

## A Hybrid Stochastic Deterministic Approach for Full Core Neutronics

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**Abstract** - A hybrid approach for neutronic modelling is developed based on combining the Monte Carlo method with deterministic neutron flux mapping. The method aims to simulate full reactor cores with good accuracy while keeping low computational costs. For this purpose, a stochastic solver is used to estimate the neutron flux distribution on a coarse spatial mesh and neutron flux synthesis using the modes of the transport equation calculated on a fine mesh is employed to reconstruct a detailed neutron flux distribution required for design optimisation and safety analysis. By following this approach, the number of neutron histories and the tallies scored by the stochastic solver can be reduced significantly which would reduce the computation time and memory demand. The approach is applied to simulate a partial reactor core. Results confirm that the hybrid method can achieve up to 90% reduction in computation time compared to Monte Carlo while keeping comparable accuracy.

### I. INTRODUCTION

Reactor design and analysis rely on understanding the neutron flux distribution within the reactor core. For this purpose, deterministic methods are employed for finding an approximate solution for the Boltzmann neutron transport equation. Current practice rely on a two step process consisting of a lattice calculation followed by a full core diffusion calculation. In the first step, the reactor is represented by an infinite lattice of single unit cells and the multigroup transport equation is numerically solved to produce a reactor database of neutron cross sections. The second step uses the reactor database to solve the few groups diffusion equation on a simplified reactor geometry consisting of spatially homogenised unit cells. Such simplifications in the reactor representation as well as the neutron properties jeopardise the accuracy of the solution. However, deterministic methods continue to be used as the main analysis tools for reactor design due to their practicality and relatively low computational costs.

Monte Carlo (MC) methods on the other hand simulate stochastically the physical behaviour of neutrons within the reactor with few simplifications; hence they provide a more accurate solution. Despite the advancement of computer platforms, the Monte Carlo method remains prohibitively computationally expensive for production calculations and has been limited in use for benchmarking and verification [1].

With the introduction of new reactor designs and fuel cycles as well as more stringent safety requirements, there is a renewed interest in the use of the MC method for production calculations. Recent efforts attempt to improve the performance of the MC method by reducing the run time through employing hybrid deterministic-stochastic approaches. Such methods successfully achieved some reductions in the run time for full core MC by accelerating the inactive portion of the simulation [2, 3]. However, an acceleration in the inactive cycles is insignificant as these constitute a small portion of the simulation.

In the presented work, a novel hybrid method for reducing the computation time for stochastic full core simulations while maintaining good accuracy on the solution is described. The

method is based on coupling the MC simulation to a deterministic flux mapping approach based on the modal expansion model of the neutron flux distribution. In the next section, the transport equation and modal expansion of the neutron flux are introduced. Then, the Monte Carlo method is briefly discussed and the proposed hybrid approach is described. The method is applied to a 3D problem for illustration and sample results are produced. Results show that the approach can achieve 90% reduction in the running time while maintaining better than 6% accuracy compared to the conventional MC method.

### II. THE TRANSPORT EQUATION AND MODAL EXPANSION

The steady state transport equation in neutron multiplying media is an eigenvalue problem which states mathematically the conservation of neutrons[4]:

$$\begin{aligned} & \Omega \nabla \phi(\mathbf{r}, E, \Omega) + \Sigma_t(\mathbf{r}, E) \phi(\mathbf{r}, E, \Omega) \\ &= \int_0^\infty dE' \int_{4\pi} d^2\Omega' \Sigma_s(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) \phi(\mathbf{r}, E', \Omega') \\ & \quad + \frac{1}{4\pi k} \chi(E) \int_0^\infty dE' \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E') \quad (1) \end{aligned}$$

where a single fissile isotope is assumed in the fission source for simplicity. Eq. (1) admits an infinite number of eigenfunctions or modes as mathematical solutions. The fundamental mode solution, i.e. the eigenfunction corresponding to the largest eigenvalue, describes the asymptotic behaviour of the neutron flux at steady state and the higher order modes describe perturbations around it.

Deterministic approaches for solving the transport equation rely on numerical discretisation of the phase space. Typically, the energy interval is split into a number of groups  $G$  over which neutron cross sections are assumed to be constant. Furthermore, neutron sources and scattering are assumed to be independent of the direction of travel  $\Omega$ . These two assumptions significantly simplify the integration of the transport equation over energy and direction. When the space is discretised into  $M$  mesh elements, the transport equation is written

in matrix form:

$$\mathbf{A}\Phi = \frac{1}{k}\mathbf{B}\Phi \quad (2)$$

where  $\mathbf{A}$  and  $\mathbf{B}$  are two matrices of the order  $M \times G$  and  $\Phi$  is a column vector whose elements are the values of the flux distribution in each mesh element and energy group. As an example, the integral multigroup isotropic form of the transport equation is commonly solved in lattice codes using the method of collision probabilities [5] where the matrices  $\mathbf{A}$  and  $\mathbf{B}$  become identical to:

$$\mathbf{A} = \mathbf{I} - \mathbf{P}\mathbf{S}_c \quad \text{and} \quad \mathbf{B} = \mathbf{P}\mathbf{F} \quad (3)$$

where  $\mathbf{I}$  is the identity matrix,  $\mathbf{P}$  is a block diagonal matrix of collision probabilities,  $\mathbf{S}_c$  is the matrix of scattering cross sections and  $\mathbf{F}$  is the matrix of fission production cross sections. Eq. (2) is a generalised eigenvalue problem which admits  $M \times G$  eigenvectors as solutions. The eigenvector with the largest eigenvalue corresponds to the fundamental mode of the neutron flux and is the only eigenvector that satisfies all physical and boundary conditions. As in generalised eigenvalue problems, a linear combination of the eigenmodes is also a mathematical solution. In fact, the general solution of the multigroup transport equation is a series summation over the complete set of modes:

$$\Phi = \sum_{i=1}^{M \times G} a_i \Psi_i \quad (4)$$

where  $\Psi_i$  denotes the  $i^{\text{th}}$  eigenvector and  $a_i$  is the corresponding amplitude. Eq. (4) is the modal expansion model of the neutron flux. In general, the amplitude of the fundamental mode is much larger than the amplitudes of higher order modes which are quite difficult to obtain. Hence, practice in deterministic methods has been to approximate the neutron flux distribution by the fundamental mode solution. Typically, eq. (2) is solved for the fundamental mode using iterative methods such as the power iteration. The higher order modes can be obtained by more delicate approaches such as deflation techniques or QZ decomposition [6, 7].

### III. THE HYBRID METHOD

#### 1. The Monte Carlo Method

In Monte Carlo simulations, the neutron flux distribution is estimated by observing the average behaviour of a large number of neutron histories tracked across the reactor geometry [8]. From their point of birth to the point of removal, neutrons can undergo different interactions that are governed by probability distributions related to the cross sections of nuclei. By using pseudo-random numbers and statistical tests to sample different interactions, the MC method simulates the transport of neutrons and reproduces their trajectory within the reactor. The neutron flux distribution is deduced using different types of estimators such as the track length or collision estimators. Typically, the method proceeds with a number of inactive cycles, where no tallies are recorded, to generate a reliable neutron source distribution for random sampling.

Then, a number of active cycles are run where different tallies are scored.

The MC method is widely accepted as an accurate modelling tool in reactor physics. However, a number of challenges [1] render it impractical for production calculations. In particular, the extreme computational burden for high confidence in the MC estimate of the neutron flux remains the main limitation for full exploitation of the method. The computational expense of MC simulations depends on different factors of which the number of neutron histories used and the number of tallies scored are the most significant. The number of histories is dictated by the desired statistical error and the size of the mesh over which tallies are scored. For the same statistical error on tallies, the number of histories for a fine mesh simulation would be much larger than that for a coarse mesh. The number of tallies scored also escalates when a fine mesh is used thus increasing the runtime. In general, reactor design, optimisation and safety analysis require a detailed estimate of the neutron flux distribution within fuel elements to study different phenomena such as burnup, heat transfer, fuel damage, etc.

#### 2. Coupling Monte Carlo to Flux Mapping

Since the physical behaviour of neutrons within the reactor is stochastically simulated in MC, the estimate it provides can be a better approximation of the general solution of the transport equation. Here, it is assumed that the flux estimate obtained by a stochastic solver can be expanded in terms of the high order modes of eq. (1) as:

$$\phi^{MC}(\mathbf{r}, E) = \sum_{i=1}^{\infty} a_i \psi_i(\mathbf{r}, E) \quad (5)$$

As mentioned in section II., the modes of the transport equation can be obtained using numerical methods applied to one of its discretised multigroup forms. MC simulation can treat the energy and space independent variables in the continuous domain, however, tallies are typically recorded on a discrete spatial mesh and multi-energy groups. In practice, the series expansion is truncated after  $N$  modes with the largest eigenvalues  $k_i$  and eq. (5) is written in matrix form as:

$$\Phi^{MC} \approx \Psi \mathbf{A} \quad (6)$$

where  $\Phi^{MC}$  is a vector whose elements are the values of neutron flux in discrete tally mesh elements,  $\Psi$  is a matrix whose columns are the dominant modes of the transport equation and  $\mathbf{A}$  is a vector whose elements are modal amplitudes.

In the proposed hybrid method, a relatively low cost MC simulation is performed with the neutron flux distribution obtained with low statistical error on a coarse spatial mesh and few energy groups. Deterministic approaches are used to calculate the modes of the transport equation or one of its approximations on a fine spatial mesh and few energy groups. Assuming that the modal amplitudes are independent of the spatial mesh, the dominant modes are condensed into a coarse mesh and coupled with the MC solution in order to calculate the modal amplitudes. Once the amplitudes are determined, a fine mesh estimate of the neutron flux distribution can be synthesised using the modal expansion model of eq. (6).

### 3. Illustration

The hybrid simulation would proceed with the MC simulation. A number of inactive cycles are executed to converge the fission source. Then, the active cycles are started and sufficient number of neutron histories for low statistical error on the tallies are tracked. The output of the active cycles would be the neutron flux scored on a coarse mesh, denoted  $\Phi^{MC}$ , over the full core and macroscopic neutron cross sections required for performing the deterministic portion of the simulation for obtaining the high order modes. Due to the difficulty of calculating fine mesh dominant modes of the transport equation for the full core geometry, modes are calculated on a unit cell or assembly level. Determination of the modes is performed on a unit cell or assembly level using a lattice calculation to obtain fine mesh approximation of the dominant modes, denoted  $\Psi_i^*$ , while keeping low computation costs. In the presented work, a predetermined number of dominant modes are produced on a fine mesh using QZ decomposition [7]. The modes are then spatially homogenised to produce coarse mesh dominant modes, denoted  $\Psi_i$ . The final stage is the calculation of the modal amplitudes and flux reconstruction. The approach is summarised in the flow chart of figure 1.

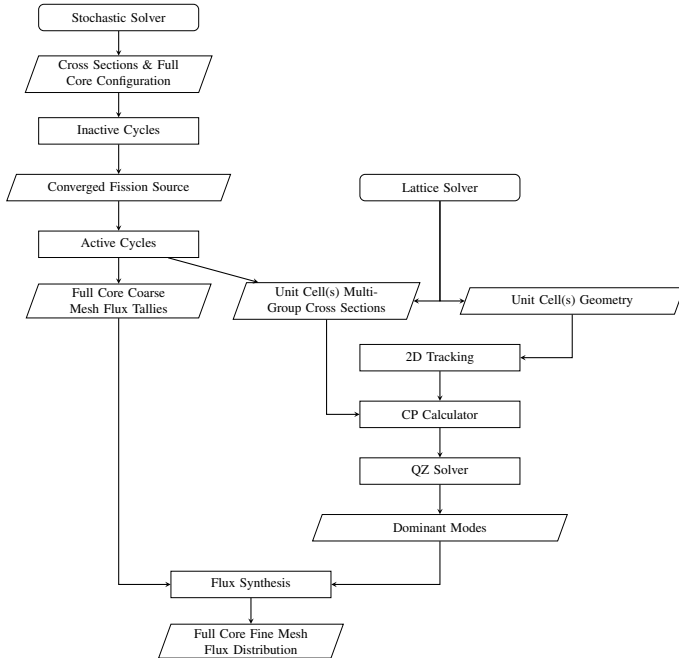


Fig. 1: Flow chart of the hybrid method

Eq. (5) is a linear system of equations with unknown  $A$ . Typically, the number of regions  $M$  is larger than the number of modes  $N$  which means that Eq. (5) is an over-determined linear system. A solution for the modal amplitudes can be obtained using a least squares approach:

$$A = (\Psi' \Psi)^{-1} \Psi' \Phi^{MC} \quad (7)$$

where  $\Psi'$  is the transpose matrix of  $\Psi_g$ . The coarse mesh solution estimated by the MC simulation and the modes, homogenised on a coarse mesh for consistency, are used for

solving Eq. (7). Once an approximation of the modal amplitudes is determined, the detailed neutron flux distribution is reconstructed by combining the fine mesh modes with their amplitudes in Eq. (8):

$$\Phi^{hybrid} = \Psi^* A \quad (8)$$

Assuming that the modal expansion model of eq. (5) is valid on a unit cell or assembly level, the approach is applied locally; different modal amplitudes are calculated for each unit cell or assembly. By following this hybrid approach, a full core neutron flux distribution is obtained on a fine mesh with an accuracy which should be comparable to the MC method while keeping the computational expenses reasonably low.

### IV. EXAMPLE PROBLEMS AND SAMPLE RESULTS

#### 1. Validation: Application to single PWR Assembly

The presented hybrid method is first validated by considering a single 2D PWR assembly with reflective boundary conditions. In this section, an attempt is made to synthesise a 2 groups fine mesh flux distribution ( $\Phi^{ref}$ ), shown in figure 2, starting from a coarse one ( $\Phi^{MC}$ ), shown in figure 3, and the accuracy of the modal expansion model is examined. The assembly considered is a typical  $17 \times 17$  lattice arrangement with 264 fuel pins and 25 water filled guide tubes. The fuel composition is chosen to represent uranium dioxide at mid-burnup from an initial 3.25% enrichment; isotopic concentrations are shown in table I. The fine spatial mesh comprises 10 burnup radial zones per fuel pellet and the coarse spatial mesh is composed of homogenised pincells. The MC code Serpent [9] is used to estimate the neutron flux in both cases. The dominant

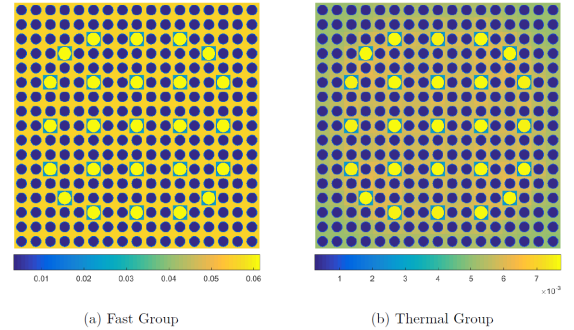


Fig. 2: Fine mesh neutron flux distribution in a PWR assembly

modes of the transport equation are evaluated using the lattice code Dragon [7]. Modal expansion using different number of modes, chosen randomly, is then utilised for flux synthesis. The hybrid estimate is compared to the reference solution by the means of the relative error:

$$e = \frac{\Phi^{ref} - \Phi^{hybrid}}{\Phi^{ref}} \quad (9)$$

#### A. Reconstruction Using 20 Dominant Modes

The modal expansion model is truncated after the first 20 most dominant modes and the relative error between the reproduced flux distribution and the reference is shown in

Isotope	Atomic Concentration (/barn-cm)	Isotope	Atomic Concentration (/barn-cm)
U234	4.6476E-6	Mb95	2.6497E-5
U235	4.8218E-4	Tc99	3.2772E-5
U236	9.0402E-5	Ru101	3.0742E-5
U238	2.1504E-2	Ru103	2.3505E-6
Np237	7.3733E-6	Ag109	2.0009E-6
Pu238	1.5148E-6	Xe135	1.0801E-8
Pu239	1.3955E-4	Cs133	3.4612E-5
Pu240	3.4405E-5	Nd143	2.6078E-5
Pu241	2.1439E-5	Nd145	1.9898E-5
Pu242	3.7422E-6	Sm147	1.6128E-6
Am241	4.5041E-7	Sm149	1.1627E-7
Am242	9.2301E-9	Sm150	7.1727E-6
Am243	4.7878E-7	Sm151	5.4947E-7
Cm242	1.0485E-7	Sm152	3.0221E-6
Cm243	1.4268E-9	Eu153	2.6209E-6
Cm244	8.8756E-8	Gd155	1.5369E-9
Cm245	3.5285E-9	O16	4.5737E-2

TABLE I: Fuel composition of the peripheral assemblies - mid-burnup

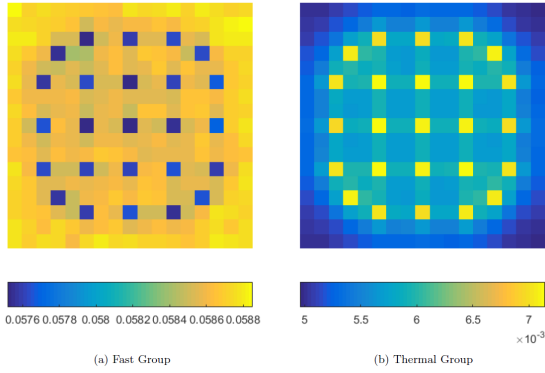


Fig. 3: Coarse neutron flux distribution in a PWR assembly

figure 4. In most regions, the relative error is below 1% in both energy groups. However, errors up to 3% are observed in few regions in the thermal energy group.

### B. Reconstruction Using 50 Dominant Modes

When the number of modes employed in modal expansion is increased to 50, the relative error on the reconstruction is slightly reduced. The maximum relative error in this case is about 2.5% in the thermal group and around 1.2% in the fast group as shown in figure 5. In general, using a larger number of modes in the series expansion could improve the accuracy of flux synthesis; however, mapping errors appear to be inevitable.

### C. Mapping Error Reduction

The expansion of the MC estimate of the neutron flux in terms of the dominant modes of the transport equation introduces a number of mapping errors. These arise from the fact that the modes obtained in the deterministic solver are an approximation. Systematic discretisation errors, assumptions

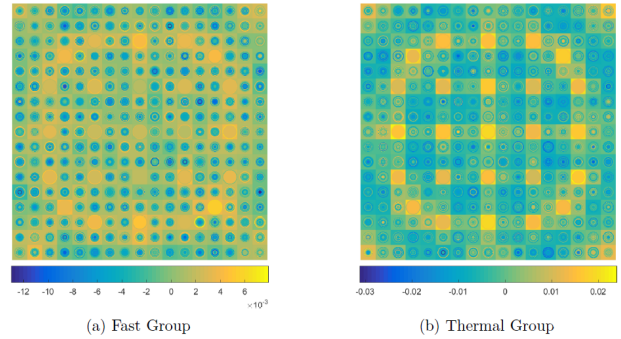


Fig. 4: Relative error on flux reconstructed using 20 dominant modes

made in the deterministic model and truncation of modal expansion collectively contribute to mapping errors. In order to improve neutron flux reconstruction, an attempt to estimate these errors is performed. The error between the coarse mesh MC solution and that reconstructed by modal expansion is given by:

$$\epsilon = \Phi^{MC} - \Psi A \quad (10)$$

Assuming that a coarse mesh element  $i$  comprises  $J$  sub-mesh elements, the total error on the reconstructed neutron flux in region  $i$  is:

$$\epsilon_i = \sum_{j=1}^J \epsilon_{ij} \quad (11)$$

Assuming that the average error is constant, the mapping error in the sub-mesh element  $j$  is then:

$$\epsilon_{ij} = \frac{\epsilon_i V_{ij}}{V_i} \quad (12)$$

Flux reconstruction with mapping error reduction as proposed here is applied to the case where 20 dominant modes are used

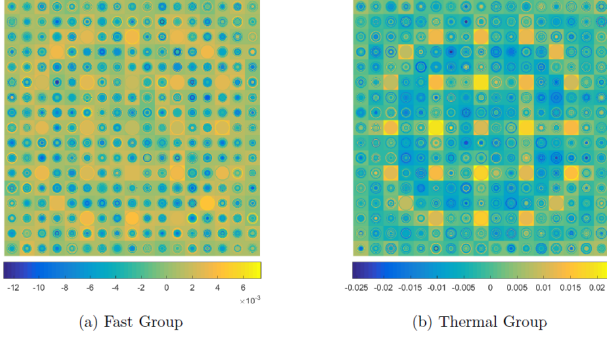


Fig. 5: Relative error on flux reconstructed using 50 dominant modes

in the modal expansion model. In this case, the hybrid estimate of the neutron flux is obtained as:

$$\Phi^{hybrid} = \Psi^* A + \epsilon \quad (13)$$

The relative error between the reference and synthesised fine mesh solution plus estimated mapping error is presented in figure 6. In this case, the maximum relative error is below

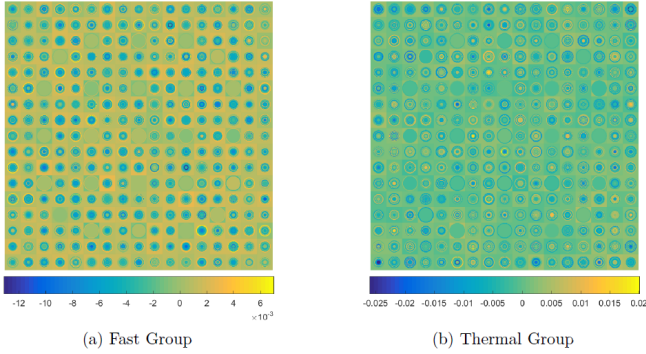


Fig. 6: Relative error on flux reconstructed using 20 dominant modes with mapping errors reduction

1.2% and 2.5% in the fast and thermal groups respectively. These values are comparable to the ones obtained with 50 dominant modes. It might be concluded that the accuracy of flux synthesis could be made less sensitive to the number of dominant modes used when mapping error estimation is applied.

## 2. Application to 3D PWR Supercell

### A. Problem Description

The approach is applied to study the neutron flux in a  $3 \times 3$  PWR 3D super-cell with the typical  $17 \times 17$  lattice arrangement. The central assembly comprises fresh fuel at 3.25% enrichment while the composition of the peripheral assemblies is that of burned fuel up to 22MWd/t from an initial enrichment of 3.25%. The isotopic composition of the fuel for the peripheral assemblies and the central one are shown in table I and II respectively. Each assembly contains 264 fuel pins of typical PWR dimensions and 25 water filled guide

tubes. The super-cell extends 366cm in the axial direction. The top view of the configuration is shown in Fig. 7.

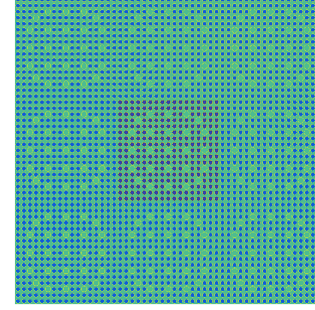


Fig. 7: PWR  $3 \times 3$  super-cell

Isotope	Atomic Concentration (/barn-cm)
U235	7.0803E-4
U238	4.6624E-2
O16	2.2604E-2

TABLE II: Fuel composition of central assembly - fresh fuel

The described configuration is studied to obtain the neutron flux distribution over a fine spatial mesh featuring the coolant channel, cladding and 10 burn-up zones per fuel cell and 3 radial regions per guide tube. All values are produced for two energy groups, the thermal group of neutrons below 0.625eV and the fast group of neutrons with greater energies. The calculation proceeds as follows:

- The MC part of the simulation is performed using the code Serpent[9]. Periodic boundary conditions are defined in the radial direction while void boundary conditions are defined in the axial direction. Neutron flux tallies ( $\Phi^{MC}$ ) in homogenised pin-cells and over 10 axial planes are scored. In addition, fine mesh average macroscopic cross sections are calculated for each type of fuel assemblies.
- Serpent output files are read by the lattice code Dragon[10] to extract neutron cross sections for calculating 2D assembly modes ( $\Psi^*$ ) using the collision probability approximation. A single assembly assuming periodic boundary conditions is defined and tracked to calculate fine mesh collision probabilities. The QZ [7] decomposition method is employed to calculate the neutron flux modes  $\Psi^*$  for each of the two assembly types.
- Once the modes are calculated, an independent amplitudes calculation is performed for each unit cell and axial plane. Cell-by-cell homogenisation of the assembly modes is performed to calculate coarse mesh modes  $\Psi$ . Coarse mesh neutron flux tallies are read plane-by-plane and assembly-by-assembly and Eq.(7) is used to estimate the modal amplitudes ( $A$ ).
- Finally, assembly modes are combined with their local amplitudes to reconstruct the neutron flux distribution ( $\Phi^{hybrid}$ ) over the fine mesh.

### B. Computational Costs

The MC simulation is performed with 20 inactive and 5000 active cycles each of 200000 neutron histories. The largest standard deviation on the neutron flux tallies is observed near the axial boundaries and is about 1% while the standard deviation on the average cross sections is less than 0.1%. The simulation is performed on a workstation with core i7-4770 CPU; parallel processing on 8 CPU threads is utilised. After the MC run completes, Dragon is executed to calculate 50 dominant modes, i.e. the ones corresponding to the largest eigenvalues, for the two assembly types in parallel where each assembly is treated on a single thread.

Once the modes are estimated, MC flux tallies in homogenised pin-cells are read and modal amplitudes are estimated on an assembly-by-assembly and plane-by-plane basis. Flux reconstruction is then performed and the results are benchmarked against a reference MC solution; the reference solution for the bottom and mid-axial planes is shown in figure 8 and figure 9 respectively. The reference solution is normalised such that the euclidean norm of  $\Phi^{ref}$  is unity. In addition, the rate of thermal and fast fission reactions estimated by the hybrid simulation are benchmarked against a reference MC estimate; the reference fission rate distribution in the bottom and mid axial planes is shown in figure 10 and figure 11. The reference simulation is performed on the same workstation using 20 inactive and 50000 active cycles each of 200000 neutron histories. The largest standard deviation on the reference neutron flux is about 1% scored in the planes near the axial boundaries. The total runtime of the hybrid method is 355 minutes compared to 3061 minutes for the reference solution. Therefore, an 88% reduction in the computational runtime is achieved.

### C. Accuracy Evaluation

In order to verify the solution obtained using the hybrid method, the relative error between the hybrid solution a reference MC estimate is evaluated. The relative error on the thermal and fast flux in the bottom and middle axial planes are plotted and shown in Fig.12 and Fig.13 respectively.

Results show that the reference flux is reconstructed with a maximum error of 4% in the fast group and 5.5% in the thermal group for the axial planes near the boundaries. Better results are obtained in the middle plane where the maximum error is less than 2% and 2.5% on the fast and thermal groups respectively. In addition, the relative error between the reconstructed fission rate and the MC reference is evaluated and shown in figures 14 and 15 for the bottom and mid axial planes. Results are coherent to those observed for the flux distribution. The maximum relative error on the reconstructed fission rate is about 5% and 2.5% for the bottom and mid planes respectively in both energy groups.

## V. CONCLUSIONS

A hybrid deterministic stochastic method for studying full core neutronics is briefly described. The method aims to preserve the accuracy of the MC method while improving the computing efficiency. Significant reductions in the computational expense of MC can be achieved through performing

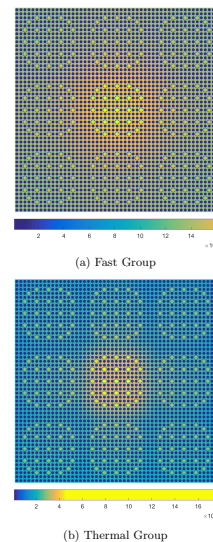


Fig. 8: Fine mesh reference neutron flux distribution in bottom axial plane

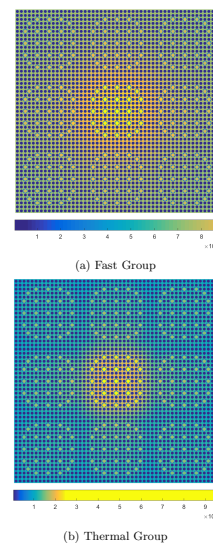


Fig. 9: Fine mesh reference neutron flux distribution in middle axial plane

the simulation on a coarse spatial mesh and deterministically reconstructing a fine mesh solution using the flux synthesis method.

The approach is applied to study the neutron flux on an example 3D problem. Results confirm that the approach can reduce significantly the computational expense for obtaining a transport solution in full core calculations while maintaining good accuracy.

Future development of the described hybrid method focuses on reducing the mapping error and improving the overall performance. For this purpose, the effects of boundary conditions and leakage in calculating modes of the transport equation are to be considered. In addition, improved methods

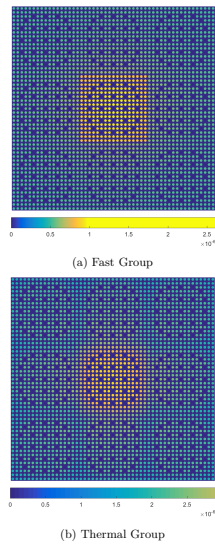


Fig. 10: Fine mesh reference fission rate distribution in bottom axial plane

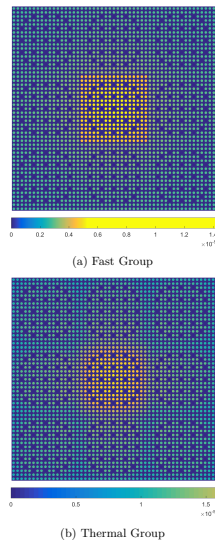


Fig. 11: Fine mesh reference fission rate distribution in middle axial plane

for estimating the mapping error are to be developed. The optimum number of modes used in modal expansion needs to be evaluated. Finally, effects of the statistical error associated with the coarse mesh solution are to be examined.

## VI. NOMENCLATURE

- $\phi$  = Neutron flux distribution
- $\Sigma_t$  = Neutron total macroscopic cross section
- $\Sigma_s$  = Neutron scattering macroscopic cross section
- $\nu\Sigma_f$  = Neutron fission production macroscopic cross section
- $\chi$  = Fission neutrons energy spectrum

- $k$  = Criticality eigenvalue
- $\psi_i$  = Eigensolution (mode) corresponding to the  $i^{th}$  eigenvalue
- $a_i$  = Modal amplitude of the  $i^{th}$  mode
- $\epsilon$  = Estimated mapping error
- $V_i$  = Volume of region  $i$
- $e$  = Relative difference between reference and hybrid solution

## VII. ACKNOWLEDGMENTS

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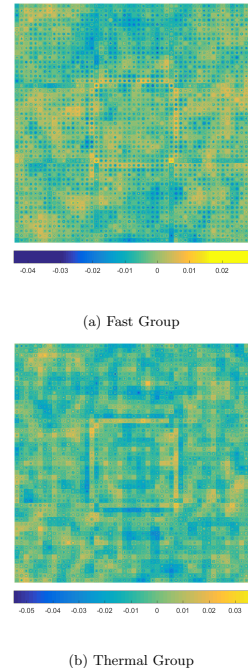


Fig. 12: Relative error on the reconstructed flux in the bottom axial plane

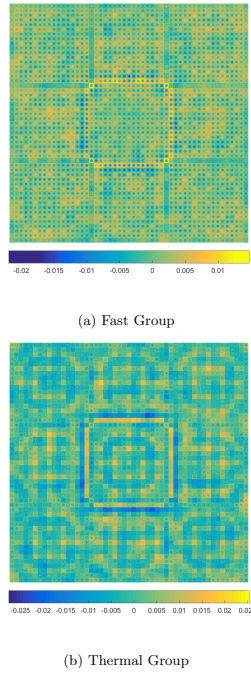


Fig. 13: Relative error on the reconstructed flux in the middle axial plane

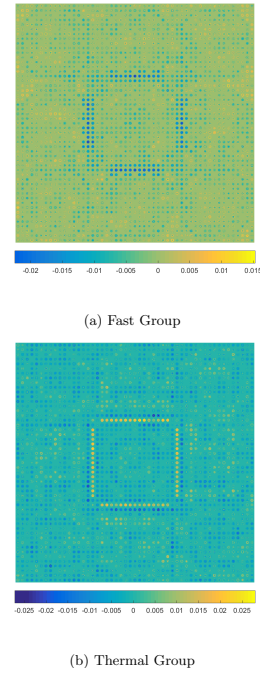


Fig. 15: Relative error on the reconstructed fission rate in the middle axial plane

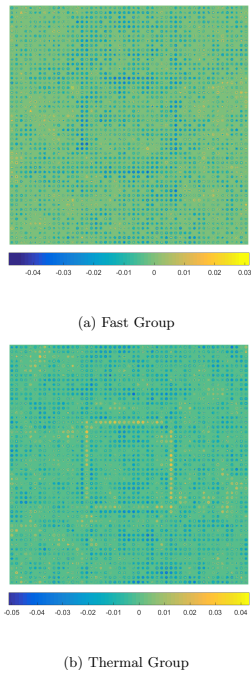


Fig. 14: Relative error on the reconstructed fission rate in the bottom axial plane

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