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The iDTMC Method for SFR Neutronics Analysis in the iMC Monte Carlo Code

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1. Introduction

The improved deterministic truncation of Monte Carlo, or iDTMC, methodology is a means of reactor neutronics analysis that combines deterministic and stochastic methods of reactor analysis. Prior work has demonstrated its ability to generate high-fidelity solutions at a modest computational cost for conventional pressurized water reactors.

Sodium-cooled fast reactors, or SFRs, are an emerging Generation IV reactor concept. It is characterized by the use of liquid sodium as the primary coolant, which allows the reactor core to be designed in a hexagonal lattice geometry with significantly lower coolant volume fractions than comparable pressurized water reactors.

The iDTMC methodology has been adapted to the analysis of reactors with a hexagonal lattice geometry, such as SFRs, and implemented in the iMC code. The iMC code is a Monte Carlo neutronics analysis code developed in-house at KAIST. This implementation was then tested on the analysis of a simplified SFR problem and its results are presented in this study.

2. Background

In this section, the principles of the iDTMC methodology are explained and its algorithm is briefly summarized.

2.1 Overview of the iDTMC Methodology

The iDTMC methodology is a technique of truncating the active cycles of the Monte Carlo neutronics analysis of a reactor by coupling the Monte Carlo calculations with a deterministic solution [1].

In iterative deterministic methods for the analyses of reactors, the iteration proceeds until the fission source distribution is considered to be sufficiently converged. The desired reactor parameters are then immediately obtained. Therefore, it may be concluded that the converged fission source contains enough information to calculate the reactor parameters.

For a conventional Monte Carlo analysis, however, the attainment of convergence for the fission source alone, following a predetermined number of inactive cycles, does not generate any useful result. The desired reactor parameters must be tallied afterwards, which implies that additional transport processes, i.e., active cycles, are necessary after the convergence of the fission source.

The key insight of the iDTMC methodology is that when the inactive cycles of the Monte Carlo simulation conclude and the fission source is sufficiently converged, the Monte Carlo results at that point already contain enough information to produce a reactor solution. The iDTMC methodology thus seeks to avoid the need to conduct a large number of active cycles by using the results of the Monte Carlo simulations with relatively few active cycles to correct a deterministic solution. It thereby obtains a solution with the accuracy of a conventional Monte Carlo solution at a significantly reduced computing cost.

The iDTMC methodology involves the mesh discretization of the reactor core geometry, where Monte Carlo-based one-group homogenized cross sections and partial current information are tallied during the active and later inactive cycles of the Monte Carlo simulations.

During inactive cycles, the tallied factors from each cycle are used to calculate partial current coarse mesh finite difference, or pCMFD, solutions. These solutions are then used to adjust the fission source weights in the Monte Carlo simulations to accelerate the source convergence process and thereby reduce the number of inactive cycles necessary to reach sufficient source convergence.

During active cycles, these tallied and cycle-accumulated factors are used to calculate partial-current fine mesh finite difference, or pFMFD, subspace solutions. These subspace solutions contain the neutron multiplication factor of the reactor and the pin-wise power distribution, which are the information of greatest interest in the neutronics analysis of nuclear reactors. It is these pFMFD solutions that are the final output of the iDTMC algorithm.

This general structure of the iDTMC methodology is depicted in Figure 1.

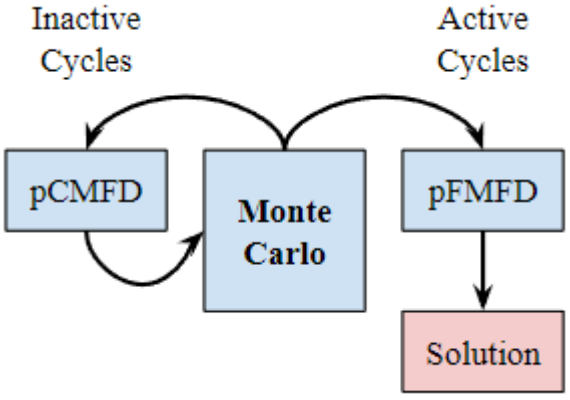

Fig. 1. The structure of information flow between the different components of the iDTMC methodology.

2.2 pCMFD Acceleration

The pCMFD method is a well-established [2] means of accelerating the convergence of the fission source during the inactive cycles of a Monte Carlo neutronics simulation. In the pCMFD method, reference partial currents are tallied from a higher-order Monte Carlo solution. These tallied partial currents are then used to adjust a lower-order finite difference method, or FDM, based deterministic solution. This deterministic solution is then used to adjust the fission source distribution for the next cycle in the Monte Carlo simulation.

The pCMFD method spatially discretizes the reactor into nodes, i.e., mesh description, then applies the neutron balance equation in each node as presented in Eq. 1. i is the index of a given cell, V_i is its volume, j is the indices of its neighboring cells, J_{ij} is the partial current outbound from cell i to cell j across their shared surface, A_{ij} is the area of that shared surface, and the notations are otherwise conventional.

$$\sum_j \frac{A_{ij}}{V_i}\left(J_{ij} - J_{ji}\right) + \Sigma_{a,i}\phi_i = \frac{1}{k_{eff}}\nu_i\Sigma_{f,i}\phi_i \qquad (1)$$

The partial currents are expressed as below.

$$J_{if} = \widetilde{D_{ij}}\left(\phi_i - \phi_j\right) + \widehat{D_{ij}}\left(\phi_i + \phi_j\right) \qquad (2)$$

$\widetilde{D_{ij}}$ is the interface diffusion constant between the two neighboring cells, defined as below.

$$\widetilde{D_{ij}} = \frac{1}{\Delta_{ij}} \cdot \frac{2D_iD_j}{D_i+D_j} \qquad (3)$$

$\widehat{D_{ij}}$ is the interface correction factor. The interface correction factors are chosen so that the partial currents calculated by Eq. 2 match the reference partial currents tallied in the Monte Carlo simulations.

Choosing the interface correction factors and then substituting the equations for partial currents into Equation 1 for each cell produces a system of linear equations with the cell fluxes and the neutron multiplication factor as the unknowns, which may be presented as an eigenvalue problem as below.

$$\boldsymbol{M}\vec{\phi} = \frac{1}{k_{eff}}\boldsymbol{F}\vec{\phi} \qquad (4)$$

Here $\boldsymbol{M}$ is the diffusion matrix, $\boldsymbol{F}$ is the fission matrix, $\vec{\phi}$ is a vector of cell-averaged one-group fluxes, and k is the neutron multiplication coefficient. Since J_{ij} only has a nonzero value if cells i and j are adjacent and a hexagonal prism has eight neighbors, with an appropriate indexing scheme $\boldsymbol{M}$ is a sparse 9-diagonal matrix and $\boldsymbol{F}$ is a single-diagonal matrix.

This eigenvalue problem may be solved by iterating between calculating the flux distribution $\vec{\phi}$ that will satisfy $\boldsymbol{M}\vec{\phi} = \vec{S}$ for a given source distribution $\vec{S}$ and updating the source distribution as $\vec{S} = \boldsymbol{F}\vec{\phi}$ with normalization. This source iteration continues until the source distribution converges sufficiently.

Finally, the Monte Carlo fission source distribution is updated. A multiplication factor is calculated for each cell. This uses the pCMFD source strength $S_{CMFD,i}$ which is simply the ith element of the $\vec{S}$ vector calculated previously, and the Monte Carlo source strength $S_{MC,i}$ which is the sum of the weights of the fission sources tallied within the volume of cell i in the previous cycle.

$$f_i = \left(\frac{S_{CMFD,i}}{\sum_i S_{CMFD,i}}\right) \div \left(\frac{S_{MC,i}}{\sum_i S_{MC,i}}\right) \qquad (5)$$

The Monte Carlo fission source distribution is updated by multiplying the weights of all tallied fission sources in each cell by the multiplication factor for that cell. This ensures that the share of the total Monte Carlo fission source represented by any given cell matches the value predicted by the pCMFD results.

The implementation of pCMFD acceleration in the iMC code uses each fuel assembly or equivalent as coarse mesh cells.

2.3 pFMFD Truncation

The pFMFD, method is mathematically identical to the pCMFD method in how partial currents tallied from a higher-order Monte Carlo solution is used to correct a lower-order, FDM-based deterministic solution. However, the pFMFD method used in the iDTMC methodology is different from the pCMFD method in several key respects.

First, as the name implies, the pFMFD method uses a finer mesh. Whereas in each cell represents a fuel assembly in the pCMFD method, in the pFMFD method each cell represents one fuel pin. Second, whereas the pCMFD method is used to accelerate the inactive cycles of the Monte Carlo simulations, the results of the pFMFD method in the active cycles are not fed back into the Monte Carlo simulations. The pFMFD subspace solution is instead used directly as an estimator for the neutron multiplication factor and the pin-wise power distribution. Finally, in order to alleviate the higher stochastic uncertainties of tallied factors caused by the smaller volume and surface area of fine-mesh cells, the pFMFD method uses cycle accumulation on its input factors.

Several factors are tallied from the Monte Carlo simulations and used in the pFMFD deterministic calculations, such as the cell-wise homogenized and group-condensed cross-sections, the partial currents across each cell surface, or the single-group cell-wise neutron flux. If $x_{c'}$ is one such factor calculated using the Monte Carlo results of cycle number c', then the actual factor used in the pFMFD calculations is an average, $\bar{x}$, calculated as below.

$$\bar{x} = \frac{1}{cc-c}\sum_{c'=c+1}^{cc} x_{c'} \qquad (6)$$

Here c is the number of skip cycles excluded from the cycle accumulation process and cc is the number of the latest Monte Carlo cycle.

3. SFR Analysis

The iDTMC methodology was adapted to the analysis of SFRs, sodium-cooled fast reactors, with a hexagonal geometry and then implemented on the iMC Monte Carlo neutronics analysis code [3, 4]. This adapted algorithm was then applied to an axially simplified model problem adapted from the NEA MOX-1000 benchmark [5] and its results were compared to those of a standard Monte Carlo analysis to verify the accuracy of the iDTMC methodology.

3.1 Simplified Reactor Problem

MOX-1000 is a benchmark model of a SFR. It has an active core consisting of 180 fuel assemblies, radially divided into three enrichment zones, interspaced with 19 control assemblies. There is a radial reflector, consisting of 114 reflector assemblies, surrounding this active core and 66 shield assemblies beyond that. The radial arrangement of assemblies in the MOX-1000 model is summarized in Fig. 2.

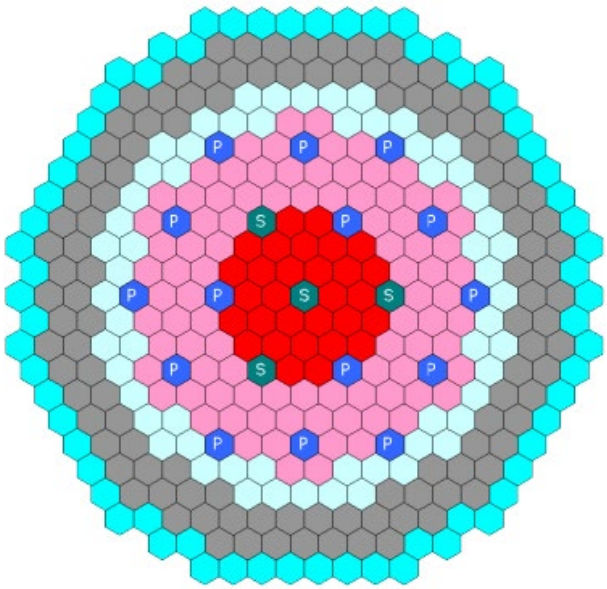

Fig. 2. The radial arrangement of assemblies within the MOX-1000 benchmark SFR model [5]. The assemblies labelled 'P' and 'S' represent the primary and secondary control assemblies, the red, pink, and pastel blue assemblies in the central region are the fuel assemblies, and the grey and sky blue near the edges represent the radial reflector and shielding respectively.

The original MOX-1000 benchmark problem is a fully three-dimensional model. The active core is bounded below by a reflector region and above by a gas plenum. Because the benchmark uses equilibrium cycle fuel compositions, the burnup of the fuel varies axially even under the beginning-of-cycle, or BOC, conditions.

For the purposes of this analysis, the model was simplified. All structural and reflective elements above and below the active core were removed and vacuum boundary conditions were imposed directly on the axial boundaries of the active core. Axial variations in burnup were also ignored and fuel compositions given for the central plane were used for the entire axial height of the active core.

3.2 Simulation Parameters

For both the iDTMC and the standard Monte Carlo analyses, 100 inactive cycles and 50 active cycles of Monte Carlo simulations were done with 1 million histories per cycle.

For the iDTMC method, 25 skip cycles were excluded from cycle accumulation. Radially, coarse mesh cells and fine mesh cells were defined to represent assemblies and fuel pins respectively. Control assemblies with no fuel pins were nonetheless also divided into fine mesh cells of the same size. Axially, the height of the reactor was represented by a single mesh node. The pCMFD and pFMFD calculations only included the active core, including the fuel assemblies and the primary and secondary control assemblies. The effect of the radial reflector was modelled by using the net current directly in Eq. 1 instead of considering it as a difference between the opposing partial currents across radial boundary surfaces of the active core.

3.3 Results

The pin-wise power distribution calculated by the iDTMC methodology is presented in the figure below.

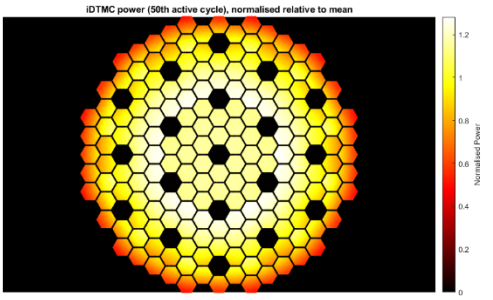

Fig. 3. The normalized pin-wise power distribution in the axially simplified model problem, calculated using the iDTMC methodology after the 50th active cycle.

The corresponding figure for the standard Monte Carlo power distribution is omitted, as it is not visually distinct from Fig. 3. Instead, the relative difference between the iDTMC and the standard Monte Carlo power distributions has been plotted in Figure 4.

Over the 50 active cycles calculated, the neutron multiplication factor calculated by the iDTMC

methodology changed from 0.977119 in the first active cycle to 0.977144 in the final active cycle, a change of 2.5 pcm. The final Monte Carlo estimate was 0.977177, with an apparent stochastic uncertainty amounting to a standard deviation of 6.4 pcm. The convergence of the neutron multiplication factor of the two methodologies is compared in Fig. 5.

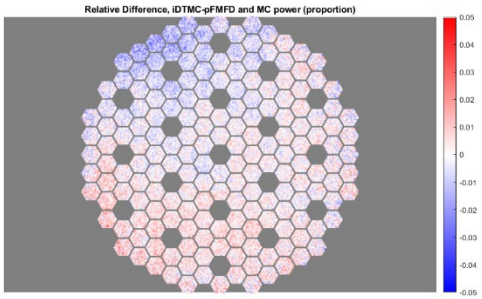

Fig. 4. The difference between the standard Monte Carlo and iDTMC pin-wise power distributions as a proportion of the standard Monte Carlo power.

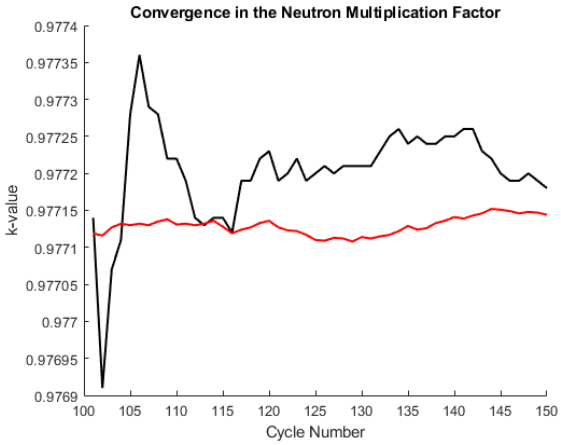

Fig. 5. The neutron multiplication factors calculated using the standard Monte Carlo and the iDTMC methodologies after each active cycle in their respective simulations.

The computing time of the Monte Carlo simulation was typically 60~70 seconds per cycle. To this, the pFMFD deterministic calculations added another 50~60 seconds per cycle.

4. Conclusions

The discrepancy between the neutron multiplication factors calculated using the standard Monte Carlo method and the iDTMC method was 3.3 pcm. Given that the apparent stochastic uncertainty of the standard Monte Carlo solution has a standard deviation of 6.4 pcm and the real uncertainty is likely to be higher, it may be asserted that the two values agree with each other.

The discrepancy in the pin-wise power distribution between the iDTMC and standard Monte Carlo methodologies may also be attributed to the stochastic uncertainty in the Monte Carlo results. It may be concluded that the iDTMC methodology implemented on the iMC code succeeds in replicating the results of the standard Monte Carlo method within stochastic uncertainties.

The value of the iDTMC methodology is clearly evident in the consistency of the calculated neutron multiplication factor across active cycles. Whereas the neutron multiplication factor calculated by the standard Monte Carlo method fluctuates heavily and converges slowly across a large number of active cycles, the iDTMC methodology produces a precise estimate from the first active cycle.

These results clearly demonstrate that the advantage of the iDTMC methodology, which is its ability to produce precise solutions from early active cycles, also applies to the analysis of SFRs. While the pFMFD calculations themselves add considerably to the computing time of each active cycle of the iDTMC methodology, in real use cases this will be more than compensated for by requiring fewer active cycles than a standard Monte Carlo solution of comparable precision.

Future work will include properly estimating the relative precision of the standard Monte Carlo and iDTMC methodologies to evaluate the scale of this improvement. The accuracy and precision of the iDTMC methodology must also be demonstrated for full-core reference problems without model simplifications.

Beyond that point, other features added to the iDTMC methodology for the analysis of conventional pressurized water reactors, such as depletion calculations and real variance estimation through hypercube sampling, may also be extended to the analysis of SFRs.

ACKNOWLEDGEMENTS

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