A Comparison of Time-Dependent Monte Carlo Frameworks: Predictor-Corrector Quasi-Static Method and Dynamic Simulation

HyeonTae Kim and Yonghee Kim*
Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology (KAIST),
291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea
**Corresponding author: yongheekim@kaist.ac.kr*

1. Introduction

From growing demand on the reactor transient analysis and by the aid of modern advanced computing resources, some of the most popular Monte Carlo-based nuclear reactor analysis codes are now trying to extend their capability to handle time-dependent problems. As the predictor-corrector quasi-static (PCQS) method had been successfully applied to reactor dynamics problems [1], McBOX [2], RMC [3], and other codes have adopted this scheme to solve the time-dependent neutron transport problem accurately regardless of time step size. Meanwhile, a major breakthrough on direct simulation of particle has been made by Sjenitzer and Hoogenboom [4], paving the way to another choice of methodology which referred to as dynamic simulation of Monte Carlo (DMC). This method is currently considered computationally expensive, but many major codes such as TRIPOLI-4 [5], SERPENT [6], RMC [7], McCARD [8], and others have reported their performances with the method.

Recently, the KAIST Monte Carlo code iMC has demonstrated its steady-state multi-physics analysis result on the centrally-shielded burnable absorber (CSBA) fuel, using a tetrahedral unstructured mesh-grid [9]. The CSBA fuel concept was suggested for suppressing excessive reactivity during the reactor operation to achieve soluble-boron-free operations [10], but it had been considered challenging in terms of fuel performance analysis due to its unusual 3-dimensional design. Since the fuel includes ball-shaped burnable poison inside the pellet, the simplified radial heat transfer model cannot be applied. The iMC multi-physics module can tally detailed intra-pellet power density distribution and calculate temperature, thermal expansion rate, and thermal stress distribution to provide accurate fuel performance analysis for such unconventional fuel geometry. Also, time-dependent multi-physics analysis is also underway with the iMC code.

This paper introduces a comparative study on the two mainstream approaches of the time-dependent Monte Carlo scheme, as we are implementing the multi-physics feature in the iMC code. The well-known C5G7-TD [11] problem was solved with the two strategies both using iMC, and results are discussed in terms of the computational time and memory usage. Some remarks on potential application for the time-dependent fuel performance analysis are made followed by the discussion.

2. Numerical Schemes of Interest

2.1 Predictor-corrector quasi-static method

The time-dependent neutron transport equation and the precursor concentration equation are the two governing equations of the time-dependent reactor analysis.

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

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

To solve the Eq. (1), we apply the implicit Euler method with a macro-step size of Δt. The discretized equation at time step t_s is,

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

with $T_{PCQS}\equiv\left(\sigma_t(\vec{r},E,t_s)+\frac{1}{v(E)\Delta t_s}\right)\psi(\vec{r},E,\vec{\Omega},t_s)$.

The PCQS method factorize the neutron angular flux into the amplitude function $n(t)$ and the shape function $\varphi(\vec{r},E,\vec{\Omega},t)$ as:

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

with the normalization condition of

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

The PCQS-MC solves the time-dependent fixed source problem in predictor and corrector steps. After the calculation of the predictor iteration, the point kinetics parameters are obtained. Based on the amplitude function from the point kinetics equation, the initial source for the corrector iteration is adjusted as follows:

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

where $Z(t_s)$ is a normalization factor defined to hold the normalization condition of the shape function.

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

2.2 Dynamic Monte Carlo

The DMC scheme for the time-dependent Monte Carlo simulation is well established and explained in Sjenitzer's previous study [4]. In this section, we list a few important features of the DMC which are essential to achieve a stable and reliable result. The DMC simulates the particle directly in the time-domain considering the flight time. The flight time of the particle is calculated by dividing the sampled distance with the particle's speed. When the cumulative flight time exceeds the time-step boundary, the particle is stored for the next time-step. To reduce the variance caused from particle generation branching during the simulation, the DMC adopted the branchless method which adjust particle weights instead of starting a new branch at a fission event.

One of the most important feature of the DMC method is the forced decay, as it reduces variance caused from the precursor uncertainty. In the forced decay strategy, each alive precursor produces a neutron in every time step, unlike a precursor produces neutron only once in reality. The weight of the emitted neutron from the forced decay (w_d) is adjusted as follows to prevent a biased result:

$$w_d = w_C \Delta t \sum_i f d_i \lambda_i e^{-\lambda_i (t-t_0)} \quad (8)$$

Meanwhile, the precursor weight (w_C) is also adjusted after each time step:

$$w_C' = w_C \frac{w_{surv}}{w_{n,av}} \quad \text{if } \xi < \frac{w_{n,av}}{w_{surv}}$$
$$w_C' = 0 \quad \text{else} \quad (9)$$

where,

$$w_{n,av} = \frac{w_C}{\Delta t} \int_{t_1}^{t_1+\Delta t} \Delta t \sum_i f d_i \lambda_i e^{-\lambda_i (t-t_0)} dt = w_C \sum_i f d_i \lambda_i e^{\lambda_i t_0} \left(e^{-\lambda_i t_1} - e^{-\lambda_i (t_1+\Delta t)} \right) \quad (10)$$

To control the population of particles to be simulated, the combing technique [12] is used. The combing technique preserves the total weight of the particle bank, but resample a limited number of particles based on their weight. The technique can be applied for both time sources and precursors to maintain reasonable computation time regardless of an external reactivity insertion.

3. Numerical Results

First, we solved a two-dimensional C5G7-TD0-5 benchmark problem based on DMC method and compared the result with the solution suggested in the benchmark specification document [11]. Figure 1 shows the geometry and the calculation results compared with the reference.

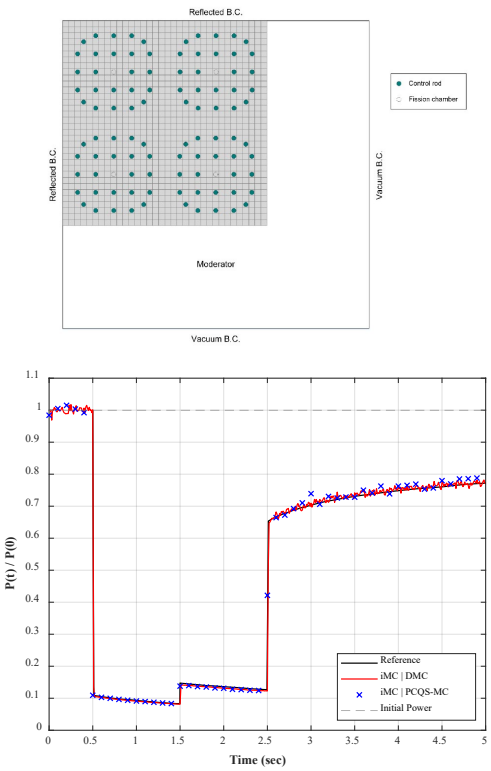

Figure 1. C5G7-TD problem geometry (top) and analysis results for C5G7-TD0-5 (bottom)

The above calculations were done on 224 parallel CPUs of an Intel Xeon E5-2697 machine with a clock

speed of 2.60 GHz using OpenMP/MPI hybrid parallelism. The calculation conditions are as described in Table I.

Table I. Calculation condition of Figure 1

	DMC	PCQS-MC
Histories per cycle	50,000	100,000
act. / inact. cycle	20 / 150	100 / 150
t_{total} / Δt	5 sec / 0.01 sec	5 sec / 0.1 sec

Since the two methods adopt different detailed numerical recipes to make them work, an 'apple to apple' comparison is impossible at the moment. Instead, we would like to compare particle simulation costs for different time step sizes. From this discussion, one may select a specific method over the other based on his problem condition of interest.

We simulated steady state calculation with DMC and PCQS-MC mode using different time step sizes, and compared particle's average collision number per cycle. One can notice that the collision number is linearly proportional to the particle transport simulation time. With this in mind, we compared the required collision number to simulate a given transient scenario with different time step sizes in both DMC and PCQS-MC. We simulated 10,000 histories per cycle for 10 active cycles with DMC, and 100,000 histories per cycle for 10 active cycles with PCQS-MC. The collision number described in Tables II and III are averaged collision number per particle being simulated, yet a comparison between the methods is meaningless as this is not an apple to apple comparison.

Table II. DMC steady-state simulation results

Δt (sec)	avg. col.	Computing time per cycle (sec)		
		Source set	Transport	MPI job
0.001	994	0.06	0.89	1.40
0.0025	2,419	0.06	2.03	1.77
0.01	9,713	0.05	7.89	2.74
0.025	24,535	0.06	18.7	4.01
0.1	100,382	0.06	57.7	7.38
0.25	259,911	0.06	173	16.5

Table III. PCQS-MC steady-state simulation results

Δt (sec)	avg. col.	Computing time per cycle (sec)		
		Source set	Transport	MPI job
0.001	62.5	0.28	1.51	9.82E-04
0.0025	63.1	0.30	1.54	7.29E-05
0.01	63.4	0.31	1.57	5.88E-05
0.025	63.5	0.29	1.56	8.11E-03
0.1	63.5	0.31	1.54	1.02E-02
0.25	63.5	0.30	1.56	1.22E-02

Based on the collision number trend against time step size, we suggest 'relative collision required per unit time' curves for the two transient Monte Carlo approaches. As one can notice from Figure 2, computational burden for DMC is almost constant regardless of the discretized time step size, while it became less time-consuming with coarser macro time step in PCQS-MC.

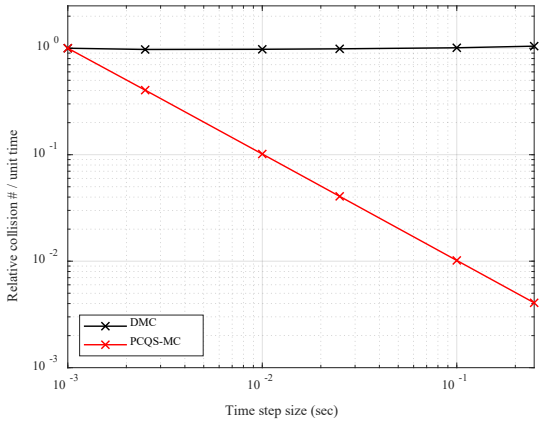

Figure 2. Relative computational burden curves of DMC and PCQS-MC verses time step size.

4. Summary and Remarks

In this study, we have presented time-dependent simulations based on two main stream numerical schemes that are implemented in the Monte Carlo reactor analysis code iMC. The validity and comparison of the methods were investigated through solving the C5G7-TD benchmark problem. In addition, we suggested computational burden of the two methods in terms of user-defined time discretization step size. From the numerical study, the DMC computational burden turns out to be rather constant regardless of the time step size, while it is inversely proportional to the time step size in the PCQS-MC scheme.

In subsequent studies, we will investigate and optimize the computational cost of the two methods in a more refined and systematic conditions considering source handling and cut-off optimization. Based on the extension and optimization, the iMC code will present time-dependent multi-physics platform for the analysis of complex fuel elements' performance studies.

ACKNOWLEDGEMENT

The National Research Foundation of Korea (NRF) Grant funded by the Korean Government (MSIP) (NRF-2016R1A5A1013919) supported this work.

REFERENCES

[1] S. Dulla, E. H. Mund, and P. Ravetto, "The quasi-static method revisited," *Prog. Nucl. Energy*, vol. 50, no. 8, pp. 908–920, 2008.
[2] Y. Jo, B. Cho, and N. Z. Cho, "Nuclear Reactor Transient Analysis by Continuous-Energy Monte Carlo Calculation Based on Predictor-Corrector

Quasi-Static Method," *Nucl. Sci. Eng.*, vol. 183, no. 2, pp. 229–246, Jun. 2016.
[3] X. Guo, X. Shang, J. Song, G. Shi, S. Huang, and K. Wang, "Kinetic methods in Monte Carlo code RMC and its implementation to C5G7-TD benchmark," *Ann. Nucl. Energy*, vol. 151, p. 107864, 2021.
[4] B. L. Sjenitzer and J. E. Hoogenboom, "Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations," *Nucl. Sci. Eng.*, vol. 175, no. 1, pp. 94–107, Sep. 2013.
[5] M. Faucher, D. Mancusi, and A. Zoia, "New kinetic simulation capabilities for Tripoli-4®: Methods and applications," *Ann. Nucl. Energy*, vol. 120, pp. 74–88, 2018.
[6] J. Leppänen, "Development of a dynamic simulation mode in Serpent 2 Monte Carlo code," *Proc. M&C*, pp. 5–9, 2013.
[7] J. Lijuna, S. Xiaotonga, G. Xiaoyua, and W. Kana, "Application of Direct Simulation Method for Neutron Space-Time Kinetics Based on RMC."
[8] N. Shaukat, M. Ryu, and H. J. Shim, "Dynamic Monte Carlo transient analysis for the Organization for Economic Co-operation and Development Nuclear Energy Agency (OECD/NEA) C5G7-TD benchmark," *Nucl. Eng. Technol.*, vol. 49, no. 5, pp. 920–927, 2017.
[9] H. Kim and Y. Kim, "Unstructured Mesh-Based Neutronics and Thermo-Mechanics Coupled Steady-State Analysis on Advanced Three-Dimensional Fuel Elements with Monte Carlo Code iMC," *Submitt. to Nucl. Sci. Eng.*
[10] X. H. Nguyen, C. Kim, and Y. Kim, "An advanced core design for a soluble-boron-free small modular reactor ATOM with centrally-shielded burnable absorber," *Nucl. Eng. Technol.*, vol. 51, no. 2, pp. 369–376, 2019.
[11] J. (Jia) Hou, K. N. Ivanov, V. F. Boyarinov, and P. A. Fomichenko, "OECD/NEA benchmark for time-dependent neutron transport calculations without spatial homogenization," *Nucl. Eng. Des.*, vol. 317, pp. 177–189, 2017.
[12] T. E. Booth, "A weight (charge) conserving importance-weighted comb for Monte Carlo," Los Alamos National Lab., NM (United States), 1996.
[13] S. H. Jang and H. J. Shim, "Monte Carlo Transient Analysis of C5G7-TD Benchmark 3D Problems Using McCARD," in *Transactions of the American Nuclear Society*, 2020, vol. 122.