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A Weighted Monte Carlo Solution of the Neutron Kinetics Equations

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Abstract - *The advance of computational technique allows Monte Carlo method being utilized for the neutronics evaluation of a nuclear reactor core. However, the solution of time dependent neutronics equation still remains a challenging problem. Correspondingly, a weighted Monte Carlo kinetics method (wMCk) is proposed based on traditional analog Monte Carlo kinetics method (aMCk). By using this method, a code named NECP-Dandi was developed mono-energetic point-kinetics simulation to focus on the time space. 11 test problems with different reactivity insertions were employed to verify the method. Numerical results demonstrate encouraging conclusions that wMCk is superior to aMCk in terms of accuracy.*

I. INTRODUCTION

Compared with deterministic method, Monte Carlo method can unfold the physical process regarding to the numerical solution of the neutron transport equation. Due to the advance of computational technique, Monte Carlo method could be employed as a first principle approach for the neutronics evaluation of a nuclear reactor core [1, 2]. Among those researches, most are concentrated on space-angle-energy phase-space, leaving the time-space as a challenging problem mainly due to the short neutron generation time. However, accurately simulating the reactor core changes over time during a transient process is very important for safety analysis.

Several research groups have devoted their effort to solving the neutron kinetics equations using Monte Carlo method. Dr. Shen [3] solved the time-dependent neutron transport equation with delayed neutrons ignored. Serpent2 [4] simulated the trajectory of each neutron to analyze multi-physics coupling process. OpenMC-TD [5] tracked both neutrons and delayed neutron precursors. G4-Stock [6] considered both prompt and delayed neutrons. However, they all employed the analog Monte Carlo kinetics method (aMCk), which suffers from large variance and low computing efficiency.

In this paper, a weighted Monte Carlo kinetics method (wMCk) is proposed and verified. To concentrate on the time-space, the spatial-angle-energy space is condensed considering the excellent flexibility in geometry, angle and energy spaces of Monte Carlo method.

II. THEORETICAL MODEL

1. Neutron Kinetics Equations

Condensing the time-dependent neutron kinetics equations in its space-angle-energy space yields the mono-energetic point neutron kinetics equations:

$$\begin{cases} \dfrac{\mathrm{d}n(t)}{\mathrm{d}t} + n(t)\Sigma_{\mathrm{t}}(t)v = n(t)\Sigma_{\mathrm{s}}(t)v + n(t)(1-\beta)\nu(t)\Sigma_{\mathrm{f}}(t)v + \sum_i \lambda_i C_i(t) \\ \dfrac{\mathrm{d}C_i(t)}{\mathrm{d}t} + \lambda_i C_i(t) = n(t)\beta_i \nu(t)\Sigma_{\mathrm{f}}(t)v \end{cases} \quad (1)$$

where i=1,2,⋯,I and j=1,2,⋯,J index the precursor group and isotopic nuclide, while other notations are common.

Define the solution vector as:

$$\boldsymbol{x}(t) = \begin{pmatrix} n(t) & C_1(t) & \cdots & C_I(t) \end{pmatrix}^{\mathrm{T}} \quad (2)$$

then Eq. (1) can be rewritten into a matrix form as:

$$\frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} + \boldsymbol{D}(t)\boldsymbol{x}(t) = \boldsymbol{P}(t)\cdot\boldsymbol{D}(t)\cdot\boldsymbol{x}(t) \quad (3)$$

where

$$\boldsymbol{D}(t) = \begin{bmatrix} \Sigma_t(t)v & 0 & \cdots & 0 \\ 0 & \lambda_1 & \cdots & 0 \\ 0 & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_I \end{bmatrix} \quad (4)$$

is the decay and transport matrix, and

$$\boldsymbol{P}(t) = \begin{bmatrix} \dfrac{\Sigma_s(t)}{\Sigma_t(t)} + \dfrac{\Sigma_t(t)}{\Sigma_t(t)}\nu(t)(1-\beta) & 1 & \cdots & 1 \\ \dfrac{\Sigma_f(t)}{\Sigma_t(t)}\nu(t)\beta_1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\Sigma_f(t)}{\Sigma_t(t)}\nu(t)\beta_I & 0 & \cdots & 0 \end{bmatrix} \quad (5)$$

is the probability and weighting matrix.

2. Integral Solution of the Neutron Kinetics Equations

To solve neutron kinetics equation by utilizing Monte Carlo method, an integral solution has to be obtained first. By using the method of variation of constant, the solution of Eq. (3) can be obtained:

$$\boldsymbol{x}(t) = \boldsymbol{T}(0\to t)\cdot\boldsymbol{x}(0) + \int_0^t \boldsymbol{T}(t'\to t)\cdot\boldsymbol{P}(t')\cdot\boldsymbol{D}(t')\cdot\boldsymbol{x}(t')\,\mathrm{d}t' \quad (6)$$

where matrix

$$\boldsymbol{T}(t'\to t) = \mathrm{e}^{-\int_{t'}^{t}\boldsymbol{D}(\tau)\,\mathrm{d}\tau} \quad (7)$$

represents the contribution from the particles at time t' to the solution vector at time t.

With a known initial value $\boldsymbol{x}(0)$, Eq. (6) can be solved iteratively:

$$\begin{aligned} \boldsymbol{x}(t) &= \boldsymbol{x}_0(t) + \sum_{m=1}^{\infty}\boldsymbol{x}_m(t) \\ &= \boldsymbol{T}(0\to t)\cdot\boldsymbol{x}(0) + \sum_{m=1}^{\infty}\int_0^t\int_0^{t_m}\cdots\int_0^{t_2}\mathrm{d}t_m\cdots\mathrm{d}t_1\boldsymbol{T}(t_m\to t)\boldsymbol{K}(t_{m-1}\to t_m)\cdots\boldsymbol{K}(0\to t_1)\boldsymbol{x}(0) \end{aligned} \quad (8)$$

where

$$\boldsymbol{K}(t_{l-1} \to t_l) = \boldsymbol{P}(t_l) \cdot \boldsymbol{D}(t_l) \cdot \mathrm{e}^{-\int_{t_{l-1}}^{t_l} \boldsymbol{D}(\tau) d\tau} = \boldsymbol{P}(t_l) \cdot f(t_{l-1} \to t_l) \quad (9)$$

is an operator representing two processes. The first part $f(t_{l-1} \to t_l)$ is the living fraction at time t_l originated from time t_{l-1}. It provides the timing of the next nuclear reaction. The second part $\boldsymbol{P}(t_l)$ provides the number of new particles generated by the last nuclear reaction and their status.

Since the contribution matrix in Eq. (7) can be reformulated as:

$$\boldsymbol{T}(t_m \to t) = \mathrm{e}^{-\int_{t_m}^{t} \boldsymbol{D}(\tau) d\tau} = \int_t^{\infty} \boldsymbol{D}(t_{m+1}) \mathrm{e}^{-\int_{t_m}^{t_{m+1}} \boldsymbol{D}(\tau) d\tau} \mathrm{d}t_{m+1} \quad (10)$$

Eq. (6) can be reformulated into the form as below:

$$\boldsymbol{x}(t) = \sum_{m=0}^{\infty} \boldsymbol{x}_m(t) \quad (11)$$

where

$$\boldsymbol{x}_m(t) = \int_t^{\infty} \cdots \int_0^{t_2} \mathrm{d}t_{m+1} \cdots \mathrm{d}t_1 \boldsymbol{D}(t_{m+1}) \mathrm{e}^{-\int_{t_m}^{t_{m+1}} \boldsymbol{D}(\tau) d\tau} \cdots \boldsymbol{K}(t_0 \to t_1) \boldsymbol{x}(0) \quad (12)$$

Thus, an integral solution of Eq. (3) that can be directly simulated by Monte Carlo method is obtained.

3. The Analog Monte Carlo Kinetics Method

According to Eq. (10) and Eq. (11), the particles at time t that construct the solution $\boldsymbol{x}(t)$ can be originated back to the initial value of $\boldsymbol{x}(0)$ by dating back m nuclear reactions, where the number m can vary from 0 to a large enough integer. If the Monte Carlo method is employed by tracking each of those particles, it is named as analog Monte Carlo kinetics method (aMCk).

The simulation process is very straight forward. (1) For a neutron generated at time t_{l-1}, its living time Δt_l can be sampled according to $f(t_{l-1} \to t_l)$ as:

$$\Delta t_l = -\frac{\ln \xi}{\Sigma_t v} \quad (13)$$

where ξ represents a random number. It means the neutron collides with a nuclide at time:

$$t_l = t_{l-1} + \Delta t_l \quad (14)$$

(2) There are three types of nuclear reactions, including neutron capture, neutron scattering and fission. The corresponding probabilities are Σ_c/Σ_t, Σ_s/Σ_t and Σ_f/Σ_t. Thus, a discrete sampling can determines the nuclear reaction type. (3) If it is the neutron capture reaction, the neutron tracking stops. (4) If it is the neutron scattering reaction, a new neutron is generated at time t_l and the simulation execution returns back to step (1). (5) If it is a fission reaction, v new neutrons would be generated. Considering that v is not an integer, the number of new neutrons would be $[v+\xi]$, where ξ represents a random number. Among those new neutrons, only one of them remains to be simulated while others would be stored waiting for their simulation sequentially. (6) For each of those new fission neutrons, there is a probability of β_i to be delayed neutron precursor of group i, while a probability of 1-β to be prompt neutron. If it is a neutron, the simulation execution returns back to step (1). (7) If it is a precursor, its living time can be sampled by using:

$$\Delta t_l = -\frac{\ln \xi}{\lambda_i} \quad (15)$$

which means it becomes a delayed neutron at time:

$$t_l = t_{l-1} + \Delta t_l \quad (16)$$

Then, the simulation execution returns back to step (1).

However, several problems would be encountered. (1) If one neutron capture reaction is happened in a particle sequence before the targeted time t, there would be no contribution to the solution for the corresponding sequence. (2) Considering the fact that fission reaction would produce more than one neutrons or precursors, those extra particles need to be stored until they can be simulated, which would make the computing code more complicated and increase the storage requirement. (3) It samples each step of the entire evolution process, which involves a strong stochastic effect, making the solution results possessed by large variance.

4. The Weighted Monte Carlo Kinetics Method

Define a weighting factor w as the contribution to the solution from a particle can yield the weighted Monte Carlo kinetics method (wMCk). There are two main differences in wMCk compared with the above aMCk.

Firstly, define new neutron capture cross-section, new fission cross-section and new average number of neutrons per fission as:

$$\Sigma'_c = 0 \quad (17)$$

$$\Sigma'_f = \Sigma_c + \Sigma_f \quad (18)$$

$$v' = v \frac{\Sigma_f}{\Sigma_c + \Sigma_f} \quad (19)$$

In this way, there would be no capture with zero contribution fully eliminated.

Secondly, the weighting factor is not going to be changed during a scattering process since the number of neutrons is taken as the same in this model. It will be changed by a factor of x in the future if (n,xn) scattering is considered. In contrast, the weighting factor is going to be changed by a factor of v' during a fission process. In this way, there is no need to temperately store any new neutrons, while will simplify the code development and save storage requirements.

In addition, the contribution from each initial neutron to the solution, in aMCk, could be 0 if the neutron was captured before the time of interest, while it could be a large integer if a sequence of fission reactions were experienced. In contrast, the corresponding contribution, in wMCk, would be the weighting factor. It will never be zero since there is no capture. And it is not going to be as large as in aMCk since $v'<v$ always holds. Thus, the variance of those contributions in wMCk would be much smaller than the variance in aMCk.

III. RESULTS

Based on the weighted Monte Carlo kinetics method proposed in this paper, a code named NECP-Dandi has been developed in Fortran 90 and verified by 11 test problems with difference reactivity insertions. The reference solutions are provided analytically or by a fully implicit backward finite difference method (FDM). The initial states of those tests are all critical with neutron density equal 1.0. The definition details of those test problems are shown in Table 1. The cross-sections are listed in

Table 2. The simulating durations are all 1ms. Test problems 1-4 and 6-7 simulates step reactivity insertion, while test problems 8-9 are designed to simulate pulse (0.1 ms) reactivity insertion. Test problems 5 and 10 are designed to simulate critical operation to demonstrate the variation of the Monte Carlo solution, while a linear reactivity is inserted in Test problem 11.

Table 1 Definition details of 11 test problems

Case	No. of precursor groups	Reactivity insertion	Reactivity insertion duration (ms)	No. of particles (million)
1	1	0	1	2500
2	6	0	1	2500
3	0	+0.0065	1	1
4	0	-0.0065	1	1
5	1	+0.0065	1	2500
6	1	-0.0065	1	2500
7	6	+0.0065	1	2500
8	6	-0.0065	1	2500
9	6	+0.0065	0.1	2500
10	6	-0.0065	0.1	2500
11	6	≈0.65*t*	1	2500

Table 2 Macroscopic cross-sections

ρ	0	+0.0065	-0.0065	0.65*t*
Σ_t (cm^{-1})	0.165258	0.165258	0.165258	0.165258
Σ_s (cm^{-1})	0.156187	0.156187	0.156187	0.156187
Σ_f (cm^{-1})	0.00365747	0.00368140	0.00363384	[1]
ν	2.48			
ν (cm/s)	3.04665510×10^6			

Before the discussion of accuracy, two definitions has to be clarified. (1) Statistic error (errS) is obtained by the central-limit theorem with confidence coefficient at 0.95. (2) Relative error (errR) is the deviation relative to reference solution.

Cases 1 and 2 are both critical problems with different number of precursor groups. The results of case 2 can be similar to those of case 1. Thus, only the results of case 1 are presented in Fig. 1 and Fig. 2. From the neutron density results as in Fig. 1, it can be found that the statistic error of aMCk (9.76×10^{-3}) is larger than that of wMCk (6.56×10^{-4}). In addition, stronger fluctuation has been observed from aMCk. In Fig. 2, the fluctuation still exists but it seems smaller due to the large increment of the precursor density.

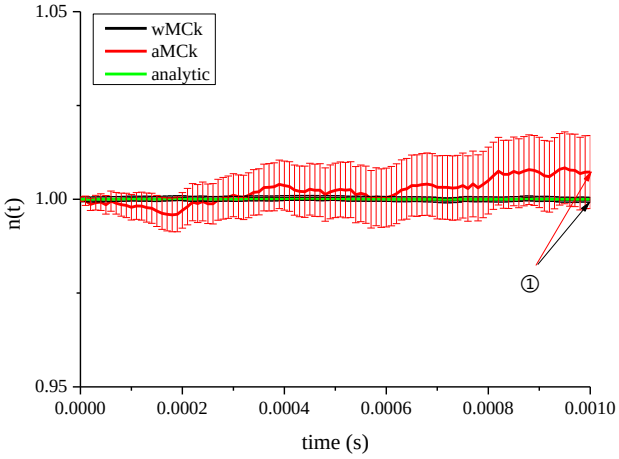

Fig. 1 Neutron density in case 1

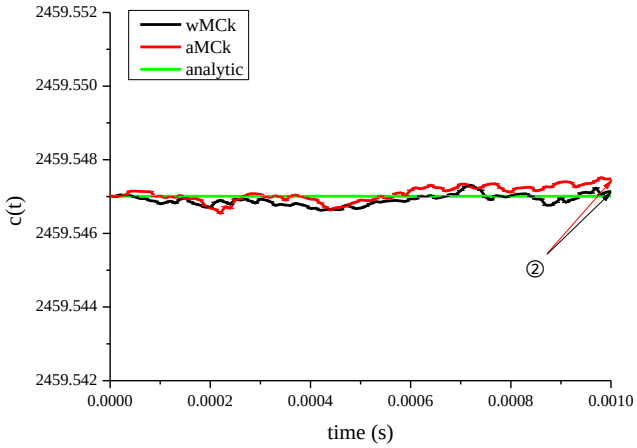

Fig. 2 Precursor density in case 1

Fig. 3 and Fig. 4 present the neutron density results of cases 3 and 4 which have no precursors. Cases 5 and 7 are both supercritical with precursors considered, while Cases 6 and 8 are both subcritical. Thus, the results of cases 7 and 8 are not represented here, while Fig. 5 to Fig. 8 shows the neutron density and precursor density comparisons. Cases 9 and 10 are positive and negative pulse reactivity insertion, which is designed to analyze rod ejection/insertion accidents. Even there is no feedback, both neutron density and precursor densities will approach their new steady states once the pulse insertion is over, as shown in Fig. 9 and Fig. 10. The largest statistic and relative errors in each cased are listed in Table 3. About one magnitude of smaller statistic and relative errors can be observed for the wMCk than the aMCk, which demonstrate the advantage of wMCk.

Case 11 represents an approximate linear positive reaction insertion to analyze neutron and precursor density change over time during a control rod withdrawal process. The results are displayed in Fig. 11. Being similar to positive and negative pulse reactivity insertion, an accurate

[1] 0.00365747+0.00237736*t*

result in terms of neutron density can be obtained by wMCk, which is impossible for aMCk with the same number of simulated particles.

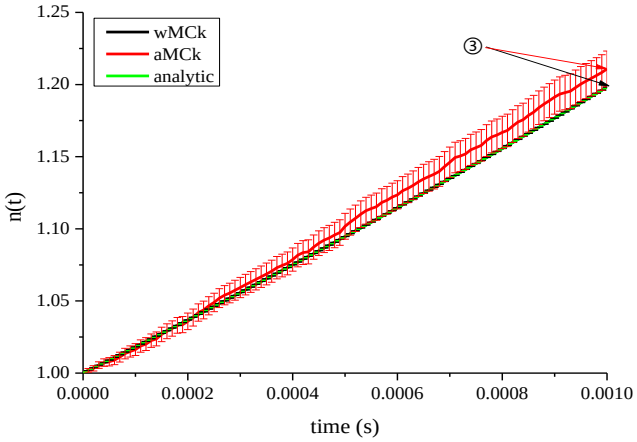

Fig. 3 Neutron density in case 3

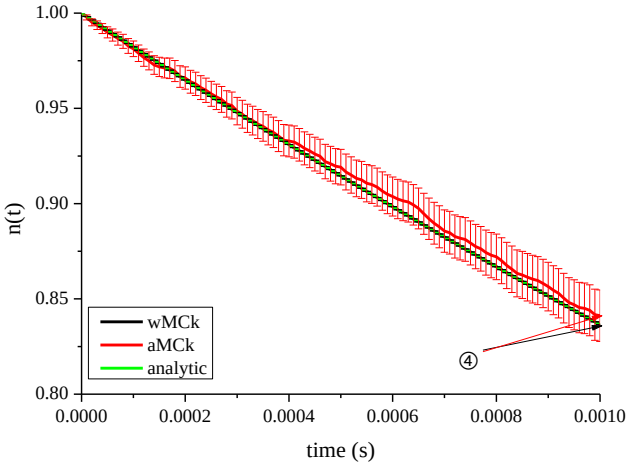

Fig. 4 Neutron density in case 4

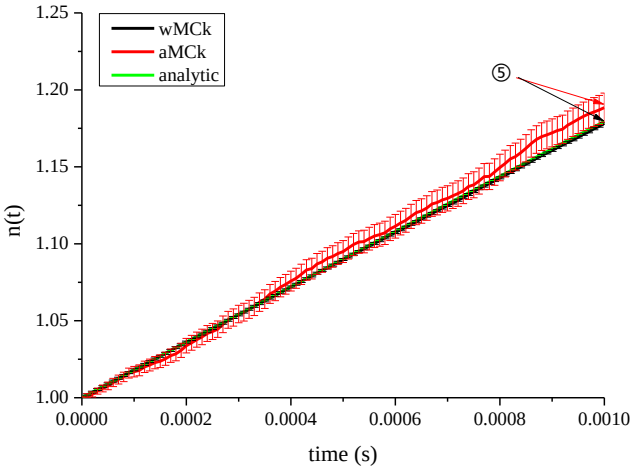

Fig. 5 Neutron density in case 5

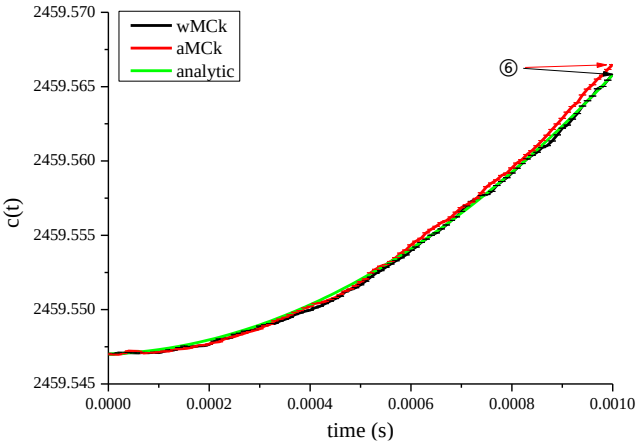

Fig. 6 Precursor density in case 5

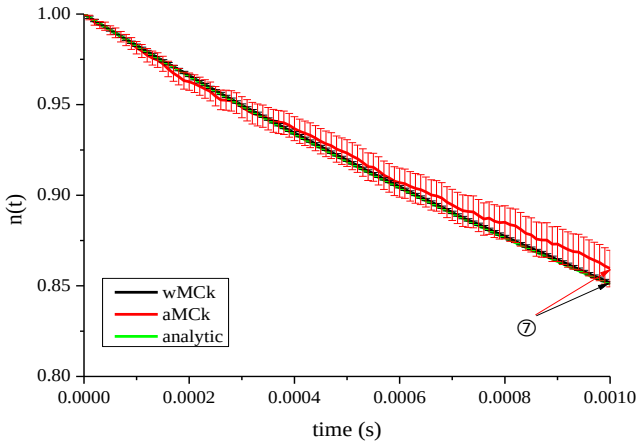

Fig. 7 Neutron density in case 6

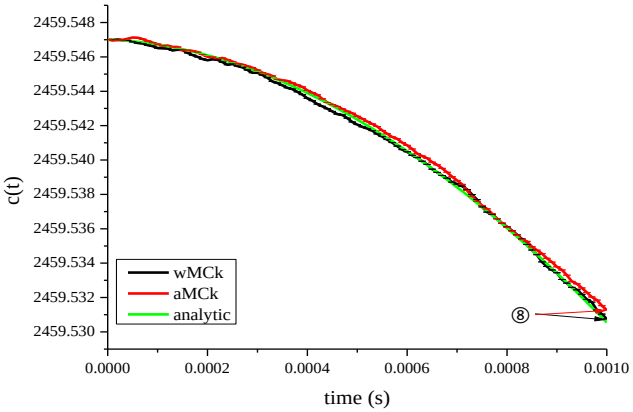

Fig. 8 Precursor density in case 6

IV. CONCLUSIONS AND DISSCUSSIONS

In this paper, to take advantage of the Monte Carlo method for solving the neutron kinetics equation, a weighted Monte Carlo kinetics method (wMCk) was proposed and compared to the currently employed analog Monte Carlo kinetics method (aMCk). Numerical results 11 test problems with zero, positive or negative step, linear

reactivity insertions demonstrate promising conclusions.

To extend this mono-energetic point kinetics solution to three-dimensional continuous energy simulation, there are two issues requiring attention as we can imagine. Firstly, the number of particles would increase dramatically due to the unfoldment of the phase space. Secondly, it is the appearance of the prompt and delayed neutron spectrums, which requires additional sampling process to determine the energy of those new fission neutrons. However, either of those issues can be overcome by simply increase the number of simulated particles or by investigating new variance reduction techniques.

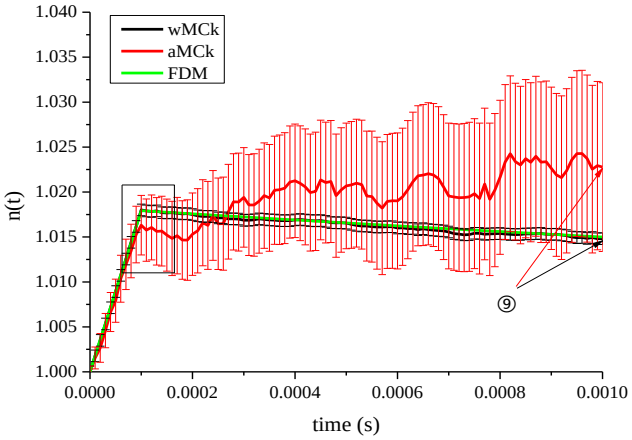

Fig. 9 Neutron density in case 9

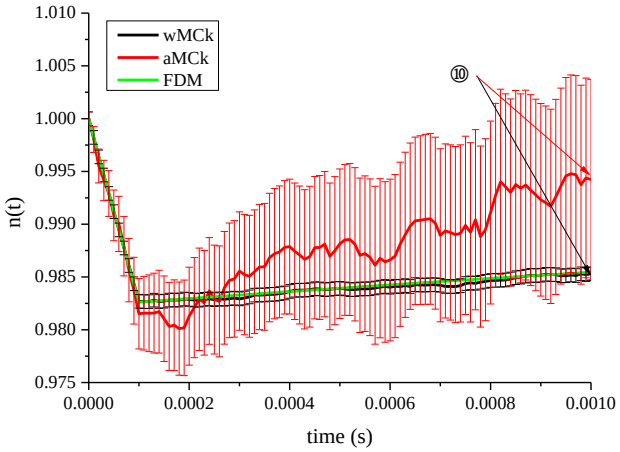

Fig. 10 Neutron density in case 10

V. ACKNOWLEDGMENTS

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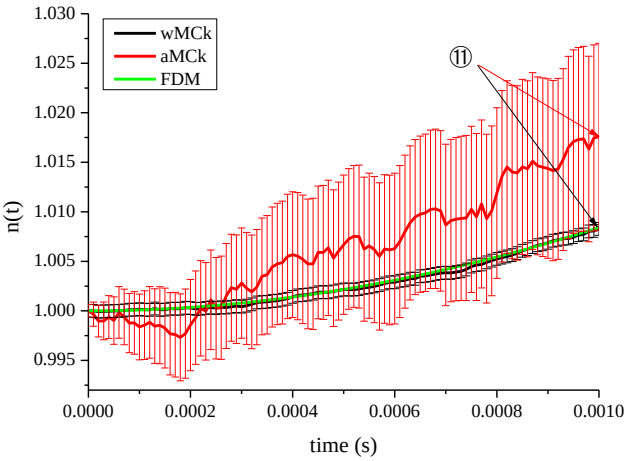

Fig. 11 Neutron density in case 11

Table 3 The largest statistic and relative errors

No.	wMCk		aMCk	
	errR	errS	errR	errS
①	-0.014%	6.56×10^{-4}	0.73%	9.76×10^{-3}
②	5.38×10^{-6}%	2.67×10^{-7}	1.91×10^{-5}%	5.51×10^{-7}
③	3.83×10^{-3}%	6.75×10^{-5}	1.06%	1.24×10^{-2}
④	-3.48×10^{-3}%	6.67×10^{-5}	0.559%	1.35×10^{-2}
⑤	-0.12%	6.62×10^{-4}	0.76%	9.44×10^{-3}
⑥	1.40×10^{-6}%	2.93×10^{-7}	2.79×10^{-5}%	5.97×10^{-7}
⑦	9.89×10^{-2}%	6.62×10^{-4}	1.02%	1.01×10^{-2}
⑧	8.44×10^{-6}%	2.45×10^{-7}	2.96×10^{-5}%	5.10×10^{-7}
⑨	-1.80×10^{-2}%	6.45×10^{-4}	0.77%	9.39×10^{-3}
⑩	-1.62×10^{-2}%	6.45×10^{-4}	0.89%	9.49×10^{-3}
⑪	-1.21×10^{-2}%	6.45×10^{-4}	0.91%	9.43×10^{-3}