Implementation of iDTMC Method for Predictor-Corrector Quasi-Static Monte-Carlo Calculation in the iMC code

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1. Introduction

Monte Carlo (MC) neutronics analysis is a precise reactor assessment method that directly simulates neutron behavior and computes reactor metrics without the need for assumptions. Unlike deterministic methods with energy and geometric assumptions, MC employs minimal approximations. However, it's computationally intensive, particularly for transients, despite improved computing power. Ongoing work focuses on optimization and acceleration to enhance efficiency.

Within the domain of MC-based transient reactor analysis, two notable approaches have gained prominence: the Dynamic Monte Carlo (DMC) and the Predictor-Corrector Quasi-Static Monte Carlo (PCQS-MC) methods. These approaches have been effectively incorporated and validated in various MC codes, including TRIPOLI-4 [1], McCARD [2], Serpent2 [3], and OpenMC [4] for DMC, as well as McBOX [5] and RMC [6] for PCQS-MC. A recent development at KAIST, known as the iMC code, offers support for both approaches, affording users the flexibility to select their preferred methodology [7].

A distinguishing feature of iMC is its integration of the Improved Deterministic Truncation of Monte Carlo (iDTMC) approach, which effectively couples the deterministic p-FMFD (partial current-based fine mesh finite difference) solution with the Monte Carlo approach [8-10]. Originally conceived and tested for steady-state calculations, the iDTMC scheme has demonstrated notable reductions in uncertainties and computational time when compared to the conventional Monte Carlo method. Additionally, recent implementations of iDTMC in depletion calculations have yielded promising outcomes [11].

This study extends the philosophy of the iDTMC method to transient MC calculations based on the PCQS-MC approach. Instead of tackling an eigenvalue problem, we solve a fixed source problem for transient simulations, with the MC-based p-FMFD solution employed to acquire kinetic parameters. The ensuing section outlines the overarching approach and presents preliminary results from the iDTMC-implemented PCQS-MC calculations.

2. Methodology

2.1 Improved Deterministic Truncation of Monte Carlo

The Improved Deterministic Truncation of Monte Carlo (iDTMC) method has been developed to enhance numerical performance and efficiency in nuclear reactor analyses [8-10]. This method employs a strategic approach, utilizing the assembly-wise coupled partial current-based coarse mesh finite difference (p-CMFD) method to accelerate the convergence of the fission source distribution during inactive cycles, while employing the pin-wise decoupled p-CMFD method to generate reactor solutions during active cycles. Figure 1 demonstrates the implementation of these methods.

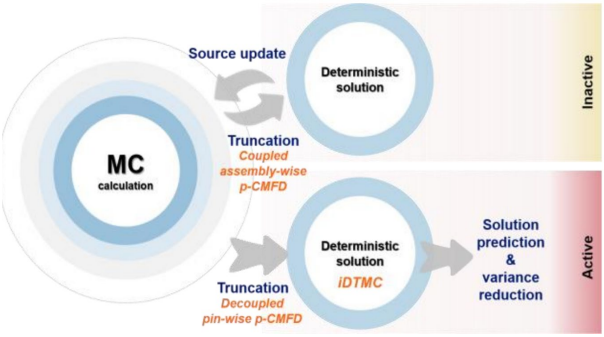


Fig 1. Visualization of the iDTMC method

2.2 *Predictor-Corrector Quasi Static-Monte Carlo*

The following set of equations mathematically represents transient behaviour of a reactor system:

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

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

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. Implementing implicit Euler method, linear variation of fission source term, and exponential transformation, the following transient fixed source problem (TFSP) is obtained.

$$\begin{aligned}&\left(L+\tilde{T}_{PCQS}-S\right)\psi(\vec{r},E,\vec{\Omega},t_s)\\ &=\frac{\psi(\vec{r},E,\vec{\Omega},t_{s-1})e^{\gamma_s\Delta t}}{v(E)\Delta t_s}+\sum_{d=1}^{G_d}\frac{\chi_d(E)}{4\pi}\lambda_d C_d(\vec{r},t_{s-1})f_{1,d}\\ &+\sum_{d=1}^{G_d}\frac{\chi_d(E)}{4\pi}\frac{\beta_d F\psi(\vec{r},E,\vec{\Omega},t_{s-1})}{k_0}f_{2,d}\\ &+\sum_{d=1}^{G_d}\frac{\chi_d(E)}{4\pi}\frac{\beta_d F\psi(\vec{r},E,\vec{\Omega},t_s)}{k_0}f_{3,d}\\ &+\frac{1}{k_0}\frac{\chi_p(E)}{4\pi}(1-\beta)F\psi(\vec{r},E,\vec{\Omega},t_s)=S_{PCQS}(\vec{r},E,\vec{\Omega},t_s),\end{aligned} \quad (3)$$

where

$$\begin{aligned}&\tilde{T}_{PCQS}\psi(\vec{r},E,\vec{\Omega},t_s)\\&=\left(\sigma_t(\vec{r},E,t_s)+\frac{1}{v(E)\Delta t_s}+\frac{\gamma_s}{v(E)}\right)\psi(\vec{r},E,\vec{\Omega},t_s).\end{aligned}\tag{4}$$

The angular flux is updated based on Eq. (3) alongside tallying of point-kinetics (PK) parameters. It is noteworthy that the calculation of the PK equation ultimately determines the power of the reactor system, which is formulated by factorizing the angular flux into an amplitude function, denoted as n(t), and a shape function as:

$$\psi(\vec{r},E,\vec{\Omega},t)=n(t)\,\varphi(\vec{r},E,\vec{\Omega},t),\tag{5}$$

To render such a factorization to be unique, an additional equation is imposed.

$$\begin{aligned}&\int dV\int d\vec{\Omega}\int dE\; W(\vec{r},E,\vec{\Omega})\frac{\varphi(\vec{r},E,\vec{\Omega},t)}{v(E)}\\&=\int dV\int d\vec{\Omega}\int dE\; W(\vec{r},E,\vec{\Omega})\frac{\psi(\vec{r},E,\vec{\Omega},t_0)}{v(E)},\end{aligned}\tag{6}$$

where $W(\vec{r},E,\vec{\Omega})$ denotes a weighting function. Substituting Eqs. (5) and (6) into Eqs (1) and (2), the PK equation can be acquired.

$$\begin{aligned}\frac{dn(t)}{dt}&=\left(\frac{\rho(t)-\beta(t)}{\Lambda(t)}\right)n(t)+\sum_{d=1}^{G_d}\lambda_d c_d(t),\\\frac{dc_d(t)}{dt}&=-\lambda_d c_d(t)+\frac{\beta_d(t)}{\Lambda(t)}n(t).\end{aligned}\tag{7}$$

- Dynamic Reactivity $\rho(t)$

$$\rho(t)=1-\frac{k_0}{k(t)}\tag{8}$$

$$k(t)=\frac{\left\langle W(\vec{r},E,\vec{\Omega}),\frac{\chi(E)}{4\pi}F\varphi(\vec{r},E,\vec{\Omega},t)\right\rangle}{\left\langle W(\vec{r},E,\vec{\Omega}),(L+T-S)\varphi(\vec{r},E,\vec{\Omega},t)\right\rangle}\tag{9}$$

- Delayed Neutron Fraction $\beta(t)$

$$\beta(t)=\sum_{d=1}^{G_d}\beta_d(t)\tag{10}$$

$$\beta_d(t)=\frac{\left\langle W(\vec{r},E,\vec{\Omega}),\frac{\chi_d(E)}{4\pi}\beta_d F\varphi(\vec{r},E,\vec{\Omega},t)\right\rangle}{\left\langle W(\vec{r},E,\vec{\Omega}),\frac{\chi(E)}{4\pi}F\varphi(\vec{r},E,\vec{\Omega},t)\right\rangle}\tag{11}$$

- Generation time $\Lambda(t)$

$$\Lambda(t)=\frac{\left\langle W(\vec{r},E,\vec{\Omega}),\frac{1}{v(E)}\varphi(\vec{r},E,\vec{\Omega},t)\right\rangle}{\left\langle W(\vec{r},E,\vec{\Omega}),\frac{1}{k_0}\frac{\chi(E)}{4\pi}F\varphi(\vec{r},E,\vec{\Omega},t)\right\rangle}\tag{12}$$

The bracket denotes integration over the whole phase space. Note that a unit vector has been generally considered for the weighing function in this work, i.e., $W(\vec{r},E,\vec{\Omega})\rightarrow 1.0$.

2.3 *iDTMC-implemented PCQS-MC*

To invoke the iDTMC calculation for PCQS-MC simulation, the governing equation should be formulated in the form of one-group diffusion-like neutron balance equation. Accordingly, the TFSP, i.e., Eq. (3), is re-written in the following manner:

$$\sum_{s,n=i,j,k}\frac{A_s}{V_{i,j,k}}(J_{s1}-J_{s0})+\Sigma_a^{i,j,k}\phi_{i,j,k}=S_{i,j,k}^{PCQS},\tag{13}$$

where V is the node volume, A is the surface area, s is the surface index, ϕ and J are the flux and current, respectively, Σ is the cross section, and S^{PCQS} is the fixed source. The CMFD parameters are calculated from the MC simulation, and the surface currents can be preserved by the correction factors.

$$J_{s1}^{+}=\mp\frac{1}{2}\widetilde{D}_{s1}(\phi_{n+1}-\phi_n)+\widehat{D}_{s1}^{\pm}\phi_{n+1/2\mp1/2},\tag{14}$$

where $\widehat{D}_{s1}^{\pm}$ is the correction factor.

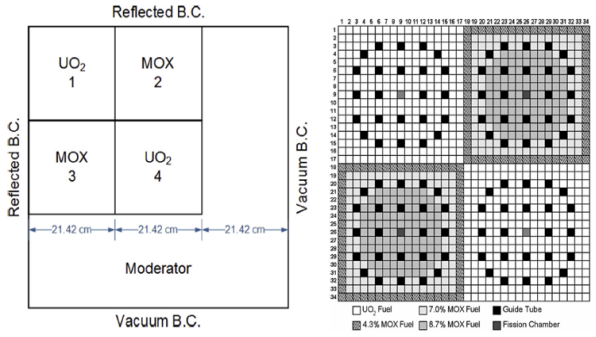
$$\widehat{D}_{s1}^{\pm}=\frac{J_{s1}^{+,MC}+0.5\cdot\widetilde{D}_{s1}(\phi_{n+1}^{MC}-\phi_n^{MC})}{\phi_n^{MC}}.\tag{15}$$

Unlike the steady-state MC calculation, where the magnitude of the fission source is preserved for every cycle, the TFSP for PCQS-MC updates t_s source term for each cycle. To accommodate such a difference, whilst solving the FMFD equation for TFSP using accumulated fine-mesh information, partial currents from each cycle was aptly scaled in its magnitude to retain identical source strength. After obtaining distribution of the pin-wise shape function, the dynamic reactivity and the correction factor that satisfy Eq. (6) can be determined from the very early initial active cycles. Note that for the iDTMC-implemented PCQS-MC calculations, the estimation of the denominator in Eq. (9) is acquired as follows.

$$\begin{aligned}&<\left(L+T-S\right)\psi(\vec{r},E,\vec{\Omega},t_s)>\\&=<S_{PCQS}(\vec{r},E,\vec{\Omega},t_s)>\\&-<\left(\frac{1}{v(E)\Delta t}+\frac{\gamma_s}{v(E)}\right)\psi(\vec{r},E,\vec{\Omega},t_s)>.\end{aligned}\tag{16}$$

3. Numerical Results

To assess the feasibility of the proposed iDTMC-implemented PCQS-MC approach, the C5G7-TD benchmark problem which involves the movement of control rods in a 2D geometry has been considered. The problem inherits the 2D geometry configuration and few-group cross-sections of the C5G7 benchmark. The overall geometry of the benchmark is shown in Fig. 2, where each fuel assembly has a 17×17 configuration that consists of 264 fuel cells, 24 guide tube cells, and a single fission chamber cell at the center. A more detailed description can be found elsewhere [12].



(a) 2-D Core Map of C5G7-TD (b) 2-D Core Pin-wise Configuration

Fig 2. Problem layout for C5G7-TD problem (2D)

Control rod movements for two different types of C5G7-TD benchmarks that have been considered are as follows:

C5G7-TD0-5

$$\begin{aligned} \Sigma_x(t) &= \Sigma_x^{GT}, && t<0 \text{ and } t\geq 2s \\ \Sigma_x(t) &= \Sigma_x^{GT} + 0.1(\Sigma_x^{CR} - \Sigma_x^{GT}), && 0<t\leq 1s \\ \Sigma_x(t) &= \Sigma_x^{GT} + 0.05(\Sigma_x^{CR} - \Sigma_x^{GT}), && 1s<t\leq 2s \end{aligned} \quad (17)$$

C5G7-TD1-5

$$\begin{aligned} \Sigma_x(t) &= \Sigma_x^{GT}, && t<0 \text{ and } t\geq 2s \\ \Sigma_x(t) &= \Sigma_x^{GT} + 0.01(\Sigma_x^{CR} - \Sigma_x^{GT})t, && 0<t\leq 1s \\ \Sigma_x(t) &= \Sigma_x^{GT} + 0.01(\Sigma_x^{CR} - \Sigma_x^{GT})(2-t), && 1s<t\leq 2s \end{aligned} \quad (18)$$

where Σ_x^{GT} and Σ_x^{CR} are macroscopic cross-sections for the empty guide thimble and control rod loaded guide thimble respectively

For both the PCQS-MC calculations conducted without and with iDTMC implementation, a time-step of 0.1 sec, 150 inactive cycles, and 300,000 histories per cycle were simulated, and pCMFD-based acceleration during the inactive cycles are applied. The primary point of differentiation between the two scenarios lies in the number of active cycles. Specifically, the conventional PCQS-MC calculation utilized 250 active cycles, while the iDTMC-incorporated case featured a reduced count of 10 active cycles. For comparative purposes, the research also includes deterministic transport solutions based on the Method of Characteristics (MOC) [13] and stochastic transport solutions using the DMC approach, alongside the PCQS-MC calculation results.

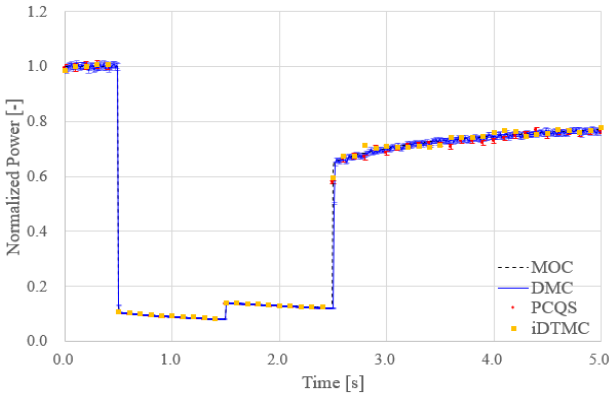


Fig 3. Calculated evolution of reactor power for C5G7-TD0-5 problem

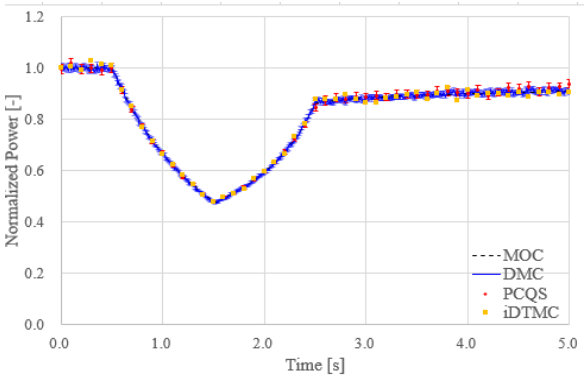


Fig 4. Calculated evolution of reactor power for C5G7-TD1-5 problem

The time-dependent evolution of reactor power for both scenarios is visually represented in Figs. 3 and 4. A brief 0.5-second transient period with no perturbations was incorporated before introducing the perturbation. The Monte Carlo (MC)-based results, including the application of iDTMC in the PCQS-MC method with only 10 active cycles, exhibit a remarkable consistency across all cases. It's noteworthy to mention that the computational burden is significantly alleviated with the implementation of iDTMC, reducing the number of active cycles from 250 to 10.

Table 1 provides a comparative analysis of the overall computational time for each problem, with particle tracking distributed across 440 parallel CPUs of an Intel® Xeon® Gold 6148 @ 2.40 GHz machine utilizing MPI/OpenMP hybrid parallelism. It's essential to mention that while the uncertainty assessment for the conventional PCQS-MC employed the PK-sampling method [14], the uncertainty evaluation for the iDTMC-implemented PCQS-MC is currently pending. It's important to note that the DMC calculation, which serves as a basis for comparison, necessitated a significantly greater amount of computational time compared to the PCQS-MC approach presented here.

Table 1. Computing time for C5G7 benchmarks

C5G7-TD0-5	
Case	Time [min]
PCQS-MC (w/o iDTMC)	1616.28
PCQS-MC (w/ iDTMC)	660.72
C5G7-TD1-5	
Case	Time [min]
PCQS-MC (w/o iDTMC)	1640.80
PCQS-MC (w/ iDTMC)	677.96

*Computing burden for DMC calculation not shown in the table (significantly heavier than the other approaches)

4. Conclusions

In this research, we delve into the integration of the Improved Deterministic Truncation of Monte Carlo (iDTMC) method into the context of PCQS-MC. The Time-Dependent Fission Source Problem (TFSP) inherent to PCQS-MC has been reformulated into a diffusion-like equation (FMFD). This reformulation allows us to derive solutions that accurately capture the dynamic reactivity of the system. Given that the TFSP adjusts the source term's strength in each cycle, we appropriately adjusted the accumulated current information's magnitude while solving the FMFD equation to achieve the iDTMC solution.

To gauge the effectiveness of our approach, we applied it to solve two distinct C5G7 benchmarks (TD0-5 and TD1-5). These benchmarks served as demonstrations that the iDTMC-implemented PCQS-MC method offers a reliable means of estimating power evolution while substantially reducing the computational workload compared to the conventional PCQS-MC approach. Our forthcoming research endeavors will be concentrated on evaluating the associated uncertainties in these calculations, thus furnishing more concrete figure-of-merit (FOM) metrics for comparative performance assessment.

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