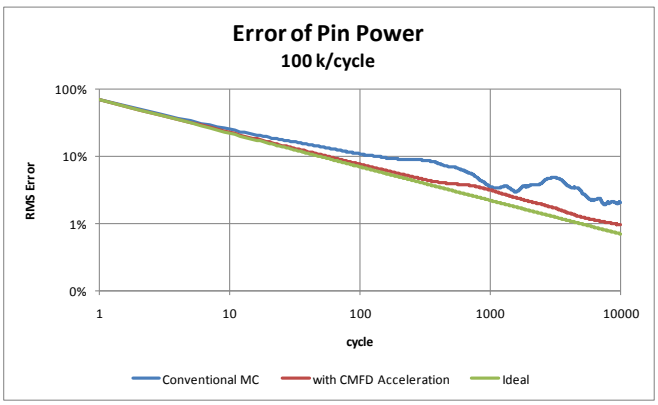


**Fig. 11** Error behavior in a single MC simulation of Test Problem 2

The ratios of observed errors to ideal errors show how much the solution is biased compared with the ideal MC simulation over 10,000 cycles. As shown in Fig. 12, the MC error is 2 to 3 times larger than the ideal error for the conventional MC while it is about 1.3 times larger with CMFD acceleration. This has a good agreement with the stated results in Table 1.

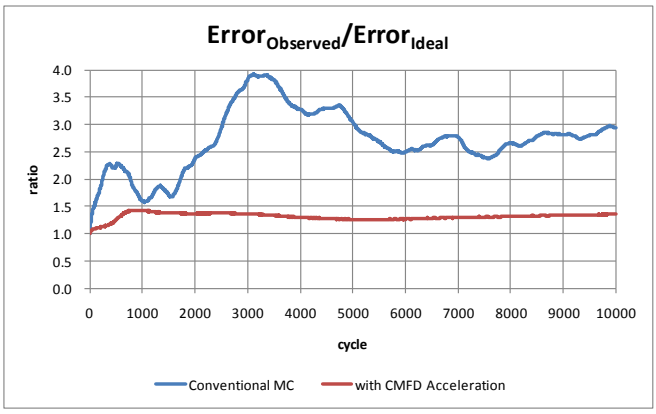


**Fig. 12** The ratio of observed error to ideal error for Test Problem 2

By comparing the error in assembly powers with the error in pin powers, it can be noted that they are highly correlated regardless of CMFD acceleration as shown in Figs. 13 and 14. However, the error in pin-to-box factors converges very well following the ideal error behavior. This means that the inter-cycle correlation introduces additional errors in the global power distribution and consequently the underestimation in real variance results from this error in the global power. Ironically, the higher uncertainty of local properties results from the higher uncertainty of global distribution. It should be noted that the CMFD acceleration, along with the weight adjustment scheme, adjusts the global fission source distribution to improve the MC solution and let the local distribution go as the conventional MC. Therefore, it can be said that the CMFD acceleration is an efficient approach for solving the fundamental problem of inefficient global propagation of information in the conventional MC eigenvalue calculation.

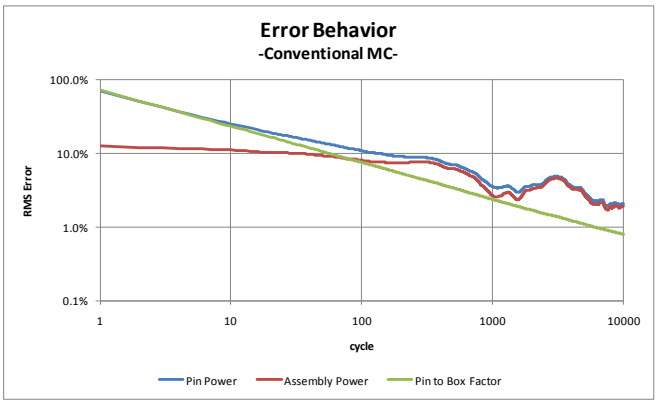


**Fig. 13** Error behavior from single MC simulation for Test Problem 2

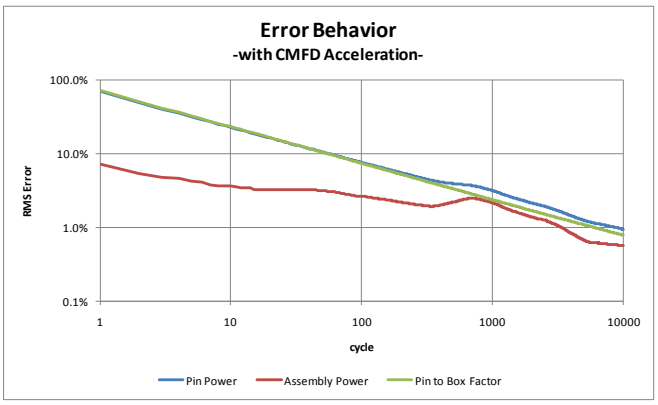


**Fig. 14** Error behavior from single MC simulation with CMFD acceleration for Test Problem 2

## IV. Conclusions

In this work we performed 25 independent MC simulations for the two 2-D full-core multigroup test problems and found that the real standard deviation appears 3 times greater than the apparent standard deviation in the pin power distribution in the case of conventional MC simulation. The error in pin powers is caused by increased uncertainties of the global power distribution, not the local one.

With the application of CMFD acceleration, the real standard deviation is reduced by about a factor of 2, which is a factor of 4 in terms of neutron population. The improvement is more outstanding for the assembly powers, since the CMFD-accelerated case still involves fluctuations for peripheral fuel pins.

From this study, it can be concluded that the CMFD acceleration is effective in reducing real standard deviation of local properties in a high dominance ratio problem. Though the inter-cycle correlation is not perfectly eliminated by CMFD acceleration, the solution from single MC simulations can be also improved by CMFD acceleration.

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