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Uncertainty Estimation by Correlated Sampling for the iDTMC Analysis of Sodium-Cooled Fast Reactors

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1. Introduction

As part of the recent attention on next-generation reactor concepts, significant efforts are being dedicated to the development of sodium-cooled fast reactor, or SFR, designs. This has created an interest in methods to conduct neutronics analyses on such reactor designs accurately, precisely, and cheaply.

There are two broad approaches to reactor neutronics analysis: deterministic methodologies and stochastic methodologies. Deterministic methodologies, however, require homogenisation and group condensation that may introduce inaccuracies, especially for SFRs which have no asymptotic neutron spectrum. Stochastic methodologies, on the other hand, require the simulation of a large number of particles and thus has a high computing cost. The iDTMC methodology, combining deterministic and stochastic methodologies to solve reactor problems with the accuracy of Monte Carlo at a significantly reduced computing cost, has been implemented on both conventional light water reactors [1] and sodium-cooled fast reactors [2].

Because the iDTMC methodology incorporates a stochastic element, iDTMC solutions have stochastic uncertainty and it is important to know the magnitude of this uncertainty. Because of the strong cycle-wise correlation in the iDTMC solution, apparent uncertainty is not useful as an estimator for the true stochastic uncertainty of the iDTMC solution. The correlated sampling method, which relies on the sampling of pFMFD factors, has been developed to assess the stochastic uncertainty of iDTMC solutions [3].

The present study seeks to extend the correlated sampling method to assess the uncertainty of the iDTMC solution for SFR problems and test the accuracy of the uncertainty estimated through the correlated sampling method.

2. Methodology

The iDTMC methodology [1] solves reactor neutronics problems by coupling a stochastic solution scheme with a deterministic solution scheme. Because it has a strong cycle-wise correlation, its apparent uncertainty is not a good estimator for its real stochastic uncertainty. Thus, a method was developed to estimate the uncertainty of the iDTMC solution through the correlated sampling of some pFMFD factors.

2.1 pCMFD Methodology

The coarse mesh finite difference, or CMFD, methodology is a scheme for the non-linear acceleration of convergence for reactor problems. It subdivides the reactor problem into coarse mesh, assembly-sized, nodes, uses cross-sections and currents from a higher-order solution to generate a numerical, deterministic solution to the reactor problem, and then uses it to adjust the neutron source distribution in the higher-order solution.

In the partial-current CMFD, or pCMFD, scheme, a simple finite difference formulation for a diffusion-like 1-group scheme is used. The neutron balance equation for a given node i with neighbours j is given below.

$$(1)\ \sum_{j=1}^{N_j}\left[\frac{A_{ij}}{V_i}\left\{\widehat{D_{ij}}(\phi_i-\phi_j)+(\widehat{D_{ij}}-\widehat{D_{ji}})(\phi_i+\phi_j)\right\}\right] +\Sigma_{a,i}\phi_i=\frac{1}{k_{eff}}\nu\Sigma_{f,i}\phi_i$$

The correction factors $\widehat{D}$ are set such that the first term of the above equation matches the net current across each node surface in the higher-order solution. In the iDTMC methodology, this is current tallied from the Monte Carlo simulations. The absorption and fission cross sections used are flux- and volume-weighted cross sections. This preserves the reaction rates of the higher-order solution. Note that SFRs commonly have a hexagonal pin and assembly geometry, and thus the width of a node cannot substitute for the ratio between the area of a node surface and the node volume.

The pCMFD calculation is only performed for the active core region, with any reflectors and other elements outside the active core being abstracted with a boundary condition. At node surfaces corresponding to the active core boundary, the following boundary condition is used instead of the normal expression for current. The boundary condition factor, also expressed $\widehat{D_{ij}}$, is such that the pCMFD leakage matches the leakage of the higher-order solution.

$$(2)\ J_{net}=\widehat{D_{ij}}\phi_i$$

Determining the correction factors and boundary condition factors for all nodes and constructing the neutron balance equations produces a system of

equations which is equivalent to the reactor eigenvalue problem.

$$(3)\quad \boldsymbol{M}\vec{\phi} = \frac{1}{k_{eff}}\boldsymbol{F}\vec{\phi}$$

This system of equations can then be solved by the usual iterative methods, with the iDTMC methodology using the biconjugate gradient stabilised method, and the neutron source weights for the next cycle of the Monte Carlo calculations can be adjusted as follows.

$$(4)\quad w'_i = w_{MC} \cdot \frac{w_{node,CMFD}}{\sum_{node} w_{i,MC}}$$

2.2 iDTMC Methodology

The improved deterministic truncation of Monte Carlo, or iDTMC, methodology is based on the observation that a deterministic pCMFD solution can not only be used to accelerate the neutron source convergence in the inactive cycles of a Monte Carlo simulation but can also be used directly as the final subspace solution generated by the calculations during the active cycles. This allows a subspace solution with the fidelity of the Monte Carlo method to be generated at very early active cycles, avoiding the cost of simulating many active cycles to tally the quantities of interest.

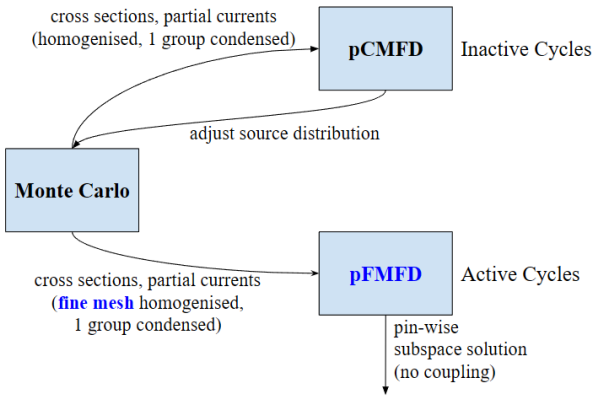

Fig. 1. Structure of the iDTMC methodology

In the iDTMC methodology, the pCMFD method is coupled with the inactive cycles of the Monte Carlo simulations to accelerate the convergence of the fission source distribution. In the active cycles, cross sections and partial currents tallied across the active cycles and the later inactive cycles of the Monte Carlo simulations are used to generate deterministic pFMFD subspace solutions, which are not coupled with the Monte Carlo simulations but are instead taken as the final reactor solution of the methodology. This structure is illustrated in figure 1.

The hexagonal pin and assembly geometry typical of SFRs means that when dividing the active core into pin-sized nodes for fine mesh tallying and the pFMFD calculations, irregular pentagonal nodes at the radial surfaces of assemblies are necessary. A top-down view of the radial division of the reactor core into coarse and fine mesh nodes is provided in figure 2.

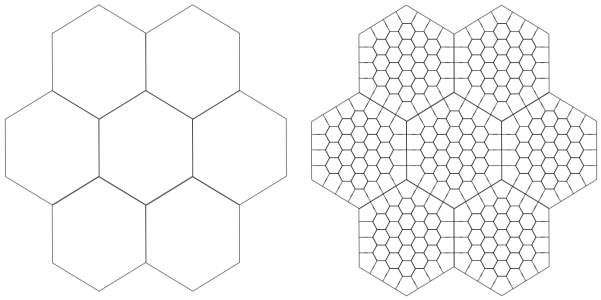

Fig. 2. Division of the core into coarse and fine mesh nodes

2.3 pFMFD Methodology

The partial-current fine mesh finite difference, or pFMFD, methodology used in the iDTMC methodology is identical to pCMFD in its mathematical formulation. The differences are that it is not coupled with the Monte Carlo simulations but is instead used to generate a final subspace solution and that it is conducted on a pin-sized fine mesh as opposed to the assembly-sized coarse mesh of the pCMFD methodology.

Because the fine mesh grid has a larger number of smaller nodes and node surfaces compared to the coarse mesh grid, the uncertainty in tallied partial currents and cross-sections is much larger. Thus, instead of relying only on the tallies of the most recent cycle, the partial currents and cross-sections used in the pFMFD calculations are tallied across the later inactive and all active cycles. This process is called cycle accumulation. The early inactive cycles which are not included in the cycle accumulation are referred to as skip cycles.

2.4 Uncertainty Estimation by Correlated Sampling

The cycle accumulation of pFMFD factors means that the factors used in the pFMFD calculations and thus the subspace solutions generated by those calculations are very strongly correlated between active cycles. Thus, apparent uncertainty, uncertainty calculated from the variability in results between cycles, cannot be used as an estimator for the stochastic uncertainty of the iDTMC methodology. The correlated sampling method has been developed to estimate the true stochastic uncertainty of the iDTMC methodology [3].

In the correlated sampling method, samples of cross-sections are generated such that the distribution of cross-sections in the samples matches the distribution of those tallied in each cycle and the correlations between the total, absorption, and fission cross-sections are the same for the samples and the tallied values. These samples are then used to calculate pFMFD solutions. The stochastic uncertainty of the original iDTMC-pFMFD solution may be estimated from the variability between the pFMFD solutions calculated from sampled factors.

Due to the fast neutron spectrum of SFRs, current and leakage have a significantly larger influence on solutions for such reactors. The correlated sampling of cross-sections alone may not produce an accurate estimate of the true stochastic uncertainty. Thus, the methodology was extended to allow for the sampling of boundary conditions and correction factors. The boundary conditions and correction factors are sampled from the corresponding distributions of factors tallied in each cycle independently of the cross-sections and each other.

3. Results

The correlated sampling method for the estimation of stochastic uncertainty was implemented on the iDTMC methodology as implemented in the iMC code [4]. This was then tested on a mini-core problem and a full-sized reactor problem by comparing the uncertainties estimated by correlated sampling and the real uncertainty calculated from independent batch analyses.

3.1 Mini-Core Model

The mini-core model is a miniaturised sodium-cooled fast reactor inspired by the MOX-1000 reference problem by the NEA [5]. The model has 1 withdrawn control assembly, 18 fuel assemblies, and 42 reflector assemblies, arranged as shown in figure 3. The internal structure of each assembly and the axial structure of the mini-core model are identical to those of the MOX-1000 reference problem. This axial structure includes a reflector region below the active core and a gas plenum region above. The active core height is 114.94 cm.

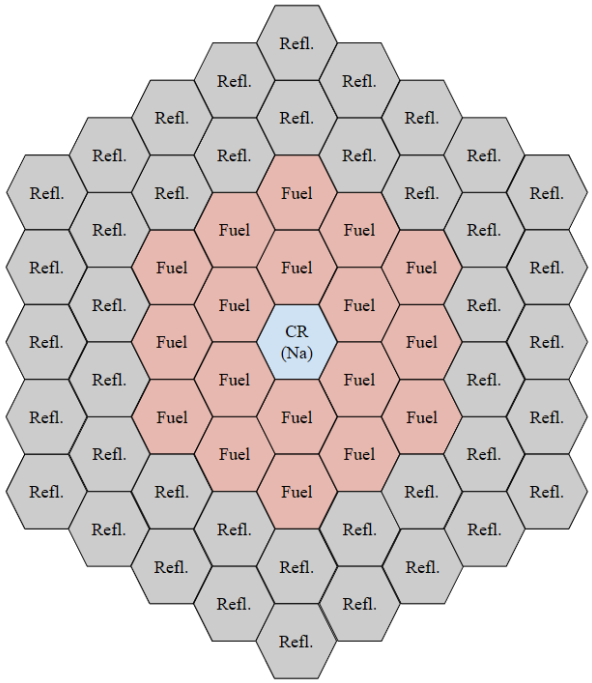

Fig. 3. Radial configuration of the mini-core model

For the pFMFD calculations, the axial length of each pin was divided into five fine-mesh nodes of equal length. No axial divisions were used for the pCMFD calculations; each assembly was one coarse mesh node.

Four calculations with correlated sampling were performed. In each case, the iDTMC calculations were done with 1 million histories per cycle, 40 inactive cycles of which 15 were skip cycles, and 10 active cycles. At the 1st and 10th active cycles, uncertainty estimation by correlated sampling was performed with 100 sets of sampled factors. 30 independent iDTMC calculations were performed with the same simulation parameters.

The real and estimated uncertainties in the neutron multiplication factor and the root mean square uncertainty in the pin power are presented in tables 1 and 2. In these tables, XS, BC, and CF refer to the sampling of cross-sections, boundary conditions, and the correction factors respectively.

Table 1: Uncertainties in the k-value, mini-core

Method	Standard Deviation (pcm)	
	1st Active Cycle	10th Active Cycle
iDTMC (real)	8.28	7.38
iDTMC (apparent)		0.73
Correlated Sampling (XS)	3.94	3.59
Correlated Sampling (XS, BC)	23.4_	19.3_
Correlated Sampling (XS, CF)	19.9_	20.9_
Correlated Sampling (XS, BC, CF)	25.2_	22.7_

Table 2: RMS uncertainty in the pin power, mini-core

Method	Standard Deviation	
	1st Active Cycle	10th Active Cycle
iDTMC (real)	0.24%	0.22%
Correlated Sampling (XS)	0.37%	0.42%
Correlated Sampling (XS, BC)	0.36%	0.33%
Correlated Sampling (XS, CF)	0.49%	0.45%
Correlated Sampling (XS, BC, CF)	0.52%	0.49%

In this model, the correlated sampling of cross sections alone produces a significant underestimate of the true uncertainty in the neutron multiplication factor but significantly overestimates the uncertainty in the pin-wise power distribution. Including the independent sampling of the boundary conditions or the correction factors produces large overestimates of both.

The inability of the apparent uncertainty in the iDTMC k-value to estimate the real uncertainty is also evident, with a very small apparent uncertainty of 0.73 pcm in the tenth cycle.

3.2 Full-Core Model

The full-core model, presented in Figure 4, is based on the MOX-1000 reference problem [5].

The axial mesh division was the same as those used for the mini-core problem. The tests run and the iDTMC simulation parameters used were also identical.

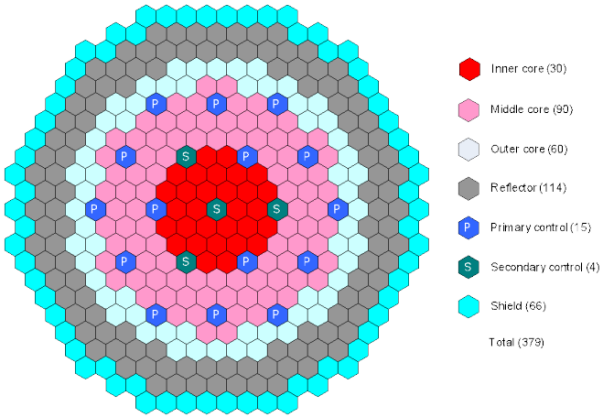

Fig. 4. Radial configuration of the full-core model.

Table 3: Uncertainties in the k-value, full core

Method	Standard Deviation (pcm)	
	1st Active Cycle	10th Active Cycle
iDTMC (real)	4.65	4.76
iDTMC (apparent)		0.38
Correlated Sampling (XS)	3.58	3.37
Correlated Sampling (XS, BC)	18.9_	14.8_
Correlated Sampling (XS, CF)	14.9_	15.0_
Correlated Sampling (XS, BC, CF)	22.0_	22.6_

Table 4: RMS uncertainty in the pin power, full core

Method	Standard Deviation	
	1st Active Cycle	10th Active Cycle
iDTMC (real)	0.67%	0.58%
Correlated Sampling (XS)	0.86%	0.86%
Correlated Sampling (XS, BC)	1.07%	0.96%
Correlated Sampling (XS, CF)	1.56%	1.47%
Correlated Sampling (XS, BC, CF)	1.99%	1.92%

The real and estimated uncertainties in the neutron multiplication factor and the pin-wise power distribution for the full-core model are presented in tables 3 and 4. Real and estimated uncertainties in the pin-wise power distribution are generally higher in the full-core model compared to the mini-core model, as the same number of simulated particle histories is distributed between a far higher number of nodes and node surfaces.

Otherwise, the results are largely comparable to those of the mini-core model. The correlated sampling of cross-sections alone underestimates the uncertainty in the k-value and overestimates the uncertainty in the power distribution, although the differences are smaller than they are for the mini-core model. Including the sampling of either boundary conditions or the correction factors results in strong overestimates of both.

4. Conclusions

For the full-core model, the uncertainties estimated through the correlated sampling of cross-sections alone provide significantly biased but reasonable estimates for the real uncertainty in the iDTMC solution. Reducing the size of the reactor, however, results in large underestimates of the uncertainty in the neutron multiplication factor, due to the larger effect of neutron leakage the uncertainty of which cannot be accounted for with the correlated sampling of cross-sections alone.

The sampling of boundary conditions or correction factors, however, produces large overestimates in the uncertainty regardless of the size of the reactor, due to their independent sampling failing to account for the correlation in pFMFD factors between different nodes or the correlation between cross-sections and the other pFMFD factors. Developing an effective mathematical treatment to reproduce these correlations in the sampled pFMFD factors is likely necessary for a truly accurate estimate of the iDTMC stochastic uncertainty through correlated sampling.

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