A New Approach for Evaluating the Uncertainty of Predictor-Corrector Quasi-Static Monte Carlo Transient Simulation

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1. Introduction

In the wake of widespread high-power computing resources and algorithmic breakthroughs, attention has been drawn to the Monte Carlo-based transient reactor analysis in both academic and practical sense in the past few years. Two major philosophical approaches for time-dependent Monte Carlo simulation are widely accepted, which are the dynamic Monte Carlo (DMC) and the predictor-corrector quasi-static Monte Carlo (PCQS-MC), and has been implemented and demonstrated in several reactor analysis programs including TRIPOLI-4 [1], McCARD [2], Serpent2 [3], OpenMC [4] and iMC [5]. It is noteworthy to mention that the recently developed KAIST Monte Carlo transport program iMC supports both the DMC and PCQS-MC calculation based on the user's preference.

Since the Monte Carlo calculation is in nature a stochastic process, both the DMC and PCQS-MC calculation results are subjected to uncertainty issue, where its evaluation is rather intricate compared to the conventional steady-state Monte Carlo calculation. For the DMC real variance estimation, a history-based batch method has been proposed to mitigate the source correlation among the cycles [6]. However, a different measure is required for appraising the real variance for the PCQS-MC method, where its deterministic-stochastic framework renders the conventional uncertainty estimation method to be ineffective.

In this paper, a new approach for systematically evaluating the uncertainty of the PCQS-MC calculation result is proposed. Such a unique method not only considers the sample uncertainty but also incorporates the uncertainty of sampled point-kinetic parameters. It is found that the proposed measure reflects the inherent nature of the PCQS-MC method, resulting in an improved uncertainty estimation.

2. Predictor-Corrector Quasi-Static Monte Carlo

The time-dependent neutron transport equation and the precursor concentration balance equation should be simultaneously solved for transient reactor analysis.

$$\frac{1}{v(E)}\frac{\partial\psi(\vec{r},E,\vec{\Omega},t)}{\partial t} = -L\psi(\vec{r},E,\vec{\Omega},t) - T\psi(\vec{r},E,\vec{\Omega},t) + S\psi(\vec{r},E,\vec{\Omega},t) + \sum_{d=1}^{G_d}\frac{\chi_d(E)}{4\pi}\lambda_d C_d(\vec{r},t) + \frac{1}{k_0}\frac{\chi_p(E)}{4\pi}(1-\beta)F\psi(\vec{r},E,\vec{\Omega},t), \quad (1)$$

$$\frac{\partial C_d(\vec{r},t)}{\partial t} = \frac{1}{k_0}\beta_d F\psi(\vec{r},E,\vec{\Omega},t) - \lambda_d C_d(\vec{r},t), \quad (2)$$

where *L, T, S,* and *F* represent the leakage, transport, scattering, and fission operators respectively, and all the other notations are that of the convention.

Through implementation of Implicit-Euler method with a time step of Δt_s, the aforementioned set of equations reduces into the following form:

$$L\psi(\vec{r},E,\vec{\Omega},t_s) + T_{PCQS}\psi(\vec{r},E,\vec{\Omega},t_s) = S\psi(\vec{r},E,\vec{\Omega},t_s) + \frac{1}{k_0}\frac{\chi_p(E)}{4\pi}(1-\beta)F\psi(\vec{r},E,\vec{\Omega},t_s) + \sum_{d=1}^{G_d}\frac{\chi_d(E)}{4\pi}\lambda_d C_d(\vec{r},t_s), \quad (3)$$

with $T_{PCQS} \equiv \left(\sigma_t(\vec{r},E,t_s) + \frac{1}{v(E)\Delta t_s}\right)\psi(\vec{r},E,\vec{\Omega},t_s)$. Note that both the neutron fission source and delayed neutron precursor concentrations should be sampled and banked during calculation.

The neutron angular flux can be factorized into the amplitude function *n(t)* and the shape function $\varphi(\vec{r},E,\vec{\Omega},t)$ as:

$$\psi(\vec{r},E,\vec{\Omega},t) = n(t)\,\varphi(\vec{r},E,\vec{\Omega},t). \quad (4)$$

Note that Eq. (4) is not an assumption, but rather demands an additional equation to render such a factorization to be unique as below:

$$\int dV \int d\vec{\Omega} \int dE\ W(\vec{r},E,\vec{\Omega})\frac{\varphi(\vec{r},E,\vec{\Omega},t)}{v(E)} = \int dV \int d\vec{\Omega} \int dE\ W(\vec{r},E,\vec{\Omega})\frac{\psi(\vec{r},E,\vec{\Omega},t_0)}{v(E)}. \quad (5)$$

In the PCQS-MC calculation, the shape function and its associated point kinetics equation (PKE) parameters are deduced in the predictor iteration. Through the PKE calculation, the amplitude function is then updated, which corrects the source distribution:

$$\psi^{corrector}(\vec{r},E,\vec{\Omega},t_s)=\psi^{predictor}(\vec{r},E,\vec{\Omega},t_s)\frac{n(t_s)}{Z(t_s)}, \quad (6)$$

where $Z(t_s)$ is a normalization factor introduced to suffice Eq. (5).

$$Z(t_s)\equiv\frac{\left\langle W(\vec{r},E,\vec{\Omega}),\ \dfrac{\psi^{predictor}(\vec{r},E,\vec{\Omega},t_s)}{v(E)}\right\rangle}{\left\langle W(\vec{r},E,\vec{\Omega}),\ \dfrac{\psi(\vec{r},E,\vec{\Omega},t_0)}{v(E)}\right\rangle}. \quad (7)$$

3. Uncertainty Evaluation for PCQS-MC

Unlike the conventional steady-state Monte Carlo calculation, not only the cycle-wise source correlation but also the uncertainty of tallied PKE parameters manifests in the PCQS-MC calculation result. To assess the extent of each uncertainty source, a null-transient simulation has been devised using the critical GODIVA device. The following three different cases were postulated: Case 1) non-controlled case that represents a normal PCQS-MC calculation, Case 2) dynamic reactivity during PKE calculation set to be zero which neglects the uncertainty associated with PKE parameters, and Case 3) suppression of cycle-wise source correlation through a large number of histories per cycle. Table 1 enumerates a more detailed description of each case.

Figure 1 depicts the calculated null-transient power evolution for each case, where uncertainty has been estimated from the cycle-wise tallied power during predictor iteration multiplied by amplitude function.

Table 1. GODIVA null-transient simulation

Case	Parameter Uncertainty	Histories per cycle / # inactive cycles / # active cycles
1	$\mathrm{Var}[\rho]\neq 0$ $\mathrm{Var}[\beta\nu\Sigma_f\phi]\neq 0$	100,000 / 200 / 100
2	$\mathrm{Var}[\rho]= 0$ $\mathrm{Var}[\beta\nu\Sigma_f\phi]\neq 0$	100,000 / 200 / 100
3	$\mathrm{Var}[\rho]\neq 0$ $\mathrm{Var}[\beta\nu\Sigma_f\phi]\approx 0$	1,000,000 / 200 / 10

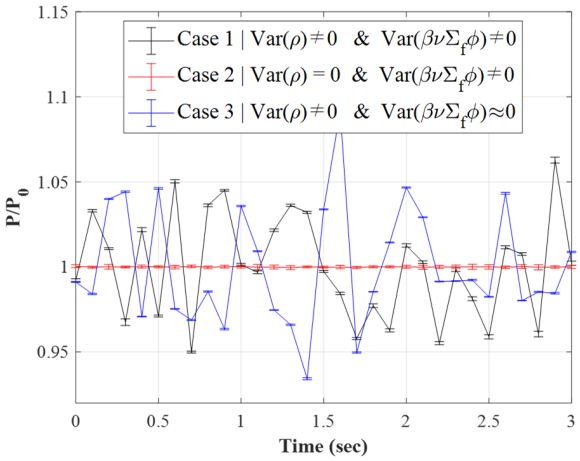

Figure 1. Null transient power evolution for each case

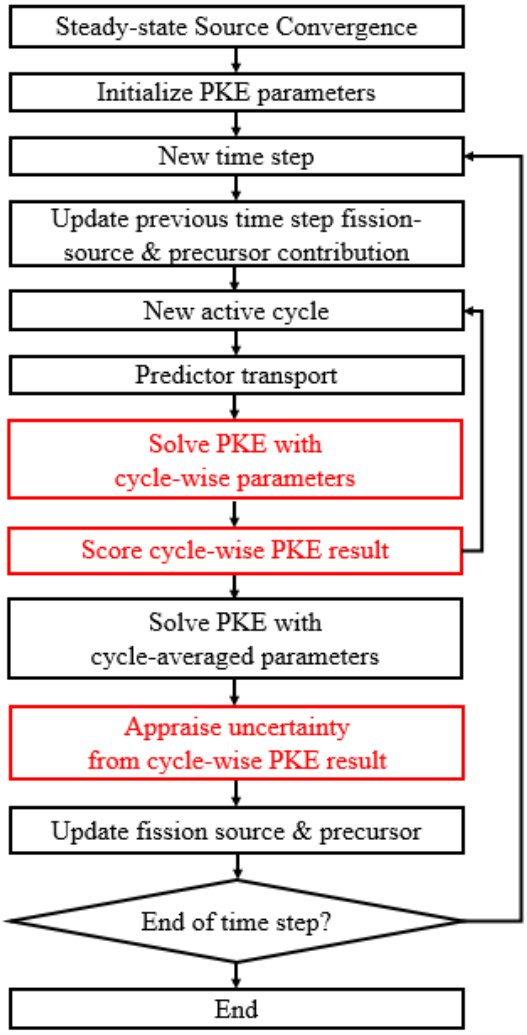

Figure 2. Calculation flow-chart of PCQS-MC for PK sampling method (red colour).

It is apparent that the uncertainty of tallied PKE parameters, especially the dynamic reactivity, has the most significant contribution to the fluctuation of PCQS-MC derived power estimation. Furthermore, the aforementioned conventional cycle-wise uncertainty assessment severely underestimates such an inherent uncertainty of the PCQS-MC framework.

To circumvent the limitation of the conventional cycle-wise uncertainty appraisal scheme in order to properly reflect the PCQS-MC method, a modified simulation scheme referred to as the point kinetics (PK) sampling method is suggested in this work. In addition to the conventional PCQS-MC framework, where PKE is solved with cycle-averaged tallied information, the PK sampling scheme additionally solves the PKE based on the cycle-wise tallied information, which does not incur any significant computing burden. Through scoring the cycle-wise PKE corrected power, both the cycle-wise and PKE parameters-related uncertainties can be considered. The overall procedure is illustrated in Fig. 2, where a red-dashed box is additionally introduced to perform PK sampling.

It is worthwhile to articulate that the uncertainty of the cycle-averaged PKE parameter-based corrected power does not correspond to the sample variance from the cycle-wise PKE corrected power due to non-linearity of PKE calculation. Nevertheless, a reasonable estimation can be made if enough numbers of histories and cycles are involved due to the law of large numbers. For such a case, both the cycle-wise dynamic reactivity and cycle-wise PKE corrected power will follow a normal distribution.

Based on the aforementioned mathematical reasoning, a screening process is proposed to harness the PCQS-MC uncertainty from the cycle-wise PKE corrected power. Note that a non-linearity associated with solving PKE could incur bias in the corrected cycle-wise power. The Shapiro-Wilk normality test [7], which is a null-hypothesis testing, is implemented to systematically exclude the scored cycle-wise corrected power until the sample follows a normal distribution.

Screening Process

Step1) Check whether the given set of samples satisfies the Shapiro-Wilk test (Significance level: α)
Step2) If not, exclude the data out of $\mu_s \pm z_{\alpha/2}\sigma_s$ range, where μ_s and σ_s denote sample mean and standard deviation of the (screened) set of samples.
Step3) Check whether the screened set of samples satisfies Shapiro-Wilk test.
Step4) If not, iteration Step2 ~ 3 until Shapiro-Wilk test is satisfied or all the elements reside within the range of screening.

4. Numerical Results

To verify the applicability of the proposed PK sampling scheme for assessing the PCQS-MC calculation uncertainty, a two-dimensional C5G7-TD benchmark has been considered in this work. A null-transient with a time-step of 0.1 sec was performed with 150,000 histories / 100 inactive cycles / 100 active cycles, and 40 independent batch runs were considered to acquire the real variance.

Figure 3 depicts both the real variance and PK sampling-based uncertainty for a time duration of 1.0 sec where each error bar corresponds to the 1-sigma range. A significance level (α) of 0.05 with a $z_{\alpha/2}$ value of 1.96 was considered during the screening process. One could observe that extent of real and PK sampling-based uncertainties are consistent throughout the simulation, where the latter always underestimates the real variance due to the presence of cycle-wise correlation. Nevertheless, the null-transient result plainly attests to the effectiveness of the proposed scheme for deducing proper uncertainty for PCQS-MC transient calculation.

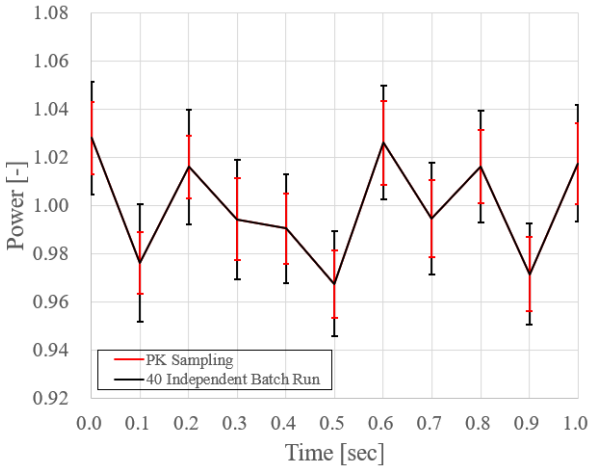

Figure 3. Null-transient result for C5G7-TD benchmark.

It is the screening process that guarantees the set of samples, i.e., cycle-wise PKE corrected power, to follow a normal distribution. Figures 4 and 5 illustrate the Q-Q (Quantile-to-Quantile) plot and the raw data that have been obtained at a time-step of 0.1 sec. The screened-out data are marked with a blue colour in Fig. 5, and the corresponding Q-Q plot visualizes that the set of samples follows a normal distribution. Identical result was obtained with different values of significance levels: α = 0.046 ($z_{\alpha/2}$ = 2.00) and α = 0.055 ($z_{\alpha/2}$ = 1.920), which are conventional values often applied for null-hypothesis testing.

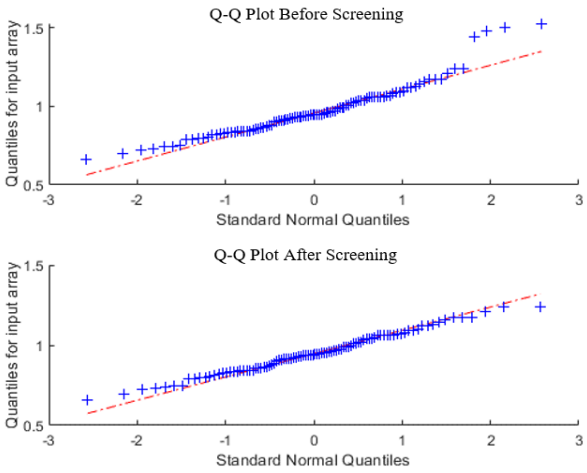

Figure 4. Q-Q plot before and after the screening.

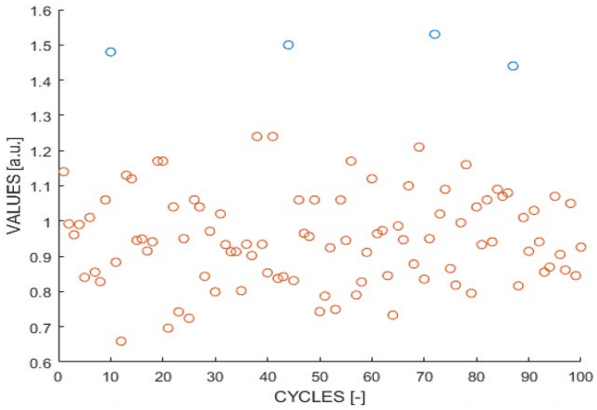

Figure 5. Set of cycle-wise PKE corrected power, where screened out data are marked with blue colour.

Using the proposed PK sampling method, the C5G7-TD2-5 transient benchmark problem was solved and the time-step-wise uncertainty of the PCQS-MC solution has been estimated. Such a problem involves the insertion and withdrawal of control rods. Figure 6 exhibits the calculated result where the PCQS-MC solution well resembles the reference MOC calculation, and the fluctuation is well confined within the estimated uncertainty (2-sigma range).

5. Summary and Conclusions

In this work, a new method for accurately estimating the uncertainty of PCQS-MC transient calculation result has been proposed, which is referred to as point-kinetics (PK) sampling method. It was verified that the uncertainty for the cycle-averaged PKE parameters, mainly dynamic reactivity, is the major contributor to the innate uncertainty of PCQS-MC calculation, which

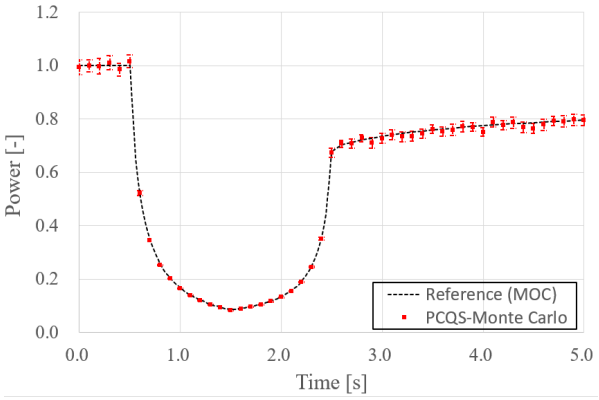

Figure 6. Solution of C5G7-TD2-5 benchmark.

cannot be accommodated through conventional cycle-wise error estimation. In contrast, by scoring the cycle-wise PKE corrected power, the PK sampling method can reflect such inherent uncertainty of the PCQS-MC framework. Note that the additional computing burden for performing cycle-wise PKE correction is marginal. From the transient simulation of the C5G7-TD benchmark, it was confirmed that PK sampling-based uncertainty well resembles the real variance.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea Grant funded by the Korean government NRF-2016R1A5A1013919

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