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Estimation of the Effective Multiplication Factor by Monte-Carlo Method Using the Importance Function

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Abstract – *The work describes the MCU code based realization of a method that allows leveling of effective multiplication factor bias in criticality calculations without any changes in simulation and receiving reliable evaluations of its statistical uncertainty. The method is based on the calculation of a discrete adjoint function of a matrix transport equation and its use for the evaluation. The effectivity of the method is demonstrated in calculation of the «Whiteside problem» weakly coupled system.*

I. INTRODUCTION

There are three problems in Monte-Carlo calculations of k_{eff} of large systems in which geometric dimensions are much bigger than a neutron path length. They are related to the usage of the generation method with a fixed number of neutrons N_{TOT} in a generation. The problems are:

1. the choice of initial neutron distribution or the choice of number of the first skipped generations N_{SKIP};
2. the estimation of bias Δ_K – systematic miscalculation of k_{eff};
3. the estimation of a statistical error σ_{corr} taking into account correlations between generations (σ_0 denotes the estimation of the standard deviation excluding the correlations).

These problems can be solved with the usage of the autocorrelation function of the contribution of generations to k_{eff} estimation [1–4].

Let's denote C_k as the covariance function of contribution of the current and the current plus k-th generations to k_{eff} when steady-state condition is reached. For a stationary random process $\{k_1, k_2, ..., k_n, ..., k_N\}$, where k_n is the evaluation of k_{eff} at generation number n, the C_k evaluation may be defined using finite sample of N elements

$$< C_k >= \frac{1}{N-k} \sum_{n=1}^{N-k} (k_n - < k_n >)(k_{n+k} - < k_n >),$$

where <·> denote the evaluation.

Correlation function $c_k = C_k/C_0$ normalized to dispersion is called the autocorrelation function of a random process. Let's denote L as their lag. Then

$$\sigma_{corr} = \sigma_0 \sqrt{1 + 2S_L}, \text{ where } S_L = \sum_{k=1}^{L} c_k.$$

Usually when calculating by MCU code [7] the following shall be satisfied

1. $N_{SKIP} \geq L$;
2. N_{TOT} is such a large number that [1]

$$\Delta_K \approx \frac{1}{< k_{eff} >} \sum_{k=1}^{L} C_k \qquad (1)$$

is inessential (as it is shown in [2], $\Delta_K - \frac{2}{< k_{eff} >} \sum_{k=1}^{L} C_k = \mathrm{O}(N_{TOT})^{-3/2}$));

3. statistical error is calculated for the so-called series, each of which includes a user-defined number of generations N_{BAT}. N_{BAT} is such a large number that S_L is minimal.

It's important to note [1–6] that $\Delta_K \sim 1/N_{TOT}$ and $D(k_n) \sim 1/N_{TOT}, S_L = < k_{eff} > \Delta_K / D(k_n) = const$; that's why the bias doesn't depend on N and P (number of processors), and depends on N_{TOT} value.

It is known that the use of importance function (adjoint function) essentially minimizes the correlation between generations and get the k_{eff} estimation with $\Delta_K = 0$ and $\sigma_K = \sigma_0$.

Work [2] suggests a method to decrease the bias of k_{eff} evaluation and correlation between the k_n evaluations using spatial transformation of transport equation. This work suggests a different approach without an integral operator modification. Instead, it is associated with the adjustment of contributions into the evaluation at the stage of tallying using the adjoint function.

The approach is realized in the MCU code [7] and numerical results of k_{eff} evaluation for the «Whiteside problem» weakly coupled system [8] are obtained using normalization on the importance function at which $\Delta_K \cong 0$ and $\sigma_K \cong \sigma_0$.

II. DESCRIPTION OF METHOD

The description of the method of unbiased k_{eff} evaluation using the importance function is the development of the work [1]. In this study, more attention is paid to a precise description of the changes in the algorithms used in the transport equation modeling.

1. Basic concepts

Let's assume that the state S of Monte Carlo simulation of a neutron transport in a criticality task is the set of M neutrons each of which is characterized by its weight w_i and a point in phase space p_i (i = 1,2,…,M). Here M is the maximum number of particles in the state ($M \geq N_{TOT}$). Thus the state may be represented as a matrix $S = [\boldsymbol{w}, \boldsymbol{p}]$, where $\boldsymbol{w}$ is a non-negative vector-column of M components and $\boldsymbol{p}$ is a column with points of the phase space.

The generation rate refers to a non-negative density in the phase space.

Three deterministic representations are correct for the states:

- total weight $W(S)=w_1+\ldots+w_M$;
- multiplication by a positive scalar $\lambda[\boldsymbol{w},\boldsymbol{p}] = [\lambda\boldsymbol{w},\boldsymbol{p}]$;
- reduction to density $(\nu(S))(p) = w_1\delta(p-p_1)+ +\ldots+w_M\delta(p-p_M)$, where p is an arbitrary point in phase space and δ is Dirac delta distribution.

It is obvious that $\nu(\lambda S)=\lambda\nu(S)$ and $\lambda W(S)=W(\lambda S)$.

Let's define two narrow sets at the variety of states.

1. Generation $F=[\boldsymbol{w},\boldsymbol{p}]$ is such a state that $w_1=\ldots=w_{NTOT}>0$, and $w_{NTOT+1}=\ldots= w_M=0$.

2. Normal generation $G=[\boldsymbol{w},\boldsymbol{p}]$ is such a state that $w_1=\ldots=w_{NTOT}=1$,and $w_{NTOT+1}=\ldots= w_M=0$.

It is obvious that $W(G)=N_{TOT}$, $G=(N_{TOT}/W(F))F$ is a normal generation.

2. The formalization of the modeling process

Monte Carlo method to simulate the transport equation in the critical tasks can be conventionally represented as two processes, each of which are produced by random variables based on certain physical quantities.

The first process is a simulation step. Using the normal generation G it builds a random state $S|G$ (S under the condition G). Wherein the condition of bias absence at a single step simulation is satisfied, i.e. for any G

$$\mathbf{E}(\nu(S \mid G)) = \boldsymbol{H}\nu(G), \tag{2}$$

where $\boldsymbol{H}$ is the secondary neutrons generation operator, $\mathbf{E}$ is the mathematical expectation.

The second process is normalization. Using the given condition of the set $S=[\boldsymbol{w}_S,\boldsymbol{p}_S]$ it builds a random normal generation $G|S=[\boldsymbol{w}_G,\boldsymbol{p}_G]$. Wherein the following conditions are satisfied:

- any point in $\boldsymbol{p}_G$ components may be found in $\boldsymbol{p}_S$ components of non-zero weights, i.e. any particle of normal generation is obtained from a particle of a state of S;
- equivalence of weights, i.e. let a_p be a sum of weights of particles of a state of the S set corresponding to some point p, and b_p is the mathematical expectation of a similar amount for normal generation, than for any points p and q at $b_p>0$ it is true that $a_q/a_p = b_q/b_p$;
- normalization is homogeneous with weight 0, i.e. for any $\lambda>0$ it is true that $G|S = G|(\lambda S)$.

It is followed from the second condition that

$$\mathbf{E}(\nu(G \mid S)) = \nu(S)N_{TOT} / W(S). \tag{3}$$

In the beginning of the iteration process of simulation the initial normal generation G_0 is chosen. Let's assume that normal generation G_t is formed. Then the state of secondary neutrons is $S_{t+1}=S|G_t$ according to the said above. The next normal generation is $G_{t+1}=G|S_t$.

The contributions to the assessment of the effective multiplication factor are

$$k_{t+1} = W(S_{t+1})/W(G_t) = W(S_{t+1})/N_{TOT}.$$

Instead, it is suggested to use the following contributions to the evaluation of k_{eff}

$$k_{h,t+1} = (h,\nu(S_{t+1})) /(h,\nu(G_t)), \tag{4}$$

where h is a non-negative function in the phase space, which is positive in all points with fuel; round brackets $(\cdot,\cdot)$ denote integration of function and density product.

It is obvious, that $k_{t+1} = k_{e,t+1}$, where e is the function identically equal to one.

Sequence $\{S_t,G_t\}$ uniquely defines the sequence of generations $\{F_t\}$. Namely, $F_0 = G_0$, further transition to the next point is carried out according to the following equations

$$G_t = F_t / c_t, \text{ where } c_t = W(F_t) / N_{TOT},$$
$$S_{t+1} = S \mid G_t,$$
$$G_{t+1} = G \mid S_{t+1},$$
$$F_{t+1} = G_{t+1}c_t W(S_{t+1}) / N_{TOT} = G_{t+1}c_t k_{t+1}.$$

In other words, $c_{t+1} = k_1 k_2 \ldots k_{t+1}$ [1].

At the same time due to (3)

$$\mathbf{E}\left(\nu(F_{t+1} \mid S_{t+1})\right) = c_t\mathbf{E}\left(\nu(G_{t+1} \mid S_{t+1})\right)k_{t+1} = c_t\nu(S_{t+1}).$$

It follows that

$$\mathbf{E}\left(\nu(F_{t+1} \mid F_t)\right) = \mathbf{E}(\left(\mathbf{E}\left(\nu(F_{t+1} \mid S_{t+1})\right)\right) \mid F_t) =$$
$$= c_t\mathbf{E}\left(\nu(S_{t+1} \mid F_t)\right) = c_t\mathbf{E}\left(\nu(S_{t+1} \mid G_t)\right) = c_t\mathbf{H}\nu(G_t)$$

due to (2). Thus

$$\mathbf{E}\left(\nu(F_{t+1} \mid F_t)\right) = \boldsymbol{H}\nu(F_t).$$

Iterating the last equation we get

$$\mathbf{E}(\nu(F_t) \mid F_0) = \boldsymbol{H}^t\nu(F_0).$$

This formula in different notation may be found in other works, e.g. [1,2].

Instead of the k_t evaluation one may use $k_{h,t}$, where h is the main adjoint function of the operator $\boldsymbol{H}$. It allows one to avoid bias in the k_{eff} evaluation, and zero out corresponding covariance at statistical uncertainty calculation.

The first follows from

$$\mathbf{E}(k_{h,t+1} \mid G_t) = \mathbf{E}((h,\nu(S_{t+1})) / (h,\nu(G_t))|G_t) =$$
$$= (h,\boldsymbol{H}\nu(G_t)) / (h,\nu(G_t)) = (\boldsymbol{H}^+h, \nu(G_t)) / (h,\nu(G_t)) = k_{eff}.$$

In particular, this equation implies that for any $q\geq 0$

$$\mathbf{E}(k_{h,t+q+1} \mid G_t) = \mathbf{E}(\mathbf{E}(k_{h,t+q+1} \mid G_{t+q}) \mid G_t) = k_{eff}.$$

Zero covariance between $k_{h,t+q+1}$ and $k_{h,t+1}$ follows from

$$\mathbf{E}(k_{h,t+q+1} \cdot k_{h,t+1} \mid G_t) = \mathbf{E}(\mathbf{E}(k_{h,t+q+1} \cdot k_{h,t+1} \mid G_{t+1}) \mid G_t).$$

Based on the fact that $k_{h,t+1}$ is constant at the condition of G_{t+1}.

$$\mathbf{E}(\mathbf{E}(k_{h,t+q+1} \cdot k_{h,t+1} \mid G_{t+1}) \mid G_t) = \mathbf{E}(k_{h,t+1}\mathbf{E}(k_{h,t+q+1} \mid G_{t+1}) \mid G_t) =$$
$$= \mathbf{E}(k_{h,t+1}k_{eff} \mid G_t) = k_{eff}^2.$$

Thus, covariance is $k_{eff}^2 - k_{eff} \cdot k_{eff} = 0$.

3. Implementation

Thus, if we know the adjoint function we may obtain non-biased estimation of k_{eff} and reliable estimate of statistical uncertainty.

Implementation of the method of calculation of the adjoint function is based on the use of fission matrix [9,10]. The set of points in phase space containing fuel is divided into a number of zones. Then the equation of criticality can be expressed as

$$k_{eff}\boldsymbol{\psi}=\mathbf{T}\boldsymbol{\psi},$$

where $\boldsymbol{\psi}$ is a vector, i-th component of which corresponds to the neutron generation rate in zone i, and $\mathbf{T}$ is the matrix, where T_{ij} is the average number of neutrons born in zone i at the condition that the fission was caused by the neutron born in zone j.

In this case the adjoint equation is

$$k_{eff}\boldsymbol{\psi}^{+}=\mathbf{T}^{\mathrm{T}}\boldsymbol{\psi}^{+},$$

here transposed matrix $\mathbf{T}$ has the meaning of the adjoint operator. Matrix elements are calculated by means of the Monte Carlo method during neutron transport simulation and the main adjoint function is calculated by means of any deterministic iteration method.

The accuracy of the calculation of the adjoint function using this method depends on the detail of the partition, which can be infinitely increased, but it also means the increase in the load on the computing resources.

After the importance function is calculated the second stage of calculation begins. Generations are produced by means standard for the MCU code. To evaluate the contribution into k_{eff} using the formula (4) $\boldsymbol{\psi}^{+}$ is used as the function h.

In the process of the simulation of the generation number t the two sums are calculated. The first one includes values of $\boldsymbol{\psi}^{+}$ for neutrons of the generation in their initial points. The second sum includes values of $\boldsymbol{\psi}^{+}$ in the points of secondary neutrons generation multiplied by the corresponding weights. If there is no non-analog simulation and at generation in the points of absorption this gives the average amount of fission neutrons. The contribution into k_{eff} is the ratio of the second sum to the first one.

Thus, the deviation from the standard calculation takes place not in the simulation, but in the tallying, which is provided in the MCU code.

III. RESULTS

The method is approved by calculation of weakly coupled system «Whiteside problem».

1. Model description

The system consists of 9×9×9=729 spheres with plutonium-239 (see Fig. 1), which are located in mesh points of the regular cubic lattice with the 60 cm pitch. The radius of central sphere is equal to 5.009 cm, the radius of the rest ones is equal to 3.976 cm. The lattice of spheres is located in the air and is encircled by the water reflector of 100 cm thickness. The temperature of all materials is equal to 300 K. In this system k_{eff} = 1.0035.

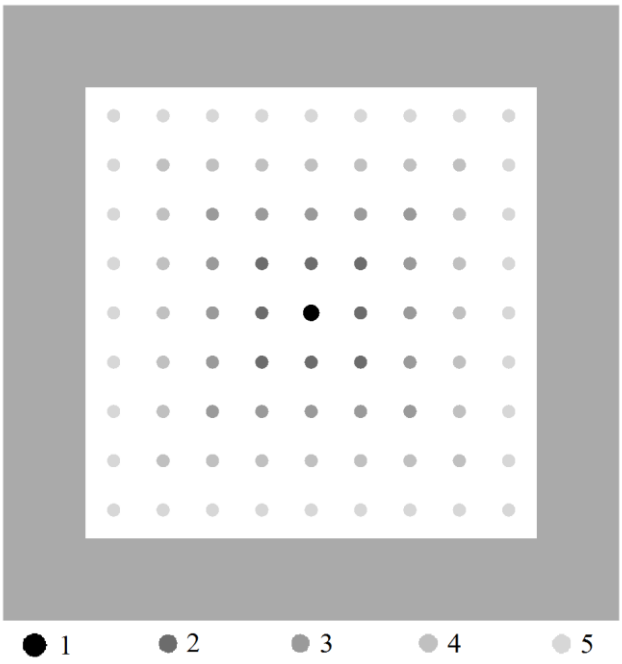

Fig. 1. Scheme «Whiteside problem» in OXY plane.

2. Calculation of importance function

All 729 spheres are grouped in 5 cubic layers, and the matrix dimension is 5×5. Enumeration of tally zones in OXY plane is shown on Fig. 1 (from inner layer (1-st zone) to outer one (5-th zone)). The scheme of enumeration in OXZ plane is the same.

Estimations of the fission matrix, the eigenfunction and the importance function are given in Tables I,II. The values of eigenfunction are divided by unit volume of a sphere and normalized ($\boldsymbol{\psi}_{norm}$). The eigenvalue of the matrix k_{eff} is equal to 1.0035.

It should be noted that in this task values of $\boldsymbol{\psi}_{norm}$ and $\boldsymbol{\psi}^{+}$ are practically the same (see Table II).

To investigate the effect of fission matrix detailing on calculation results a fission matrix of 729×729 (each sphere is a different tally) was evaluated.

Calculations by the MCU code have been performed with the various number of neutrons in the generation N_{TOT}=2000, 5000, 10000, 20000, and 50000. Calculation results of effective multiplication factor with the normalization using the importance function k_{adj} (5 zones) and k_{adj729} (729 zones) are compared with the standard calculation of k_{std} (see Table III and Fig. 2). For convenience of comparing all calculations use the same

number of histories (≈$5\cdot10^9$). Statistical uncertainty (a standard deviation) is equal to 0,004 %.

Table I. Fission matrix **T**

*i**j*	1	2	3	4	5
1	1.0030	0.0014	0.0005	0.0004	0.0004
2	0.0164	0.7774	0.0091	0.0067	0.0062
3	0.0265	0.0330	0.7736	0.0271	0.0237
4	0.0485	0.0535	0.0586	0.7932	0.0555
5	0.0753	0.0856	0.0879	0.0950	0.8257

Table II. The eigenfunction and the importance function

No.	ψ_{norm}	ψ^+
1	0.9740	0.9736
2	0.0097	0.0101
3	0.0061	0.0060
4	0.0053	0.0053
5	0.0049	0.0050
Sum	1.0000	1.0000

Table III. Effective multiplication factor estimations in dependence on N_{TOT}

N_{TOT}	K_{std}	k_{adj}	k_{adj729}
2000	1.00208	1.00332	1.00340
5000	1.00296	1.00346	1.00352
10000	1.00326	1.00350	1.00353
20000	1.00340	1.00353	1.00354
50000	1.00349	1.00354	1.00353

The results with different division show that evaluations with higher detailing (729 tallies) have smaller bias. However, the difference is small and does not exceed 0,01 %.

These data indicate that the importance function can be calculated with coarse approximation. That is why it is possible to use the importance function, which has been calculated for similar models.

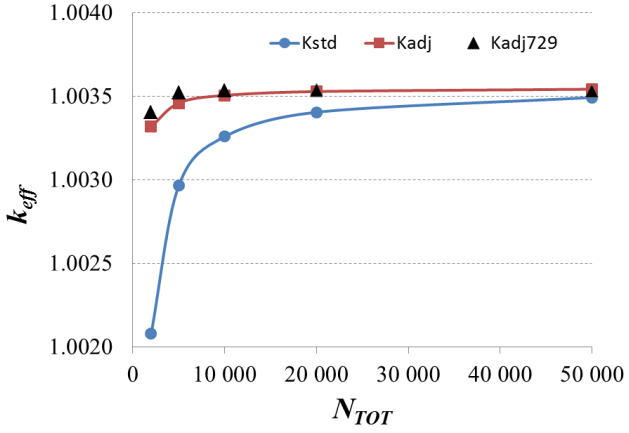

Fig. 2. Calculation k_{eff} of with normalization using the importance function (k_{adj}, k_{adj729}) and without that (k_{std}).

It should be noted essential irregularity between neutron sources in different spheres. It is shown on Fig. 3 where calculation of eigenfunction and importance function was obtained for 729 zones. The neutron source in central sphere is essentially more than others. It characterizes weakly coupled system.

Also it should be noted that eigenfunction divided by unit volume is nearly equal to importance function for detail matrix too.

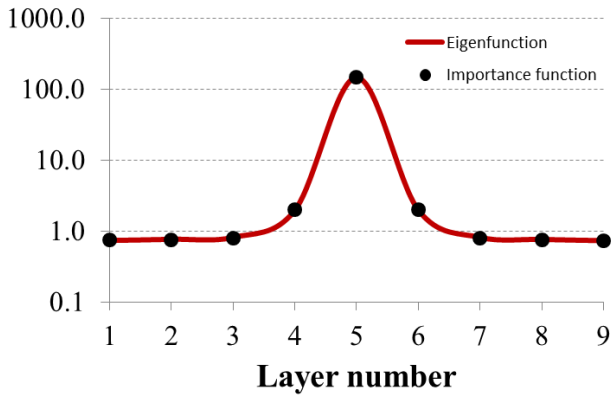

Fig. 3. Values of eigenfunction are divided by unit volume of a sphere and importance function for central row by height which are obtained as a result of fission matrix solution with 729 zones. Both ψ_{norm} and ψ^+ are normalized so that sum of elements of each is equal to 729.

3. Calculation of the k_{eff} evaluation bias and its statistical uncertainty

The calculation of bias of k_{eff} is performed using the formula (1). The standard calculation with N_{TOT}=2000 gives the bias Δ_K=0.15 % (see Table IV and Fig. 4), whereas the calculation with the normalization on the estimation of the importance function gives the bias of only Δ_K=0,02%. Hereafter the results are from calculations with importance function obtained using five tally division.

Table IV. Standard deviation and bias calculation's results

	Standard calculation			Calculation taking into account importance function		
N_{TOT}	σ_0, %	σ_{corr}, %	Δ_K, %	σ_0, %	σ_{corr}, %	Δ_K, %
2000	0.0020	0.0040	0.147	0.0040	0.0042	0.023
5000	0.0020	0.0040	0.059	0.0040	0.0042	0.009
10000	0.0020	0.0040	0.029	0.0040	0.0042	0.005
20000	0.0020	0.0040	0.015	0.0040	0.0042	0.002
50000	0.0020	0.0040	0.006	0.0040	0.0042	0.001

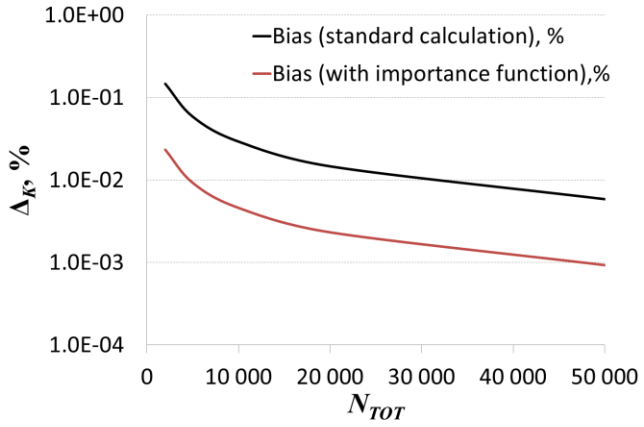

Fig. 4. Bias calculated depending on N_{TOT}.

Figure 5 illustrates the behavior of k_{eff} in dependence on the number of simulated generations at N_{TOT}=2000. One may see that the standard calculation gives bias while the calculation with the normalization using the importance function gives almost the correct answer.

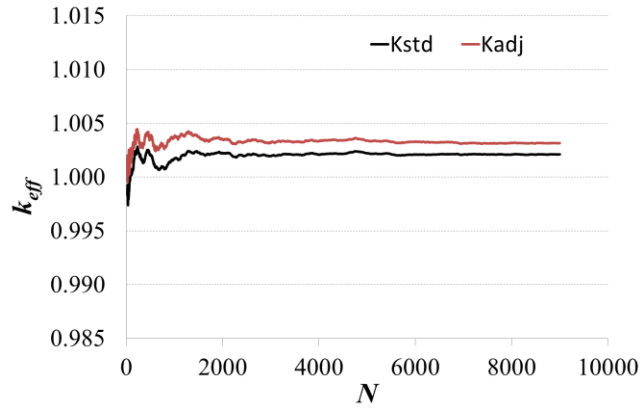

Fig. 5. Dependence of k_{eff} on the number of simulated generations.

In the standard calculation the sum of L=100 elements of autocorrelation function at $NTOT$=2000 is equal to (see Fig. 6)

$$S_L = \sum_{k=1}^{L} c_k = 1.6,$$

what means that statistical uncertainty taking into account correlation between generations is $\sigma_{corr} / \sigma_0 = \sqrt{1+2S_L} \approx 2$ times higher than statistical uncertainty obtained using the standard formula for the variance of the random variable. Statistical uncertainty of k_{eff} excluding correlations between generations is σ_0=0.002%, and σ_{corr}=0.004 % including them. In the calculation with the normalization using the importance function the statistical uncertainty of k_{eff} calculation obtained by the standard formula is σ_0=0.004%. Thus, normalization using the importance function does not decrease the statistical uncertainty, but it allows obtaining it using the standard formula for the variance of the random variable offsetting the impact of correlations between generations.

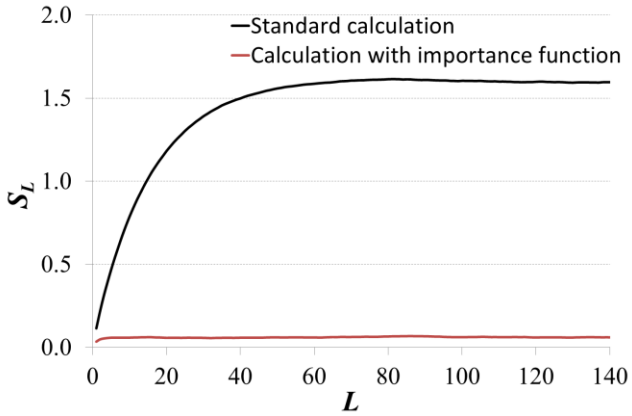

Fig. 6. Sums of the first L elements of autocorrelation function.

IV. CONCLUSION

The paper describes a method that allows one to level the bias of the effective multiplication factor calculation without making any changes to the simulation process and receive reliable value of its statistical error. The proposed method is very simple to implement and practically does not increase the neutron history simulation time. Moreover, its use reduces the number of neutrons in the generation and, consequently, the total calculation time by order of magnitude.

The effectiveness of the method is demonstrated by the example of the calculation of a weakly coupled system «Whiteside problem».

As a result, the work allows concluding the following.

1. The usage of the normalization using the estimation of the importance function reduces significantly the value of the maximum lag. Calculations of the autocorrelation function using the standard normalization gives the value of the lag L=100, in case of the normalization using the importance function, it is L=5.

2. The usage of the normalization using the importance function reduces significantly the value of the bias of k_{eff} estimation. At rather small N_{TOT}=2000 such normalization gives almost non-biased k_{eff} estimation. To obtain the similar result statistically it is necessary to use N_{TOT}=20000.

3. The normalization using the importance function doesn't reduce the statistical error of the calculation but allows one to obtain it by the standard formula for the dispersion of a random value without taking into account correlations between generations because this correlation is almost equal to zero.

4. The solution of the matrix equation almost coincides with k_{eff} obtained by Monte-Carlo method with the normalization using the importance function.

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