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ARTICLE

Evaluation of the Statistical Error in the Results of Calculations of Full-Scale Three-Dimensional Model of VVER-1000 by Means of the Monte Carlo Method

Mikhail A. KALUGIN, Dmitry S. OLEYNIK*, Denis A. SHKAROVSKY and Eugenia A. SUKHINO-KHOMENKO

Russian Research Centre "Kurchatov Institute", Kurchatov Sq. 1, Moscow, 123182, Russia

When simulating neutron transport in systems with size many times bigger than the neutron migration area there are some difficulties associated with the choice of the parameters of the Monte Carlo method, such as the initial distribution, the number of neutrons in a generation, the number of the first active series. In addition, there is a problem with the calculation of the statistical error of the results.

This paper proposes algorithms for calculation of statistical error, taking into account the correlations between the generations, built on the basis of statistical analysis of the results of calculations by Monte Carlo. In addition, simple rules are formulated for choosing the parameters of a Monte Carlo calculation scheme that have been tested on several problems, including the full three-dimensional model of the VVER-1000 core. The results of these VVER-1000 calculations are used in this paper.

It is shown that the formula for the variance in the light of correlations gives results similar to those obtained on multiprocessor computers, where each processor estimates the average value of the functional independently.

The performance of the algorithm of selection of the first active series in the case when the initial distribution of the source is obviously far from reality is demonstrated.

To justify the selection of the number of neutrons in a generation some preliminary results of calculations of Maiorov's correction (theoretical value of bias in functional evaluation) are presented.

KEYWORDS: Monte Carlo, statistical error, stochastic process, random variable, Maiorov's correction, effective multiplication factor, reaction rates, full-scale three-dimensional model VVER-1000

I. Introduction

When simulating neutron transport in systems with size many times bigger than the neutron migration area there are some difficulties associated with the choice of the parameters of the Monte Carlo method, such as the initial distribution, the number of neutrons in a generation, the number of the first active series. In addition, there is a problem with the calculation of the statistical error of the results. This was the subject of many studies and a number of important theoretical results were obtained.[1-6] Maiorov derived the formula to evaluate the systematic error of the results of any Monte Carlo calculation of functionals of the neutron flux. [1] Besides, he also studied another important issue of taking into account the influence of the correlation contribution to the functional in the neighboring generations on the accuracy of estimates of statistical error in the solution of the homogeneous neutron transport equation by Monte Carlo.

This paper proposes algorithms for calculation of statistical error, taking into account the correlations between the generations, built on the basis of statistical analysis of the results of calculations by Monte Carlo. In addition, simple rules are formulated for choosing the parameters of a Monte Carlo calculation scheme that have been tested on several problems, including the full three-dimensional model of the VVER-1000 core. The results of these VVER-1000 calculations are used in this paper. Also the paper contains numerical results for the comparison of theoretical and experimental k_{eff} biases.

Algorithms for statistical analysis of simulation results are implemented in the MCU code by means of which the test calculations were carried out.[7]

II. The General Scheme of the Monte-Carlo Method

In solving problems of criticality by means of the Monte Carlo method one usually use generations with a fixed total weight of the neutron sources in one generation. In this scheme the phase coordinates of neutrons of the initial (zero) generation can be chosen arbitrarily. To calculate the non-linear functionals F such as the effective multiplication factor (k_{eff}) and the reaction rate in the registration areas a random variate ξ is used. Its sample values are elementary estimates x_n, calculated for the so-called series, each of which includes a user-defined number of generations – N_{BAT} (with $N_{BAT} = 1$ notions of series and generation coincide) and each generation includes N_{TOT} neutron histories. Thus if N_{GEN} is total number of generations, N is number of series and N_{HIST} is total number of neutron histories in calculation then

$$N = N_{GEN}/N_{BAT}, \quad N_{HIST}=N_{TOT}\, N_{BAT}\, N.$$

*Corresponding author, E-mail: oleynik@adis.vver.kiae.ru

Estimations are done in such a way that their mathematical expectations $M\xi$ would be equal to F:

$$M\xi = \bar{x} = F\,. \tag{1}$$

The functionals are calculated as the arithmetic average values of elementary estimates:

$$X = \bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_n\,, \tag{2}$$

where N is the number of simulated series. The solution is ensured by fulfilling the condition $M\bar{x} = F$.

Hereafter we use the notation x_n for both the sample values of the random variable ξ and the random variable itself. Similarly, the designation $\bar{x}$ is used for both the sample mean values and for the random variable.

Evaluation of the variance of the random variable x_n (sample variance) is calculated by the formula

$$D(x_n) = \frac{1}{N-1}\sum_{n=1}^{N}\left[(x_n - \bar{x})^2\right]\,. \tag{3}$$

Standard deviation in this case is $s = \sqrt{D(x_n)}$.

For estimation of the variance of the random variable $\bar{x}$ on the assumption of the independence of random variables x_n and constancy of their distribution functions for all n the usual formula is used:

$$D(\bar{x}) = D\left(\frac{1}{N}\sum_{n=1}^{N} x_n\right) = \frac{1}{N^2}\left(\sum_{n=1}^{N} D(x_n)\right) = \frac{D(x_n)}{N}\,. \tag{4}$$

By the central limit theorem confidence interval for the evaluation of the functional $\bar{x}$ with 95% reliability (with a significance level of 0.05) is defined as

$$P\left\{|\bar{x} - m| < \frac{2s}{\sqrt{N}}\right\} \approx 0.95\,,$$

where m is the mathematical expectation, s is the dispersion.

Thus, the error of calculation by Monte Carlo or, equivalently, the confidence interval for the mean X is determined by the variance $D(\bar{x})$ which is usually calculated using Eq. (4) on the assumption of independence of x_n.

III. General Formula for Variance Considering Correlations between Serial Estimates

Let's apply the formula for the variance $D(\xi) = M\xi^2 - (M\xi)^2$ to the sum of x_n

$$D\left(\sum_{n=1}^{N} x_n\right) = \left(M\left(\sum_{n=1}^{N} x_n\right)^2 - \left(M\sum_{n=1}^{N} x_n\right)^2\right). \tag{5}$$

After simple transformations we get

$$D\left(\sum_{n=1}^{N} x_n\right) = \sum_{n=1}^{N}\left(Mx_n^2 - (Mx_n)^2\right) + 2\sum_{1\le l<m\le N}\left(Mx_l x_m - Mx_l Mx_m\right)\,. \tag{6}$$

The first term of Eq. (6) is the sum of the variances of x_n, the second – the sum of the covariance coefficients $K_{l,m}$ of two random variables x_l and x_m.

Applying Eq. (6) to Eq. (4) we obtain a general formula for the variance of the mean

$$D(\bar{x}) = \frac{1}{N^2}\left(\sum_{n=1}^{N} D(x_n) + 2\sum_{1\le l<m\le N} K_{l,m}\right). \tag{7}$$

In practical calculations of the variance using Eq. (7) there is a problem of determining of $D(x_n)$ for all n=1,N and covariance coefficients $K_{l,m}$.

First problem can be solved using the assumption about the constancy of the distribution function of random variables x_n. In this case $\sum_{n=1}^{N} Dx_n = NDx_n$. However, rigorous justification of this provision requires additional research. As for the covariance coefficient $K_{l,m}$, calculation of its value for all l, m is associated with certain computational difficulties. Practically, the implementation of these two items, though possible, but extremely difficult, so we need to convert Eq. (7) so as to obtain a simple formula for calculation of the variance of the mean.

IV. Elements of the Stochastic Processes Theory

For each tallied functional there is a sequence $\{x_1, x_2, \ldots, x_n, \ldots, x_N\}$ which is, generally speaking, a stochastic process, because each element of the sequence x_n is a random variable.

Recall that a stochastic process $X(t)$, defined on the set of T, is a function of t, whose values at each $t \in T$ represent a random variable.[8,9] There are stochastic processes with continuous time (T - interval on the real axis) and discrete-time. In our case T is a natural row: $T = \{1, 2, \ldots, n, \ldots, N\}$, where n is the index of series.

An important role in the theory is played by stationary stochastic processes whose probability characteristics do not change depending on t.[8] Consequently, the average value $m(t)$ is constant and the covariance function $B(t,s)$ depends only on the distance between the arguments, i.e. $|t - s|$. From the last assertion it implies that the value of variance $D(X(t))$ is also constant.

One of the main characteristics of stationary stochastic processes is the autocorrelation function $r(k)$ or r_k

$$r(k) = \mathrm{corr}(X(t), X(t+k)),$$

where $k > 0$ is integer. Value of k is called a delay or lag, for which the correlation coefficient is calculated.

To estimate the average value of a stochastic process using a single realization the following estimation is used:

$$\bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_n\,.$$

In the theory of stochastic processes it is proved that this average may serve as an estimate of the mathematical expectation of $X(t)$, if a stochastic process is stationary and the autocorrelation function $r_k \to 0$ at $k \to \infty$.[8]

If a stochastic process is stationary then the estimation $M\bar{x} = F$ is unbiased. The second condition provides the

consistency of the estimate $D(\bar{x}) \to 0$ at $N \to \infty$. Namely, at increase in the number of simulated generations the estimate of $\bar{x}$ verges towards the true value of the functional.

Thus, the analysis of the function $\bar{x}$ and the autocorrelation function in dependence of N is required for statistical processing of Monte Carlo calculation results. Such an analysis has been performed for the model considered in this paper (see Section VI for the model description).[10] This analysis shows that the process for the reaction rates and k_{eff} at uniform initial approximation is stationary and the autocorrelation function $r_k \to 0$ at $k \to \infty$.

V. Calculation Formula for Variance Considering Correlations between Serial Estimates

Let's transform Eq. (7) taking into account the stationarity of the process. By calculating the autocorrelation function by the formula

$$r_k = \frac{\sum_{n=n_0-k}^{N-k}(x_n - \bar{x})(x_{n+k} - \bar{x})}{\sum_{n_0}^{N}(x_n - \bar{x})^2} = \frac{\sum_{n=n_0-k}^{N-k}(x_n - \bar{x})(x_{n+k} - \bar{x})}{D(x_n)}, \quad (8)$$

where $n_0 - k = N_{SER0}$ ($k > n_0$) is the number of the first active series, one can also calculate the variance

$$D(\bar{x}) = \frac{D(x_n)}{N} + \frac{2}{N^2}\sum_{m=1}^{N-1}\sum_{k=1}^{N-m}\mathrm{cov}(x_n, x_{n+k}) = \frac{D(x_n)}{N}\left(1 + \frac{2}{N}\sum_{m=1}^{N-1}\sum_{k=1}^{N-m} r_k\right). \quad (9)$$

Equation (9) is well-known and was published, for example, by Sveshnikov[11] or by Gast and Candalore[12].

Member $\frac{2}{N}\sum_{m=1}^{N-1}\sum_{k=1}^{N-m} r_k$ in Eq. (9) is the sum of the elements of the correlation matrix with the exception of elements on the main diagonal

$$\mathbf{r} = \begin{bmatrix} 1 & r_1 & r_2 & r_3 & \dots & r_{N-1} \\ & 1 & r_1 & r_2 & r_3 & \dots & r_{N-2} \\ & & 1 & r_1 & r_2 & r_3 & \dots & r_{N-3} \\ & & & \cdots\cdots\cdots & & & \\ & & & & & 1 & r_1 \\ & & & & & & 1 \end{bmatrix}, \quad (10)$$

so, $D(\bar{x})$ is calculated as (see, for example,[9])

$$D(\bar{x}) = \frac{D(x_n)}{N}\left(1 + 2r_1\frac{N-1}{N} + \dots + 2r_L\frac{N-L}{N}\right), \quad (11)$$

where L is the number of elements of the autocorrelation function, significantly different from zero.

In the MCU code it is assumed that r_k is significantly different from zero if $|r_k| > \sqrt{\frac{1}{N}(1 + 2\sum_{l=1}^{k-1} r_l^2)}$.[9] At large values of N, i.e. $N > 1{,}000$, Eq. (9) may be simplified

$$D(\bar{x}) = \frac{D(x_n)}{N}\left(1 + 2r_1 + 2r_2 + \dots + 2r_L\right). \quad (12)$$

This formula is used in MCU to calculate the variance. Recall that $D(x_n)$ is calculated by Eq. (3).

With the use of multiprocessor computing the variance can be calculated by the equation identical to Eq. (4)

$$D(\bar{x}) = \frac{1}{P}D(x_p) = \frac{1}{P}\left(\frac{1}{P}\sum_{p=1}^{P} x_p^2 - (\bar{x})^2\right), \quad (13)$$

where $\bar{x} = \frac{1}{P}\sum_{p=1}^{P} x_p$, P – number of processors, x_p – estimation of the functional obtained on p-th processor over N series. Estimations x_p are independent, which is guaranteed by the implementation of multi-processor calculations in MCU and the choice of a pseudorandom number generator.[13,14] The normalization process is conducted within each processor.

VI. Brief Description of VVER-1000 Core Model

The results of calculations by means of the Monte Carlo method of a few states of a full three-dimensional model of the Volgodonsk nuclear power plant VVER-1000 power unit No. 1 are analyzed.[15] The modeled unit is at the minimum controlled power level achieved during the physical startup. Specifications of the model (the geometric dimensions of the fragments of the reactor, material composition, etc.) are based on design data and startup experiments data.

The core consists of 163 hexagonal fuel assemblies (FA) of different types with different material composition of fresh fuel (enrichment of the isotope ^{235}U – 1.6, 2.4, 3.3 and 3.7% by weight) and is surrounded by a reflector on all sides. The model takes into account the position of control rods, complex structure of the reflector under core, the actual configuration of the baffle, etc.

The results of calculations considered are k_{eff} and the spatial distribution of energy by height of the core. This paper presents the results of calculations of the model with the core divided into 14 layers by height, and thus the energy release was calculated in 2,282 nodes.

The calculations were performed using the MCU code. The distinctive feature of the code is the possibility of calculating the statistical characteristics at the stage of processing the results obtained during the simulation. For this evaluation functionals of all generations are recorded during the simulation in a separate file and processed after the end of the calculation.

VII. Calculated Results

Obviously, to calculate accurate estimates of the variance it is sufficient to nullify the effect of correlations between the generations. Earlier, the MCU code used a standard method; N_{BAT} successive generations are united into series.[16] In this case it was assumed that for sufficiently big values of N_{BAT}, the variance can be calculated by Eq. (4) without taking into account the correlations between the series. However, as computational studies show (see **Fig. 1**), the

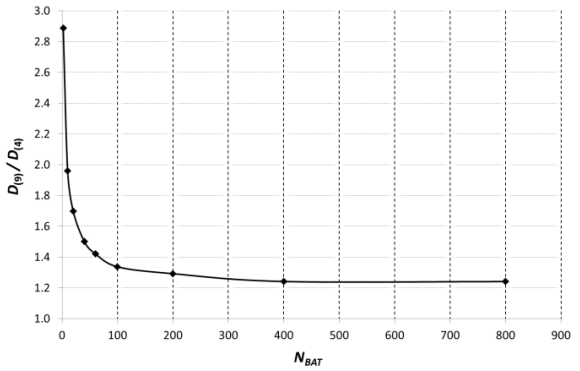

Fig. 1 The ratio of the variance $D_{(9)}$, calculated by Eq. (9) to the variance $D_{(4)}$, calculated by Eq. (4) for different values of N_{BAT} in the node with maximum power of the VVER-1000 core

correlation corrections can be reduced, but it is impossible to make it equal to zero.

To test the algorithm for variance evaluation by Eq. (9) calculations have been performed using the model described in Section VI. **Figure 2** shows the comparison of calculated variances for some states of the model (the number of neutrons in the generation N_{TOT} = 2,000, the total number of simulated histories = 4.8×10^9, uniform initial distribution) with those obtained using independent calculations on 24 processors according to Eq. (13) (each processor modeled 2×10^8 histories).

Despite the fact that the statistical error in calculating the variance by Eq. (13) was ~30%, the results show good agreement as demonstrated in Fig. 2 by the fact that the difference in the results behave in a stochastic manner with the average sample value close to zero (when analyzing all 2,282 nodes).

Obviously, the stationary stochastic process in the first series may influence the initial distribution of neutrons, which is far from correct, and correctly chosen parameter N_{SER0} can guarantee stationarity of the process starting with the first series. To solve this problem MCU uses two approaches.

The first one is described, for example, by Oleynik.[17] It is proposed to choose the initial distribution of neutrons as the result of the approximate solutions of matrix equation. Studies have shown that for all considered states the uniform distribution is good enough to make results of calculations with N_{SER0} = 1 and 2,000 coincide with the "exact" solution (for sufficiently large $N = 10^5$) even for the state with stuck control rods in one of the FA's in which variation factor is of the order of 20.[10]

Thus, together with the initial distribution of neutrons obtained from the solution of the approximate matrix equation with coextensive fractioning of the core into 163 (FA = object) and 2,282 objects (FA layer = object) the behavior of a stochastic process with an unreal initial approach have been analyzed. Namely, it is the case when a point source is located far enough from the most power stressed region of the core for the mentioned above state with stuck control rods.

Figure 3 demonstrates the behavior of estimates of k_{eff} in dependence on the number of simulated generations (N_{TOT} =

Standard deviation S_1 with regard to correlations (unit: 0.01%)																			
											34								
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Standard deviation S_2 obtained from the calculation on 24 processors (unit: 0.01%)																			
											38								
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$(S_1-S_2)/S_2\times100(\%)$																			
											-11								
									3				-12						
							3				-16								
					0				0				-5						
			-6				4				0								
		14			0				8				10						
-12			0				25				7								
		-6			13				4				-3						
			-24				14				19								
					-5				15				9						
							24				21								
									23				-3						
											38								

Fig. 2 Comparison of statistical errors obtained by Eqs. (9) and (13) for power production in the central layer of the core of VVER-1000 at 60 degrees turn symmetry, %.

3,000, N_{BAT} = 400) for different initial distributions of neutrons. When it was taken from the approximate solutions of the distribution matrix, the mathematical expectation of the stochastic process behaves as a constant starting from the first series in contrast to the point source.

The second approach is based on the fact that the first serial estimation taken into account should be in close proximity to the final result that is obtained by simulating a sufficient number of series such that the value Dx_n is not so big. Then it can be assumed that the distribution of neutrons in the recorded field is close enough to the real one. Thus, the algorithm checks if the estimation of the functional for this series is within two standard deviations of the random variable x_n from the mathematical expectation. If the estimate does not belong to this interval, the estimate of the functional for this series is discarded. To prevent accidental hitting the specified interval the algorithm requires that the

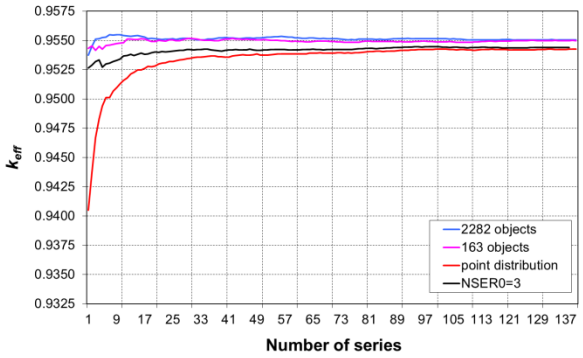

Fig. 3 Dependence of k_{eff} on the number of the simulated series.

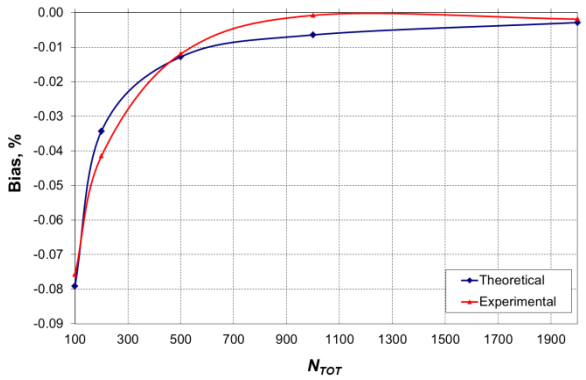

Fig. 4 Comparison of theoretical and experimental estimates of bias in k_{eff} for VVER-1000 core.

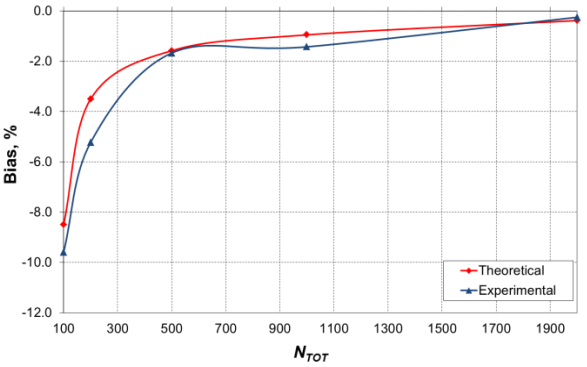

Fig. 5 Comparison of theoretical and experimental estimates of bias in the node with maximal energy in the central height layer of VVER-1000 core.

condition had been met three times in a row. For the task in consideration the algorithm gives N_{SER0} = 3 (the first two serial estimates were not included, and the subsequent fall into the interval).

Figure 3 shows that at this approach the mathematical expectation of the stochastic process is almost constant.

It should be noted that the calculation results presented in Fig. 3 are preliminary, and in the future we plan to explore the influence of the initial distribution of neutrons on stationarity of the stochastic process in more detail.

It is well known that in Monte-Carlo calculations with normalization process (number of fission neutrons is reducible to fixed number N_{TOT}) estimates of functionals calculated by Eq. (2) are biased and the bias decreases with the increase of the number of neutrons in generation.[3,18] In the MCU code normalization process is used after simulation of each generation by scheme which was developed by Frank-Kamenetsky[16]. A lot of works are dedicated to the theoretical solution of the problem. A significant result was obtained by Maiorov.[1] He strictly deduced the asymptotic formula for the systematic error of the 1-st kind Δ_M of arbitrary estimation of any functional (Maiorov's correction Δ_M): k_{eff}, reaction rates in tallies and etc. Maiorov's correction is calculated by the formula:[1]

$$\begin{aligned}\Delta_M &= \bar{x} - F \\ &= -\frac{1}{k_{eff}} \sum_{l=1}^{N-1} \frac{1}{N} \sum_{n=1, n>l}^{N} (x_n - < x_n >)(k_{n-l} - < k_n >),\end{aligned} \tag{14}$$

where F – the desired value of the functional, N - the number of simulated generations, $<k_n>$ - the total weight of the neutron generation number n.

This formula is implemented in MCU and allows us to estimate the systematic error of the first kind of results calculated with a given value of N_{TOT}. It provides the reliability of the estimates. The use of this approach gave us some preliminary results.

Figures 4 and **5** show the theoretical and experimental bias depending on different values of N_{TOT} for k_{eff} and power production in the most stressed node of the core in one of the critical states of three-dimensional full-scale model of the VVER-1000. The values of the experimental bias are obtained at comparison with the "exact" results of calculations for a large value of N_{TOT} = 10^4 neutrons. Theoretical (Maiorov's correction) and experimental estimations of bias are practically the same, which confirms the practical value of Eq. (14). In the future we plan to address the problem of bias using other problems including pin-by-pin calculations of VVER cores.

VIII. Conclusion

In this paper we have described algorithms for calculation of statistical error, taking into account the correlations between the generations and built on the basis of statistical analysis of the results of calculations by means of the Monte Carlo method. It is shown that the formula for the variance in the light of correlations gives results similar to those obtained on multiprocessor computers, where each processor estimates the average value of the functional independently. The adjusted estimate of statistical errors allows more reliable selection of the required number of simulated generations to achieve the required accuracy.

We have presented some preliminary results of calculations of the full three dimensional model of a VVER-1000 reactor core and demonstrated performance of the algorithm of selection of the first active series in the case when the initial distribution of the source is obviously far from reality. The results for N_{SER0} = 3 are compared with results for N_{SER0} = 1 obtained using near-real initial distribution which was taken from the solutions of matrix equations. Good agreement is observed.

To justify the selection of the number of neutrons in a generation N_{TOT} preliminary results of calculations of Maiorov's correction (theoretical value of bias in functional evaluation) are presented. It is shown that the value of Maiorov's correction is in good agreement with the experimentally obtained results of the bias.

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