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Uncertainty Propagation Analysis in Time-Dependent Monte Carlo Calculations with Combing Technique

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1. Introduction

Due to flexibility of the Monte Carlo neutron transport analysis for cross section and geometry treatment, it has been in the spotlight recently with the development of computer science [1-4]. The transient behavior and safety analysis of nuclear system requires to solve the space-time dependent neutron transport equation. MCNP has simulated the time-dependent behavior of a nuclear system, based on the Monte Carlo neutron transport method, using the direct simulation method (DSM) [5]. In the development version of SERPENT 2 code, a time-dependent simulation mode has also been implemented. In this mode, sequential population control mechanism has been proposed for modeling of prompt super-critical systems [6]. For super-critical or sub-critical systems, the neutron population increases or decreases over a period of time. The neutron population is uniformly combed to return it to the neutron population started with at the beginning of time boundary [7].

In the Monte Carlo (MC) eigenvalue calculations, various schemes have been devised to estimate real variance [8-11]. However, in the time-dependent Monte Carlo (TDMC) calculations, the real variance estimation method is not studied sufficiently. The main purpose of this paper is to estimate the real variance of the tally in TDMC calculations using uncertainty propagation model. In this paper, uncertainty of the fractional core fission rate is quantified. The effectiveness is examined for C5G7-TD benchmark which specifies a series of space-time neutron kinetics problems without consideration of any feedback effects [12].

In non-critical system, the neutron population can increase or decrease exponentially. To prevent this fluctuation, the combing technique is usually applied to TDMC calculations [13]. Through the combing process, the neutron population is regulated to a user-defined value and the combed neutrons have the same weight.

2. Time-Dependent Monte Carlo Scheme

In this study, the conventional TDMC method is implemented, which can also be called as neutron history-based method (NHBM). In TDMC calculation, the tally mean and the variance are calculated from each time-step. From the very beginning to the end of each time boundary, all the neutron histories are tracked with creating branches by fission reactions instead of new neutron histories. Figure 1 shows the general scheme for performing TDMC calculation. Before the simulation for i^{th} time-step, the system properties, such as material and geometry, are read. After a single neutron is simulated, the branches from this neutron due to fission and splitting are simulated directly. When a neutron crosses the time boundary, it is stopped and stored in the bank for the next time-step. If all the neutron histories are simulated in this manner, the tally is estimated and the simulation for the time-step is terminated.

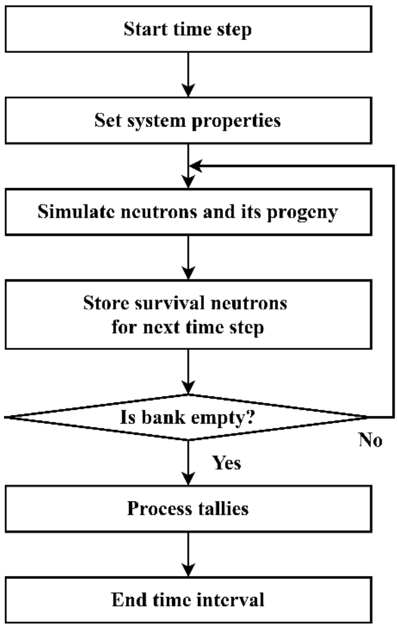

Fig. 1. Scheme for Performing Time-Dependent Monte Carlo Calculation.

There is no time information with the neutrons simulated in the MC eigenvalue calculations. On the other hand, the time information must be stored to describe the time-dependent behavior of neutrons. Therefore, the time is discretized into several time-steps and the time-step index i is introduced in the TDMC algorithm.

2.1. Combing Algorithm

The neutron population and weights are controlled by combing algorithm. The combed weights of the neutron at the beginning of every time-steps are normalized to unity by introducing scale factor. Physically, the scale factor is the expected value of the weight of neutron history at the beginning of m^{th} time-step generated by a neutron history at the beginning of the first time-step. Mathematically, the scale factor at m^{th} time-step can be written as;

$$F_m = f_1 f_2 \cdots f_{m-1} = \prod_{i=1}^{m-1} f_i \qquad (1)$$

where f_i is defined by;

$$f_i = \frac{1}{N} \sum_{j=1}^{N} w_{i,k}^{S} \Big/ w_i^0 \qquad (2)$$

where N and w_i^0 are the number of neutron histories and the initial weight of neutron histories at the beginning of the i^{th} time-step, respectively. $w_{i,k}^S$ is the survival weight from k^{th} history at i^{th} time-step. Substituting the value of Eq. (2) into Eq. (1), the scale factor can be rewritten as;

$$F_m = \prod_{i=1}^{m-1} \left(\frac{1}{N} \sum_{j=1}^{N} w_{i,k}^{S} \Big/ w_i^0 \right) \qquad (3)$$

3. Real Variance Estimation for Time-Dependent Tally

The statistical uncertainty of each time-step is accumulated with the uncertainty propagating through the calculation from the preceding time-step. Without considering the uncertainty propagation, the uncertainty in TDMC simulations can be underpredicted, which means the existence of variance bias in tally [14]. In this study, with the help of uncertainty propagation model, diagnostic method for real variance of time-dependent tally is derived.

3.1. Time-Dependent Tally Estimator

An integral form of the time-dependent Boltzmann transport equation for the collision density$\Psi(\mathbf{P})$, where $\mathbf{P}$ denotes the state vector of a neutron in the seven-dimensional phase space $(\boldsymbol{r}, E, \widehat{\boldsymbol{\Omega}}, t)$ can be written as;

$$\Psi(\mathbf{P}) = S(\mathbf{P}) + \int d\mathbf{P}' K(\mathbf{P}' \rightarrow \mathbf{P}) \Psi(\mathbf{P}') \qquad (4)$$

where $\Psi(\mathbf{P})$ and $K(\mathbf{P}' \rightarrow \mathbf{P})$ is collision density and transport kernel, respectively. The transport kernel is;

$$K(\mathbf{P}' \rightarrow \mathbf{P}) = C\left(\mathbf{r}', t'; E', \boldsymbol{\Omega}' \rightarrow E, \boldsymbol{\Omega}\right) \times T\left(E, \boldsymbol{\Omega}, t; \mathbf{r}' \rightarrow \mathbf{r}\right) \qquad (5)$$

where $C(\boldsymbol{r}', t'; E', \widehat{\boldsymbol{\Omega}}' \rightarrow E, \widehat{\boldsymbol{\Omega}})$ is collision kernel and $T(E, \widehat{\boldsymbol{\Omega}}, t; \boldsymbol{r}' \rightarrow \boldsymbol{r})$ is transition kernel [15].

After reviewing Neumann series solution, the desired tally at the end of m^{th} time-step can be calculated as;

$$Q_m = F_m \sum_{k=1}^{N} \sum_{j} w_{m,k}^{j} q_{m,k}^{j} \qquad (6)$$

where $w_{m,k}^j$ and $q_{m,k}^j$ is the weight of neutron and the tally response for the j^{th} collision of k^{th} history at m^{th} time-step. The scale factor is global parameter which only depend on time-step index m. Therefore, the variance of the tally Q_m can be written;

$$\sigma^2\left[Q_m\right] = \sigma^2\left[F_m\right] + \sigma^2\left[Q_m\right] \qquad (7)$$

where $\widetilde{Q_m}$ is defined by;

$$Q_m = \sum_{k=1}^{N} \sum_{j} w_{m,k}^{j} q_{m,k}^{j} \qquad (8)$$

Because the second-order derivative of scale factor comes out to be zero, using Taylor expansion of Eq. (1), the total derivative term of scale factor can be written as;

$$dF_m = \sum_{i=1}^{m-1} \left(\frac{\partial F_m}{\partial f_i} \right) df_i \qquad (9)$$

By definition, the variance of scale factor is;

$$\sigma^2\left[F_m\right] = E\left[\left(dF_m\right)^2\right] \qquad (10)$$

Substituting the value of derivative in Eq. (9) into Eq. (10), the variance of the scale factor can be rewritten as;

$$\sigma^2\left[F_m\right] = \sum_{i=1}^{m-1} \sum_{j=1}^{m-1} \left(\frac{\partial^2 F_m}{\partial f_i \partial f_j} \right) \mathrm{cov}\left[f_i, f_j\right] \qquad (11)$$

The relative partial derivative of scale factor is;

$$\frac{1}{F_m} \left(\frac{\partial F_m}{\partial f_i} \right) = \frac{1}{f_i} \qquad (12)$$

Combining Eq. (11) and Eq. (12), the relative variance of the scale factor can be written as;

$$\frac{\sigma^2\left[F_m\right]}{F_m{}^2} = \sum_{i=1}^{m-1} \sum_{j=1}^{m-1} \frac{\mathrm{cov}\left[f_i, f_j\right]}{f_i \cdot f_j} \qquad (13)$$

By substituting the value of Eq. (2), the inter-step covariance $\mathrm{cov}[f_i, f_j]$ can be written as;

$$\mathrm{cov}\left[f_i, f_j\right] = \frac{1}{N^2 w_i^0 w_j^0} \times \sum_{k=1}^{N} \sum_{k'=1}^{N} \mathrm{cov}\left[w_{i,k}^S, w_{j,k}^S\right] \qquad (14)$$

By substituting the value of the inter-step covariance in Eq. (14) into Eq. (13), we can obtain;

$$\frac{\sigma^2\left[F_m\right]}{F_m{}^2} = \frac{1}{N^2 w_i^0 w_j^0} \times \sum_{i=1}^{m-1} \sum_{j=1}^{m-1} \sum_{k=1}^{N} \sum_{k'=1}^{N} \frac{\mathrm{cov}\left[w_{i,k}^S, w_{j,k'}^S\right]}{f_i \cdot f_j} \qquad (15)$$

As a result of combing process, one neutron history is expected to generate one neutron history at the next time-step. One can see that the probability the k^{th} neutron history at i^{th} time-step generates k'^{th} history at the next time-step depends only on the difference between history index. Thus, we can introduce the real lag l covariance:

$$C_R[l] = \mathrm{cov}\left[w_{i,k}^S, w_{j,k+l}^S\right] \tag{16}$$

For the lag l covariance, we use the following estimator $C_S[l]$:

$$C_S[l] = \frac{1}{N-l-1} \times \sum_{k=1}^{N-l}\left(w_{i,k}^S - w_i^S\right)\left(w_{j,k+l}^S - w_j^S\right) \tag{17}$$

where w_i^S is the average survival neutron weight at i^{th} time-step, which is calculated by;

$$w_i^S = \frac{1}{N}\sum_{k=1}^{N} w_{i,k}^S \tag{18}$$

If we assume that $C_S[l]$ is $C_R[l]$, inter-step covariance can be estimated by;

$$\mathrm{cov}\left[f_i, f_j\right] = \frac{1}{N^2 w_i^0 w_j^0} \times\left(NC_S[l] + 2\sum_{l=1}^{N-1}(N-l)C_S[l]\right) \tag{19}$$

By substituting Eq. (19) into Eq. (13), the final estimator for real variance of scale factor can be written as;

$$\sigma^2[F_m] = \frac{F_m^{\ 2}}{N^2 w_i^0 w_j^0} \times \sum_{k=1}^{N}\sum_{k'=1}^{N}\frac{1}{f_i \cdot f_j}\left(NC_S[l] + 2\sum_{l=1}^{N-1}(N-l)C_S[l]\right) \tag{20}$$

4. Numerical Results and Analysis

The reference value of real variance of fractional core fission rate is calculated by repeating 500 TDMC runs with different random number sequences. The mean value of the variance estimates from every single run is treated as the numerical result of real variance estimate. The individual TDMC calculation is performed for 10,000 neutron histories and 100 time-steps with time-step size 0.01 msec.

4.1. C5G7-TD Phase I – TD0-5

In this problem, the postulated transient event is approximated in the 2-D calculations as a step change of the material composition, i.e., an instantaneous replacement of the moderator-filled guide tube material by control rod material. Eq. (21) gives mathematical expression of the cross section mixing.

$$\begin{aligned} \Sigma_x(t) &= \Sigma_x^{GT} & ,t=0 \\ \Sigma_x(t) &= \Sigma_x^{GT} + 0.1\left(\Sigma_x^R - \Sigma_x^{GT}\right) & ,t>0 \end{aligned} \tag{21}$$

Figure 2 shows the real and estimated relative standard deviation (RSD) of fractional core fission rate. Real RSD is calculated from Eq. (7). One can see that new method predict more accurately the real RSD of fractional core fission rate tally. Figure 3 shows the real to apparent standard deviation (SD) of fractional core fission rate.

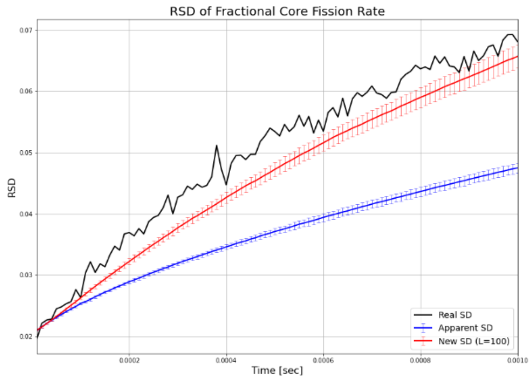

Fig. 2. Comparison of Estimated RSD's with Real RSD for Fractional Core Fission Rate Tally in C5G7-TD Phase I – TD0-5

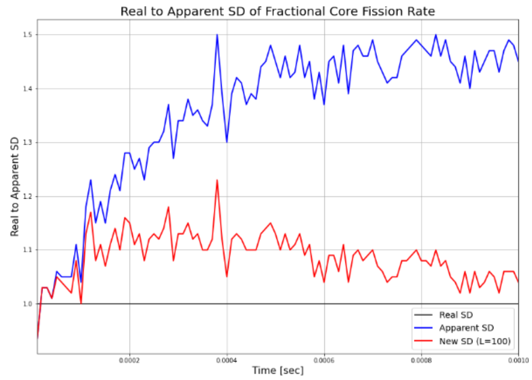

Fig. 3. Comparison of Estimated Real to Apparent SD for Fractional Core Fission Rate Tally in C5G7-TD Phase I – TD0-5

4.2. C5G7-TD Phase I – TD2-5

In this problem, the postulated transient event is approximated in the 2-D calculations as a ramp change of the material composition, i.e., a linear replacement of the moderator-filled guide tube material by control rod material. Eq. (22) gives mathematical expression of the cross section mixing.

$$\begin{aligned} \Sigma_x(t) &= \Sigma_x^{GT} & ,t=0 \\ \Sigma_x(t) &= \Sigma_x^{GT} + 100\left(\Sigma_x^R - \Sigma_x^{GT}\right)t & ,t>0 \end{aligned} \tag{22}$$

The real SD is estimated in the same manner with Problem 1. Figure 4 and 5 shows the RSD and real to apparent SD of this problem.

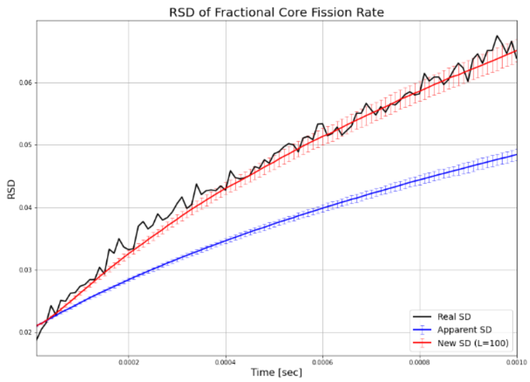

Fig. 4. Comparison of Estimated SD's with Real SD for Fractional Core Fission Rate Tally in C5G7-TD Phase I – TD2-5

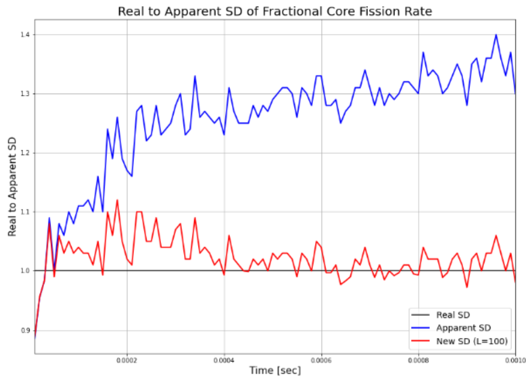

Fig. 5. Comparison of Estimated Real to Apparent SD for Fractional Core Fission Rate Tally in C5G7-TD Phase I – TD2-5

In Figure 2 and 4, the error bar means the sample SD of estimated SD's for fractional core fission rate from 500 individual TDMC run.

5. Conclusions

In this paper, a combing technique to control the neutron population for non-critical systems is implemented. The desired tally level is represented by introduction of scale factor. In TDMC calculations with combing technique, the uncertainty propagation of tally is shown to be driven by the uncertainty propagation of scale factor. Two test problem, 2-D heterogeneous transient system, are demonstrated for verification of uncertainty propagation in fractional core fission rate tally. In first case, the material composition changes suddenly and there is no more change. On the other hand, in second case, the material composition changes during simulation. The new method predicts the real SD well by comparing it to the existing estimate for both test problem.

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