Application of the FW-CADIS Variance Reduction Method to Calculate a Precise N-Flux Distribution for the FRJ-2 Research Reactor - 15603

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ABSTRACT

In order to avoid unnecessary radiation exposure and to minimize the radioactive waste and respectively cost by the decommissioning of nuclear facilities, the radiological characteristics and the activity atlases are required. Therefore, a significant step is the accurate determination of the neutron fluenz distribution resulting from the operation of a reactor. For this purpose, computer codes based on the Monte-Carlo method are employed because of the flexibility in the modelling of the complex structures and physical processes. In the scope of the research project founded by the German Federal Ministry of Education and Research (BMBF), and implemented by the Institute of Nuclear Engineering and Technology Transfer (NET) - RWTH Aachen, sophisticated simulation tools are developed, which have the capability to cover the range of demands for activity and dose rate distribution using the example of the German research reactor FRJ-2. Due to the complex geometry of FRJ-2, which consists of different structures and configuration, the MCNP5 Monte Carlo Code is the optimal method for a precise neutron transport simulation. This work presents a method to achieve a precise N-Flux distribution for the FRJ-2 research reactor using hybrid deterministic Monte Carlo method.

INTRODUCTION

The production of the detailed activity and dose rate atlases (ADAs) is one of the indispensable measures in the decommissioning process of nuclear reactors which helps to determine the radiation field for optimal radiation protection as well as to quantify and characterise nuclear waste for disposal. High-detailed simulation models capable of performing neutron and radiation transport calculations at different levels of precision and details are applied for this purpose.

In the field of nuclear engineering and radiation safety, MCNP (Monte Carlo N-Particle Transport Code) is widely used to solve neutron and radiation transport problems which cannot be solved by deterministic methods at a high level of accuracy and geometrical resolution [1]. The use of Monte Carlo method for the complex reactor system has, however, some numerical and statistically based limitations resulting from the attenuation of the neutron field at large distances and deep penetrations. For this purpose and to improve the computational efficiency, variance reduction (VR) methods are widely used within MCNP which helps to reduce the statistical errors by sampling more particle histories in the regions of interest [2, 3].

The application of the basic VR methods such as the weight window (WW) generator and geometry splitting in MCNP is rather straight forward but it could be ineffective for a complex geometry since it requires the determination of the VR parameters and detailed geometry nodalisation [7]. In addition, to optimize WW-parameters for extended particle sampling, many iterative steps must be performed that do not inevitably lead to the improvement of the results and numerical convergence [4]. To overcome inherent statistical limitations in high performance Monte-Carlo simulation, different VR methods have been developed, such as the importance sampling technique using deterministically generated importance functions which allow to considerably increase the computational efficiency and simulation performance respectively for large models [5].

FW-CADIS (Forward-Consistent Adjoint Driven Importance Sampling) represents the state of the art methodology for effective importance sampling and generation of optimal VR parameters [7]. This method has been developed at Oak Ridge National Laboratory (ORNL) and is implemented in the MAVRIC sequence of the program package SCALE6 [8]. The present work's focus is to prepare and use this methodology to generate WW-parameters for the MCNP model of the German research reactor FRJ-2 and to perform neutron transport calculation at high precision and low variance. This innovative approach to simulation is implemented within the framework of the research project "decommissioning of nuclear research and power reactors" which is funded by the German Federal Ministry of Education and Research (BMBF).

COMPUTATIONAL MODEL ON THE REACTOR

The FRJ-2 is a heavy water cooled and moderated DIDO-type research reactor which has been operated for 44 years and was shut down on May 2nd 2006. To calculate the n-Flux, the reactor core configuration containing 11250 geometrical and material cells is replaced by a surface source surrounding the core. This contains the surface element coordinates as well as the angle and the energy distribution of all neutrons crossing and leaving the enclosed surface. For neutron transport simulation as the basis for activity calculations, the existing CAD-model of FRJ-2 was converted into the MCNP syntax by employing the CAD-converter tool McCad developed by the Karlsruhe Institute for Technology [9] resulting in a very detailed geometry model. The recorded surface source data was incorporated into the CAD-based MCNP model in the form of a fixed source definition.

APPLICATION OF FW-CADIS METHOD

The variance of the MCNP calculations is mainly influenced by the number of particles tracked in different material and geometrical zones of the whole model and depends on the sampling method applied. A particularly important issue is the simulation efficiency as well as the precision of the flux distribution that is achieved by the application of different variance reduction techniques. The common variance reduction techniques encompass a wide range of statistical methods which allow to modify the random-walk process in such a way that the neutron histories with the lowest contributions on the results are scored more frequently. This is achieved by adjusting the corresponding weights to assure preserving the statistical validity of the simulation by appropriate biasing of the scores.

The Application of the basic VR methods to the CAD-based MCNP model of FRJ-2 leads to results with high statistical uncertainties, mainly in structures with a large distance from the core area (s. Fig. 1). Despite the high CPU time and large number of particle histories in many parts of the entire reactor model very low or no particle sampling and neutron track density is achieved. This is a consequence of limited particle sampling in these regions resulting in a high level of variance. Increasing the number of particle histories would directly contribute to the numerical and statistical precision. Nevertheless, this does not improve the statistics efficiently, as a reduction of the simulation error and uncertainty from 10% to 1% requires 100 times more particle histories and simulation time respectively.

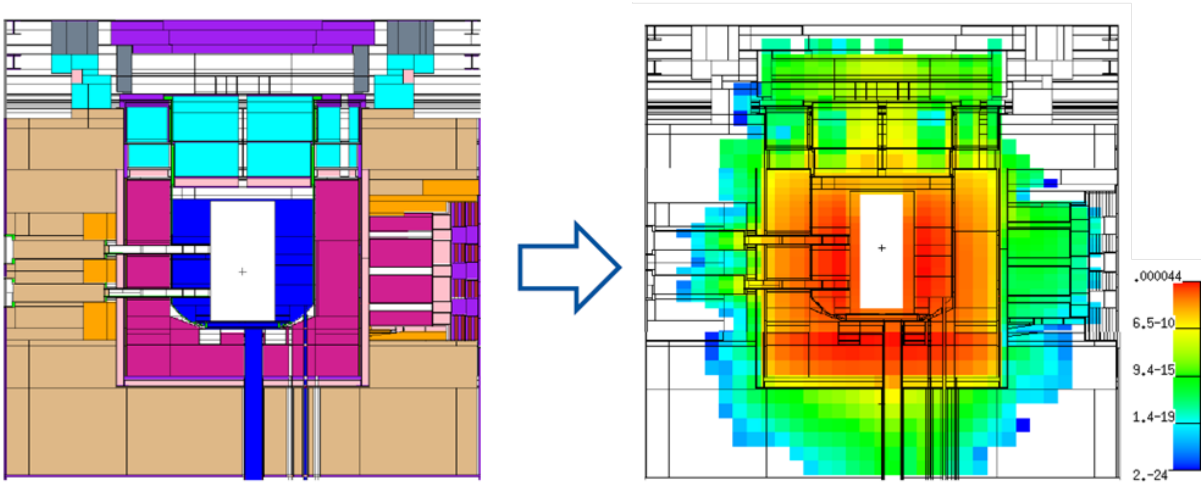

Figure 1: CAD-based MCNP model of FRJ-2 (left), N-Flux distribution via MCNP VR methods (right)

For this reason FW-CADIS is applied to improve the particle sampling and scoring by generation and application of properly distributed particle weights and importances. This method is based on the forward and adjoint flux calculation using the deterministic method for neutron transport simulations [7, 8]. Deterministic methods provide the approximate solution of the forward as well as adjoint transport equation using the method of discrete coordinates (S_N-approximation). For this purpose the code package SCALE6 (**S**tandard **C**omputational **A**nalysis for **L**icensing **E**valuation) consisting of different tools, subroutines and flux solvers for forward and adjoint calculations was used.

FW-CADIS, embedded in the MAVRIC (**M**onaco with **A**utomated **V**ariance **R**eduction using **I**mportance **C**alculations) sequence, allows automatic variance reduction through source and consistent transport biasing. Its main goal is to uniformly distribute the particle density over the zones and tally area respectively, where the number of Monte Carlo particles is related to the physical particle density and to the mean weight. By sampling the particle from biased sources, the weight is adapted to fulfil the consistency of the application. By this way the weights of the source particles match the weight window [6].

As depicted in Fig. 2, MAVRIC runs the DENOVO (three-dimensional, discrete ordinates (S_N) transport code) flux solver for 3D deterministic calculations as well as Monaco for the forward multi-group Monte Carlo calculations. In the next step, MAVRIC applies the FW-CADIS method to define and determine the adjoint source by the estimated inverse forward flux for use in the subsequent adjoint calculations (as per S_N-Method) to construct an importance map or weight window parameters for a uniform particle density and uniformly distributed statistical uncertainties respectively [7].

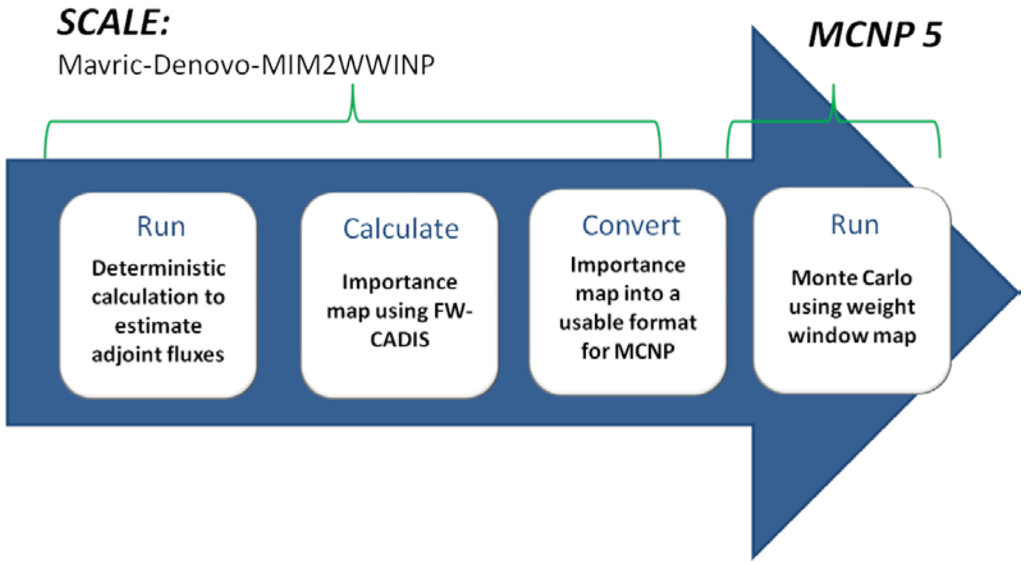

Figure 2: Process of the hybrid deterministic/Monte Carlo method

The innovative hybrid deterministic/Monte-Carlo method was considered for application to the complex FRJ-2 model to produce optimized importance map and WW-parameters respectively. A parameter study showed that the importance map created with a rough geometrical model is applicable to the highly detailed model of FRJ-2 that allows saving simulation and CPU time. For this reason a fairly simple geometry model with a homogenized core is created for deterministic calculations. This simplified model (Fig. 3) keeps the main characteristics of the CAD-model of FRJ-2 such as geometrical dimensions, exact definitions of different shielding material layers surrounding the core, as well as some important instrumentation tubes and shielding plugs including the material definitions.

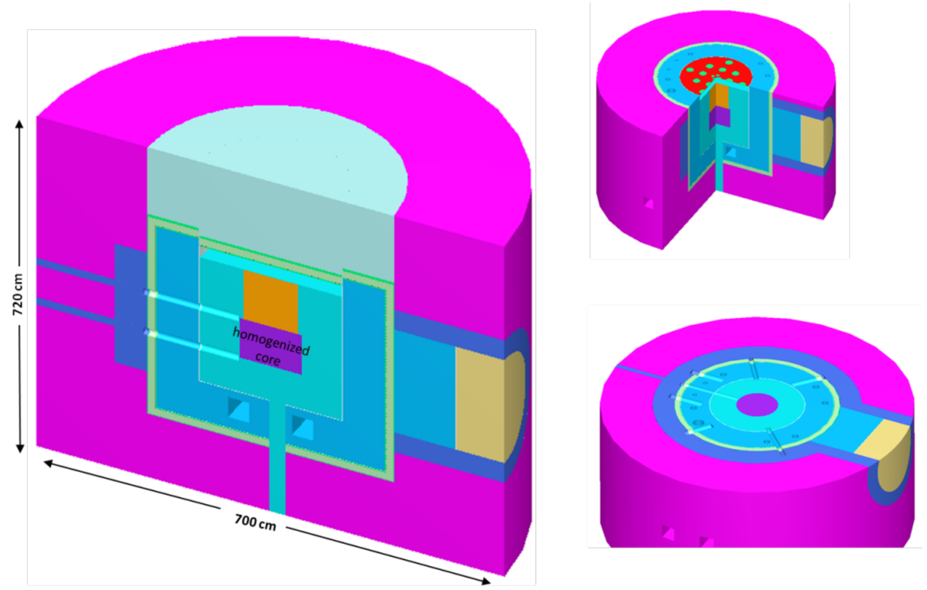

Figure 3: Simplified FRJ2-Model for computations with SCALE6

To estimate the expected tally results, a forward and an adjoint flux calculation is performed. Then the standard FW-CADIS approach is used to generate an importance map which is converted into a weight window format for MCNP application.

EFFICIENCY OF THE FW-CADIS

For the adjoint calculation and generation of the WW-parameters with the SCALE6 code using the discrete ordinate approach, a rectangular grid geometry model with less detail is needed. This model consisting of a grid of uniform mesh size (WW-mesh element size) for the WW generation, is a rough and simplified variant of the MCNP-model of FRJ2 which is constructed at a high level of nodalization for detailed neutron transport calculations.

The mesh element size of the geometry model is a significant parameter for the importance sampling through hybrid calculation (DENEVO module of SCALE6) and has a considerable effect on the computational performance for forward and adjoint calculation. To investigate the simulation performance of the method the distribution of the relative error in the entire model was considered in terms of cumulative distribution function (CDF as given in Fig. 4). These represent the distribution of the relative errors of the simulation results in the mesh elements of the entire model for different weight window mesh sizes. For instance the number of the mesh elements getting a relative error of up to 10% considerably increases with the decrease of the weight-window mesh size for a given simulation time. Each case was performed for a Monaco computational time of 15 min corresponding to 1000 source neutrons per batch.

A reduction of the weight-window mesh size leads to a more efficient particle sampling. Furthermore, the smaller the size of the mesh element the steeper the CDF profile becomes, corresponding to a fast variance reduction. This implies that low variance simulation results are produced with less particle histories and batches respectively when small-sized mesh grids are applied. However the use of the complete SCALE6 model with mesh sizes below 15 cm led to numerically inconsistent DENOVO runs, so a mesh size of 15 cm was chosen for the importance sampling and generation of the weight window map for further MCNP calculations.

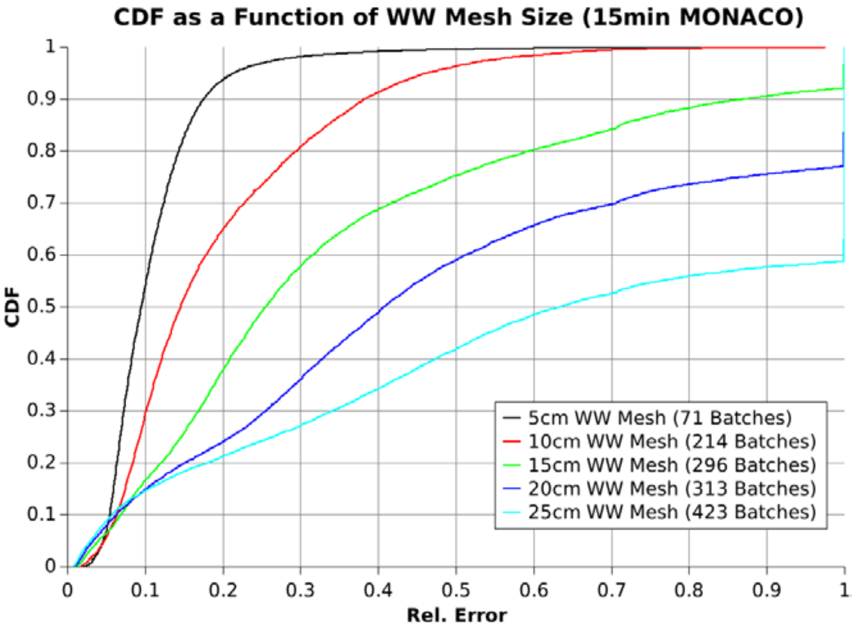

Figure 4: Benchmark to investigate the effect of the WW-mesh element size

Besides the DENOVO mesh size, the weight window ratio (upper to lower weight and bound respectively) is the most significant parameter of FW-CADIS and its optimum value is case dependent. The effect of this ratio was studied with a quarter of the reactor model and a constant WW-mesh element size of 15 cm. The result of this parameter study is shown in Figure 5. The optimum distribution was achieved with a weight window ratio of 500, which was then used for further simulations.

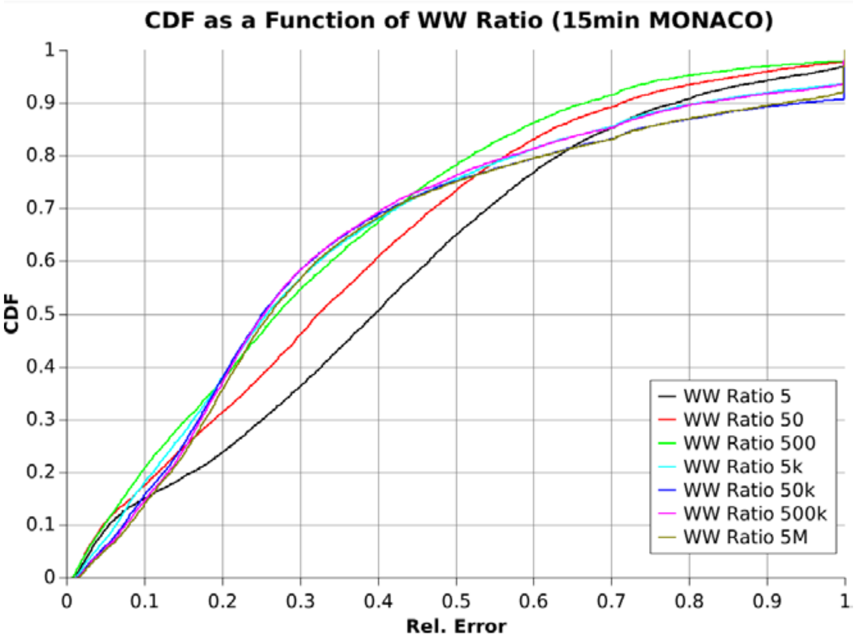

Figure 5: Benchmark to investigate the effect of the WW-ratio

Due to the geometrical and attenuation effect, the variance of the neutron flux normaly increases with distance from the neutron source of the core. Figures 4 and 5 depict clearly that with the application of a hybrid method for importance sampling and an appropriate weight window mesh size, a significant and far-reaching variance reduction in the entire geometry model is achieved. This implies a substantial rise in simulation performance and efficiency in comparison to the simulations based on the standard MCNP variance reduction methods.

As a result of the importance sampling, the optimum weight window map was generated with the SCALE6 geometry model of FRJ-2 which was then used for the detailed MCNP calculation with the CAD based MCNP outer core model and the designed surface source definition for the core. The forward deterministic estimate of the neutron flux is the first result from the FW-CADIS sequence of MAVRIC which is depicted in Figure 6, covering 12 orders of magnitude. The results, normalized to 100 particles were used to weigh the adjoint flux as given in Figure 7.

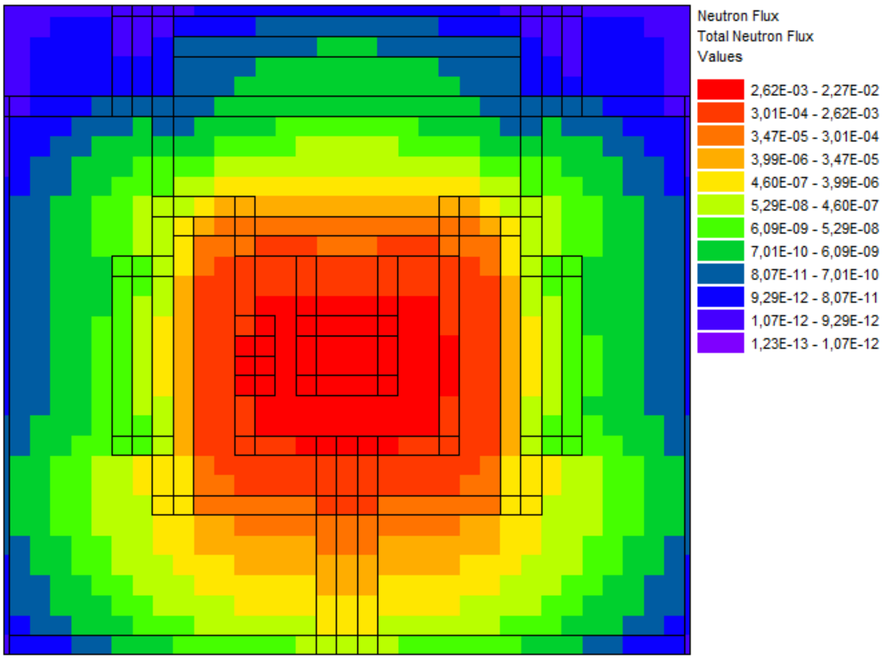

Figure 6: Distribution of the deterministic forward flux [n/s cm²]

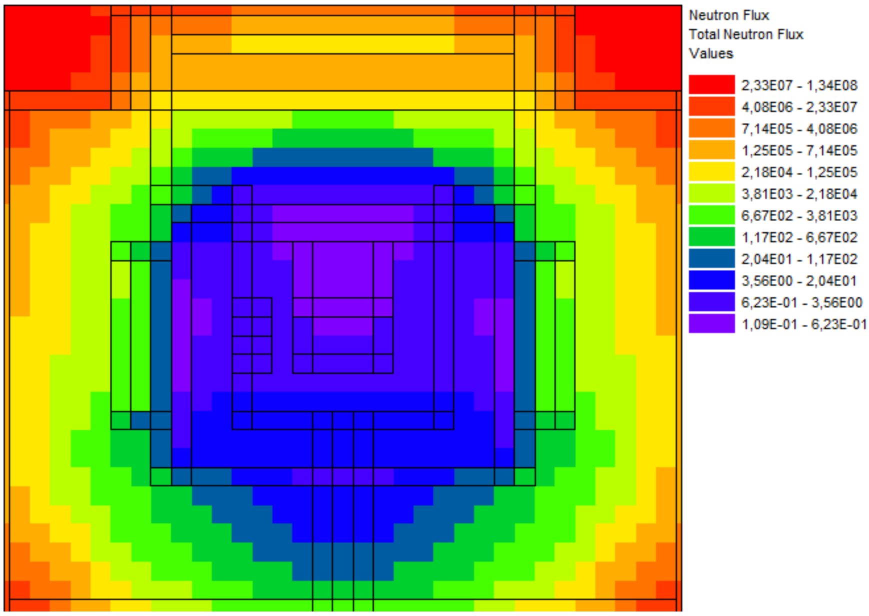

Figure 7: Distribution of the deterministic adjoint flux [n/s cm²]

The distribution of the adjoint flux in Figure 7 shows how difficult it is to simulate with low variance in the out-core structures like the biological shield. This area requires the largest importance or the lowest weight window bound to ensure a uniform distribution of the relative uncertainties in the whole geometry. The constructed importance map (Fig. 8) which is generated from the estimated forward and adjoint flux is used in the MCNP model of FRJ-2 for high precision and low variance neutron transport simulations.

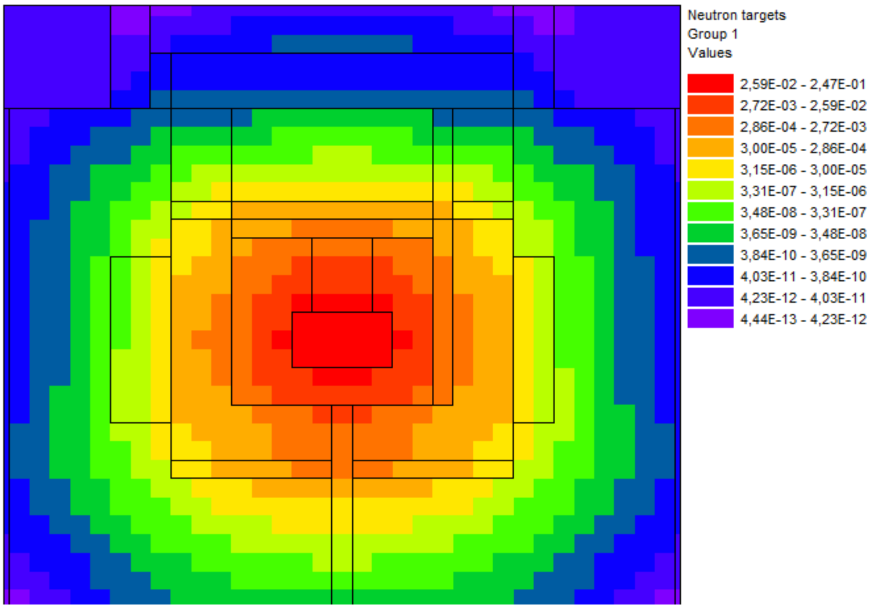

Figure 8: Distribution of weight window lower-bounds

RESULTS OF THE OPTIMIZED MONTE-CARLO-SIMULATION

The final MCNP simulation based on the converted outer core model combined with the designed surface source and optimized weight window parameters from MAVRIC sequence of SCALE6 was performed using high-performance computer systems at RWTH-IT centre.

In order to achieve sufficient neutron flux at every point of the model, a detailed 3D FMESH-grid tally with 5x5x5 cm^3 elements is applied on the whole geometry. FMESH command in MCNP allows to define a mesh tally superimposed over the whole geometry and to calculate the particle flux in units of particles/cm^2 s. The shape of the FMESH grid is independent from the geometry shape and can be rectangular or cylindrical. In this case, a rectangular shape was chosen for the simulation.

Additionally, the average values of the Figure of Merit ($\mathrm{FOM} \equiv 1/\mathrm{R}^2\mathrm{T}$, where T is the computer time in minutes and R the relative error) were calculated and compared with the analog-MCNP, using the importance map generated by FW-CADIS to determine the performance of the new method. The FOM is an indicator for the efficiency of the MCNP calculation and denotes the time required by MCNP not to exceed a given relative error. The computational time is taken from the last MCNP calculation which does not include the generation and iteration time needed for the weight window parameters (Tab. 1). Accordingly, the utilization of adjoint driven technique (FW-CADIS) leads to a significant improvement of the simulation performance in terms of statistical certainties in the whole geometrical model.

Figures 9 and 10 show the 3-D visualization of the neutron flux and the corresponding relative errors. Accordingly the relative uncertainty in the majority of the geometry is below 0.002, indicating a high level of reliability and precision. However, there are still some small regions where the statistical error is higher than 0.1. This is due to the strong shielding effect and results in lower neutron flux that could be improved by a longer simulation time.

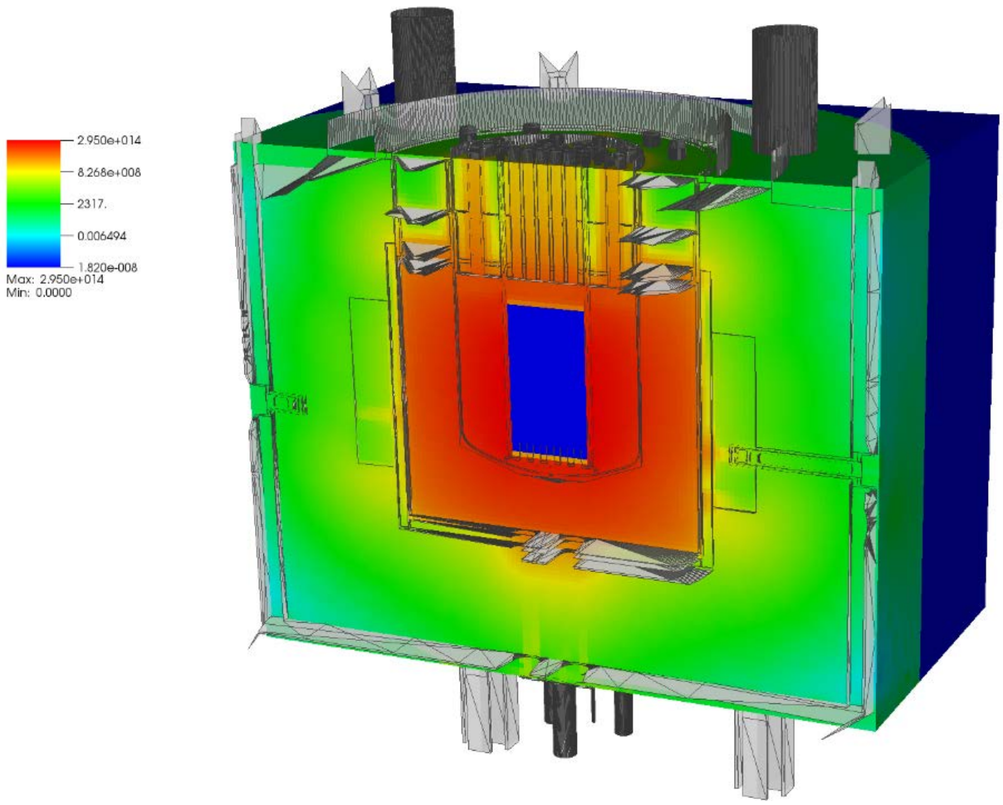

Figure 9: 3D distribution of the neutron flux over the entire geometry

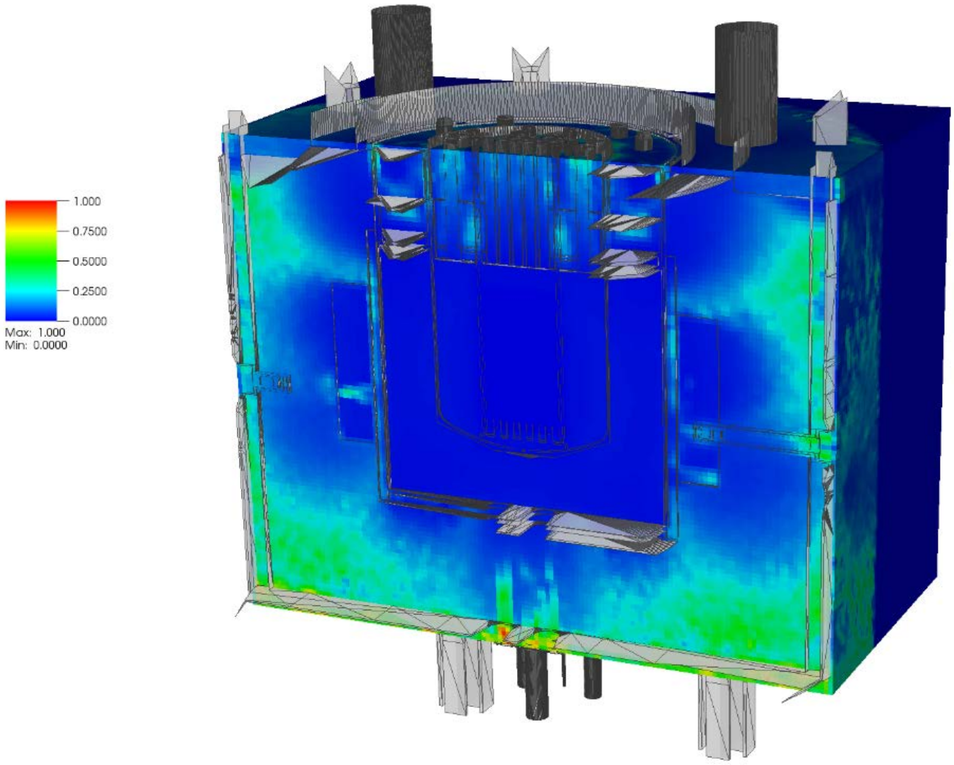

Figure 10: 3D distribution of the relative errors over the entire geometry

As mentioned above, the performance of different MCNP simulations using different variance reduction techniques was evaluated by the comparison of the FOM for different cases as given in Table 1. The results show that the larger and more constant the FOM becomes, the more efficient an MCNP simulation is. This is due to the fact that less computational time is needed to reach a given relative error and certainty level.

According to the table the average statistical error amounts to only 0.17 after a computing time of 864 hours. This computational precision and certainty (0.17) could not be achieved even after a higher computing time of 1425 hours using the standard MCNP variance reduction methods. Beside of a 1.6 times higher computational time, the average relative error remained at 55%. Comparing the methods (Tab. 1) indicates that reducing the relative errors is more influenced by the chosen variance reduction technique, particularly when using FW-CADIS. In this case the relative error is reduced by a factor of 3.2 (from 0.55 to 0.17), causing a higher FOM representing a total efficiency factor of 22.

This implies that the utilization of the new hybrid importance sampling by the FW-CADIS for MCNP applications has efficiently improved the statistical certainty and considerably reduced the variance of the neutron flux in the entire geometry, in both deep structures and distances of FRJ-2.

Parameters	**Analog MCNP**	**MCNP basic VR**	**FW-CADIS**
CPU Time [h]	1192	1425	864
Rel. Error	0.855	0.55	0.17
Avg. FOM	1.6E-03	2.3E-03	5E-02

Table 1: Comparison of the CPU-time, relative error, and average FOM for different simulation methods

DISCRIPTION AND DISCUSSION

For the decommissioning of nuclear facilities in Germany, activity and dose rate atlases (ADAs) are required to create and manage a decommissioning plan and optimize the radiation protection measures. Additionally, detailed ADAs can contribute to minimize radiation exposure of the staff involved in the dismantling and disposing activities. Finally, ADAs have the potential to efficiently reduce the cost for decommissioning as nuclear wastes can be characterized and quantified in detail which helps to minimize the total waste volume. In regard to the demand for highly detailed ADAs, an elaborate automated simulation tool was developed.

By the example of the research reactor FRJ-2, a detailed MCNP model for Monte-Carlo neutron and radiation transport calculations based on a full scale outer core CAD-model was generated. To cope with the inadequacies of the MCNP code for the simulation of a large and complex system like FRJ-2, the FW-CADIS method was embedded in the MCNP simulation runs to optimise particle sampling and weighting. The MAVRIC sequence of the SCALE6 program package, capable of generating importance maps, was applied for this purpose. The application resulted in a significant increase in efficiency and performance of the whole simulation method and in optimised utilization of the computer resources. As a result, the distribution of the neutron flux in the entire reactor structures – as a basis for the generation of the detailed activity atlas was produced with a low level of variance and a high level of spatial, numerical and statistical precision.

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