

High-Fidelity Coupled Monte-Carlo/Thermal-Hydraulics Calculations

Aleksandar Ivanov^{1*}, Victor Sanchez¹, Kostadin Ivanov²

¹Karlsruhe Institute of Technology (KIT), Institute for Neutron Physics and Reactor Technology (INR), Germany
Hermann-von-Helmholtz-Platz 1, Geb. 521, 76344 Eggenstein-Leopoldshafen

²The Pennsylvania State University, 206 Reber Building University Park, PA 16802, USA

*Corresponding Author, E-mail: Aleksandar Ivanov, aleksandar.ivanov@kit.edu

Monte Carlo methods have been used as reference reactor physics calculation tools worldwide. The advance in computer technology allows the calculation of detailed flux distributions in both space and energy. In most of the cases however, those calculations are done under the assumption of homogeneous material density and temperature distributions. The aim of this work is to develop a consistent methodology for providing realistic three-dimensional thermal-hydraulic distributions by coupling the in-house developed sub-channel code SUBCHANFLOW with the standard Monte-Carlo transport code MCNP. In addition to the innovative technique of on-the fly material definition, a flux-based weight-window technique has been introduced to improve both the magnitude and the distribution of the relative errors. Finally, a coupled code system for the simulation of steady-state reactor physics problems has been developed. Besides the problem of effective feedback data interchange between the codes, the treatment of temperature dependence of the continuous energy nuclear data has been investigated.

KEYWORDS: MCNP, SUBCHANFLOW, Monte-Carlo, Criticality, Coupled calculations

I. Introduction

MCNP [1] is a well-known code for performing criticality and fixed source neutronics calculations. These calculations are usually done using homogeneous distributions of the thermal-hydraulic boundary conditions. This assumption is a rather crude approximation. Both, the eigenvalues and flux distributions, computed in this manner, are only approximate and can be much different from the actual steady state conditions in the reactor core, especially at reactor operating conditions. MCNP has not been designed for performing coupled thermal-hydraulics calculations. Defining distributions in MCNP using only the default features of the code is very inconvenient. This reduces to explicitly defining material cells, where the distribution values are supplied. In practical terms this means defining a huge number of cells. This is necessary even for simple (at first glance) problems, such as single fuel assembly model. In order to overcome this difficulty, a more generic approach of coupling via common modules and supplying the feedback data on the fly is proposed.

Proper introduction of the thermal hydraulic feedback is only one side of the problem. Another major issue is the non-uniform distribution of the relative errors. Calculating large loosely coupled criticality problems typically results in very large variances, difficult to resolve with simple increase of the neutrons histories. Such a strategy is highly inefficient due to the non-uniform distribution of the relative errors. Using it, one obtains significant effect on the relative errors in regions with high flux values, while only small gain is obtained in the regions with small flux estimates. Increasing

the number of the neutron histories results also in an unacceptable increase of computing time. In this paper, the technique of defining weight windows, based on the flux estimate, is applied [4]. Using this technique it has been possible to produce both uniform distribution of the relative errors and their reduction in magnitude.

II. Coupling between MCNP and SUBCHANFLOW

MCNP uses multi-level geometry notion, meaning that the neutrons have set of coordinates, defined at each level of the problem geometry. The multi-level notion of the MCNP geometry is connected to the universe and repeated structure concepts, allowing the insertion of separate geometry units in other units or lattices. For instance the positioning of the individual pins within the core can be described by using the following geometry structure:

```
PIN_CELL <  
  <PIN_LATTICE[ ipin, jpin, kpin ]<  
<ASSEMBLY_LATTICE[ iassembly, jassembly, kassembly ]
```

In MCNP neutrons are tracked, and at every instant of their path each one of them has a specific set of lattice indices attached. These lattice indices are used for the definition of a bijective mapping between the neutronic and the thermal-hydraulic domains. Using this mapping and knowing the neutron coordinates, continuous supply of thermal-hydraulic feedback parameters is done, while the neutron is moving throughout the space. According to this method only the geometry dimensions should be properly

defined. The initial material specification is arbitrary, since it is continuously updated during the criticality calculation. A graphical illustration of the coupling strategy is shown in **Figure 1**:

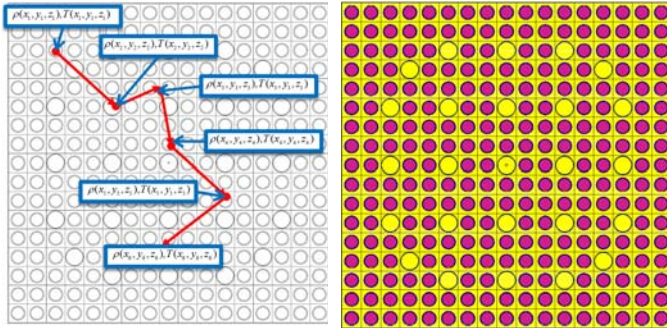


Figure 1: Continuous supply of feedback data and the effective geometry seen by the neutron as it moves.

In practical terms the implementation of the method relies on the fact that MCNP recalculates the values of the macroscopic nuclear cross sections according to the position and the energy of the neutron. If the standard version of MCNP is to be used, the code will retrieve the material distribution defined in the input. Using the current method, however, the coupled scheme intervenes before the values of the relevant macroscopic cross sections are calculated and supplies the proper nuclear data in accordance to the thermal hydraulic feedback. If the cell is filled with moderator, the proper density values have to be supplied. In this manner one introduces a thermal hydraulic distribution independent on the initial input. To account for the temperature dependence of the nuclear data the pseudo material mixing (PM) has been used [3]. Although simple for the single differential data, dealing with the double differential cross section is more involved. In this case one has to assign also the proper thermal scattering data tables. Since it is not possible to use two different thermal scattering evaluations for the same isotope within single material, the PM has to be modified. This is done by introducing artificial isotopes of hydrogen corresponding to the different temperature evaluations. Using this strategy, the pseudo material mixing reduces to **Figure 2**.

```
m1  1004.97c  0.333333  $ H 523.6 K
    8016.97c  0.166667  $ O 523.6 K
    1006.99c  0.333333  $ H 623.6 K
    8016.99c  0.166667  $ O 623.6 K
mt1  lwa106.31t lwa108.31t
```

Figure 2. Illustration of the pseudo material thermal scattering mixing for 573.6 K

Therefore, a special subroutine capable of selecting the proper thermal scattering data has been included. MCNP must be run in parallel for all serious problems larger than few pins. Therefore, when introducing feedback one should make sure that all of the slave processes receive proper feedback information. MCNP calls the MPI routines via FORTRAN-C binding DOTCOMM. The same formalism has been kept for the extensions regarding the

intermodal communication. SUBCHANFLOW has been included in the MCNP source as a separate subroutine. In the coupled scheme the thermal-hydraulic calculations are run on the master node, and once they have converged the results are transferred to all of the slave processes. From this point further the criticality calculation is initiated. To speed up the calculation, the necessary information for building the temperature dependent macroscopic cross sections is stored into arrays on the master node. Therefore, during the actual neutronic calculation, ready to use information is retrieved and the nuclear data selection process is avoided. All the necessary nuclear data has to be loaded into the memory, before the selection subroutine starts. This is done by using dummy material. For the thermal-hydraulic analysis the SUBCHANFLOW code, which is under development at the KIT has been used. It is a 3-equation based sub channel code, used to solve energy, mass and momentum conservation equations for vertical flow conditions.

III. Testing the code modifications

Since we are introducing a method, which is expected to be completely equivalent to the standard MCNP input, verifying the coding is rather straightforward. The first test case has been a 3x3 pins BWR problem with 60 axial nodes. The second case has been a 17x17 pins PWR assembly problem. Finally, in order to verify the embedded surface case, the 3x3 BWR problem has been embedded into a larger 2x2 lattice. In all the cases a thermal hydraulic distribution has been simulated with the internal coupling and compared to the standard MCNP input. In both the cases both the fission heat deposition and the eigenvalues were absolutely identical.

IV. Coupled calculations with the newly developed code system

Each coupled calculation begins with a SUBCHANFLOW run, assuming a cosine axial power profile and a flat radial pin power distribution. Following the previous work performed at KIT [3], the variation of the node averaged fuel temperature has been used for monitoring the convergence. The following criterion (1) has been imposed on the fuel temperature, and has been used as an estimate for the convergence.

$$\Delta T_{ij} = \left| \frac{T_{ij}^{\text{last}} - T_{ij}^{\text{prev}}}{T_{ij}^{\text{last}}} \right| < \varepsilon \quad (1)$$

Here, the indices “i” is the pin number and “j” is the axial cell number. The indices run over all pin cells in the problem. It should be taken into account that the tallies used to sample the power profile distribution have statistical uncertainties affecting the fuel temperature.

V. Accelerating the coupled calculation

Running simple consecutive iterations of the thermal-hydraulics and neutronics codes will not produce a

steady convergence behavior. To accelerate the coupled calculation a stochastic approximation scheme has been used. Complete mathematical derivation of the scheme can be found in references 6,5.

The steady state power distribution is a fixed point of the following nonlinear problem.

$$\varphi = G(T(\varphi), H(\varphi)). \quad (2)$$

$H(\varphi)$ and $T(\varphi)$ are the density and temperature distributions. The value of $G(T(\varphi), H(\varphi))$ is estimated by the Monte Carlo code with superimposed statistic noise ε . The Monte-Carlo estimate of the left hand side of (2) is defined as (3)

$$Y(\varphi) = G(T(\varphi), H(\varphi)) + \varepsilon \quad (3)$$

The problem as given by (2) can be in principle solved by an iterative scheme, consecutively updating $H(\varphi)$ and $T(\varphi)$. However, this is a very inefficient method. Moreover, the convergence will be limited by the magnitude of ε . Therefore, in order to achieve convergence one must run a large number of iterations, applying huge number of particle histories. Based on this, it is recommended to use an acceleration scheme. In the past relaxation scheme, acting on the thermal-hydraulic parameters only, has been used 3. The old relaxation scheme is described by the equation set (4), where “ i ” is the iteration step number.

$$\begin{aligned} T_{\text{fuel},i+1}^{\text{weighted}} &= (1-\omega)T_{\text{fuel},i-1} + \omega(T_{\text{fuel},i}^{\text{actual}}), \\ T_{\text{H}_2\text{O},i+1}^{\text{weighted}} &= (1-\omega)T_{\text{H}_2\text{O},i-1}^{\text{actual}} + \omega(T_{\text{H}_2\text{O},i}^{\text{actual}}), \\ \rho_{\text{H}_2\text{O},i+1}^{\text{weighted}} &= (1-\omega)\rho_{\text{H}_2\text{O},i-1}^{\text{actual}} + \omega(\rho_{\text{H}_2\text{O},i}^{\text{actual}}). \end{aligned} \quad (4)$$

This scheme accelerates the convergence. Unfortunately the value of the convergence parameter is still correlated to the statistical noise. The natural method of acceleration for problem (2) is to use a stochastic approximation technique 5,6. The theorem of Robbins and Monro is the key ingredient need to justify the new relaxation scheme. The formulation of the theorem as well as the proof can be found in 7. The basic idea is, that by observing random variables $Y(\varphi_n)$ having unknown distribution, roots of the unknown underlying distribution can be found. In the particular case this description fits precisely the estimate of (3). Applying the Robins - Monro theorem the following expression for the flux after running (n) iterations has been derived

$$\varphi^{(n+1)} = \frac{1}{n} \sum_{i=1}^n Y(\varphi_i) \quad (5)$$

Formula (5) gives the explicit formulation of the relaxation scheme. The flux (power profile) in the next coupled iteration is obtained to be the mean value of all the previous iterations. Since the tally estimates from all the runs are added together, simple error propagation with partial derivatives on (5) shows a decreasing error when increasing the number of iterations. Moreover, it follows that all

iterations are reflected in the final solution with weight $1/n$. Therefore, any desired convergence parameter can be achieved, if enough number of iterations are run. This is still possible even with low number of histories. Nevertheless, the number of histories and the number of inactive cycles should be chosen adequate, to ensure the fission source convergence. Moreover, the effect of increasing the number of histories in the old scheme is achieved by running more iterations in the new scheme.

In **Figure 2** the scheme of the coupled system MCNP5/SUBCHANFLOW is shown.

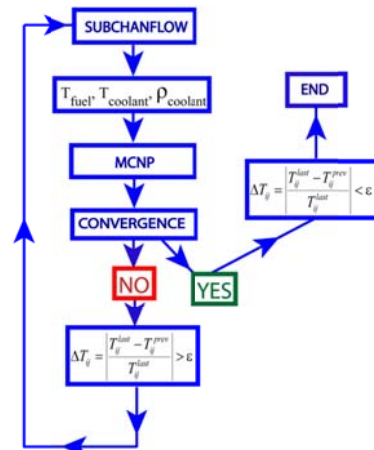


Figure 2: Couple MCNP5/SUBCHANFLOW system

VI. Variance reduction with flux based Weight Windows

Performing coupled iterations requires tallying of the neutron fission rate in geometries containing thousands of cells. Achieving proper statistical uncertainties is necessary, if one desires to reduce the number of iterations needed for convergence. Achieving this goal is not a trivial task. The main problem is the non-uniform distribution of the relative errors. Therefore, brute-force increase of the number of histories would be very inefficient. The utilization of a variance reduction scheme is a more adequate alternative method.

Assume that the problem is subdivided into cells and one would like to obtain as small as possible relative error in each cell. In the particular case, these are the lattice unit cells. Moreover, the relative errors should have uniform distribution. This can be achieved if one can ensure equal particle population in each cell. Using Weight Windows (WW), MCNP can be forced to split the particles when entering low populated cells. Suppose the middle of the WW in each cell is set proportional to the flux estimate in it. In regions with low flux levels, WW with low upper bounds and exactly the opposite for highly populated cells are obtained. Therefore, the particle population is increased in the due cells without biasing the total score. This idea has been proposed in 4. There, the lower bounds of the WW have been set according to the following formula

$$W_{low} = ((\beta + 1)/2)^{-1} \frac{\varphi_i}{Max\varphi_i} \quad (6)$$

Close observation of (6) shows that the reference cell is the one having the largest flux estimate. In all other cells the particles are split in order to obtain the same population as that in the reference cell. In those regions where the flux score is low, almost all particles entering the cell have weights higher than the upper bound of the WW. Therefore, they would be divided into number of daughter particles with weights modified to fit into the WW. The parameter β is the ratio of the upper and lower bounds of the WW. The default value of MCNP, $\beta=5$, has been used. In practice the method involves generating a WW file (WWINP) with a MCNP flux tally. The WW mesh should be set to precisely overlap the mesh tally. The WW file is updated with each

coupled iteration. To illustrate the results of this technique consider the following plots showing the distribution of the relative errors **Figure 3, Figure 4**. It is evident that applying large number of neutron histories has not solved the problem of large relative errors and their non-uniform distribution. Using flux based WW mesh however has produced a very uniform relative error distribution, having similar in magnitude values in comparison to the analog calculation. It should be noted that UOX and MOX assemblies with different enrichments are present in the problem, which explains the slightly different values. For performing these comparison tests, thermal hydraulic boundary conditions from the first coupled iteration have been used.

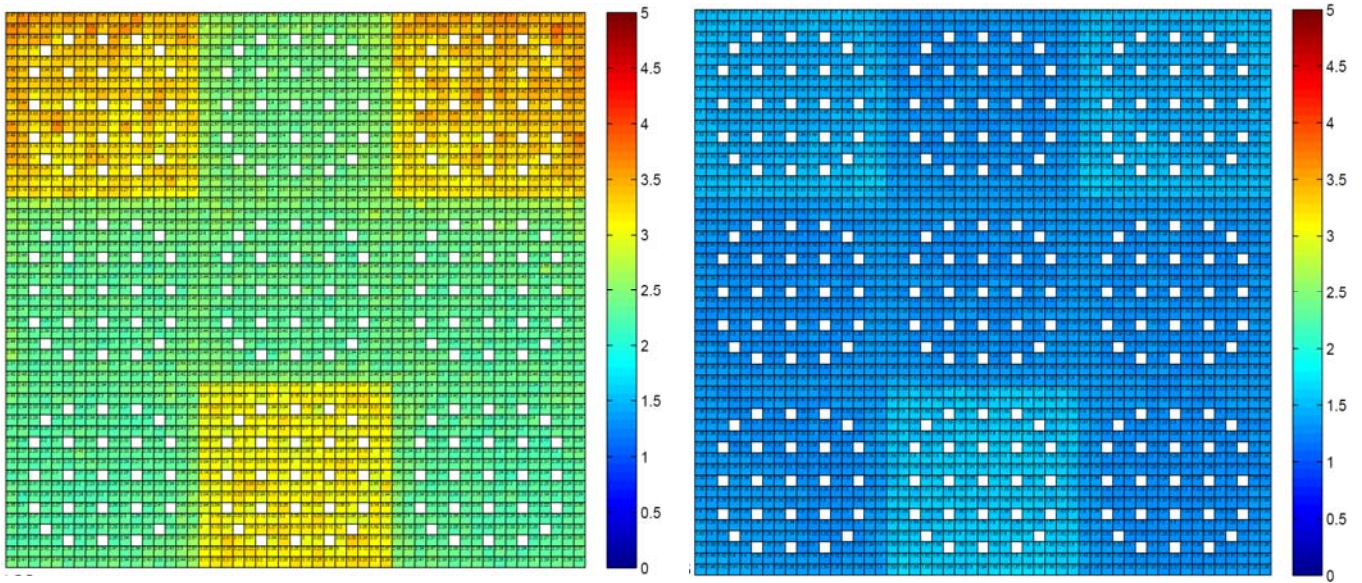


Figure 3: Plot of the relative error distribution for the first axial level. The values shown in the left plot are obtained with 220k histories per cycle and no WW. The values in the right plot are generated with WW and 100k histories per criticality cycle.

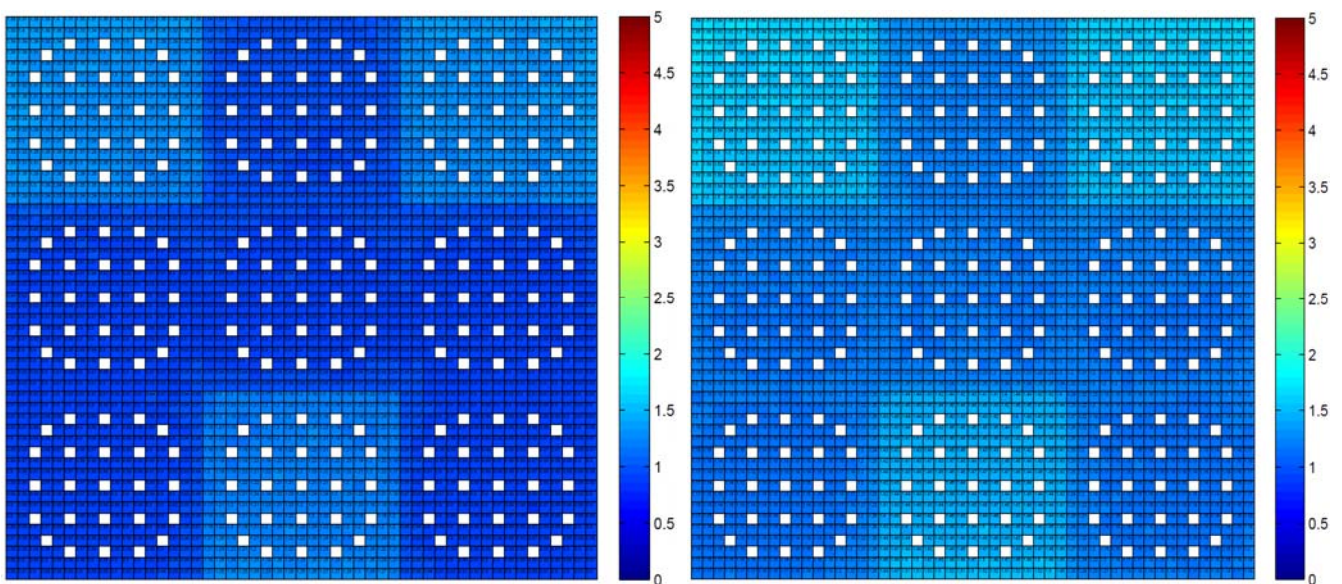


Figure 4: Plot of the relative errors distribution for the mid plane. The same problem as in Figure 2

V. Applying the coupled scheme to a PWR mini-core

Having described the coupled scheme and the convergence acceleration strategies, it is possible to proceed further describing the computational problem. A PWR 9x9 fuel assembly problem has been selected. This large problem was chosen with the purpose of demonstrating the capabilities of the coupled scheme. Due to this reason, it was chosen to run a pin-by-pin calculation. The geometry and the material definitions have been derived from the PWR UOX-MOX benchmark 8). Variation in comparison to the benchmark has been introduced by using only one type of pins. Two types of fuel assemblies have been used, MOX with 2.5 wt% Pu and fresh UOX with 3.8 wt% U235. Coolant containing 1500 ppm Boron has been used. The fuel assembly map is shown below.

MOX	UOX	MOX
UOX	UOX	UOX
UOX	MOX	UOX

This enrichment pattern has been selected to introduce more pronounced differences in the assembly power distribution. The thermal-hydraulic boundary conditions have been identical to those described in the benchmark. The total of 104040 individual cells has been defined. The fission rate has been tallied in 52020 volumes. Each assembly has been divided into 20 axial nodes. The power profile has been tallied with a mesh tally. This input would have been impossible to define and compute with the standard capabilities of MCNP. The resulting input for the neutronics would have consisted of over a million input lines. Using the method of internal coupling between the thermal-hydraulic and neutronic codes, it has been possible to define a very simple input and run the problem without any obstacles. The coupled

calculation has been run on 80 processors and each MCNP run took approximately 35 mins. In spite of the complicated geometry, uniform convergence behavior has been observed. It has been possible to achieve convergence $\epsilon=0.114\%$. The convergence parameter has been observed to fall below 0.5% after running 7 coupled iterations. The coupled calculation has been run 25 iterations and therefore, it was possible to reach values of the convergence parameter significantly lower than 1%. This has been done only to test the stability. Variations of 0.5% are on the order of 1.5 K in absolute value. The criticality eigenvalue has shown large inertia towards the change in the thermal-hydraulics conditions. Converged in terms of the criticality eigenvalue have been considered those runs with criticality eigenvalue not oscillating outside of the band defined by the eigenvalue statistical uncertainty. The eigenvalue convergence was reached after running 3 coupled iterations. The first results from the coupled calculation to be shown are two dimensional plots of the fission rate from the first and core mid planes. Note the very low estimate in the first node compared to the values from the core middle corresponding to cosine-like distribution **Figure 5** Note also the differences in the assembly powers, corresponding to the different enrichments.

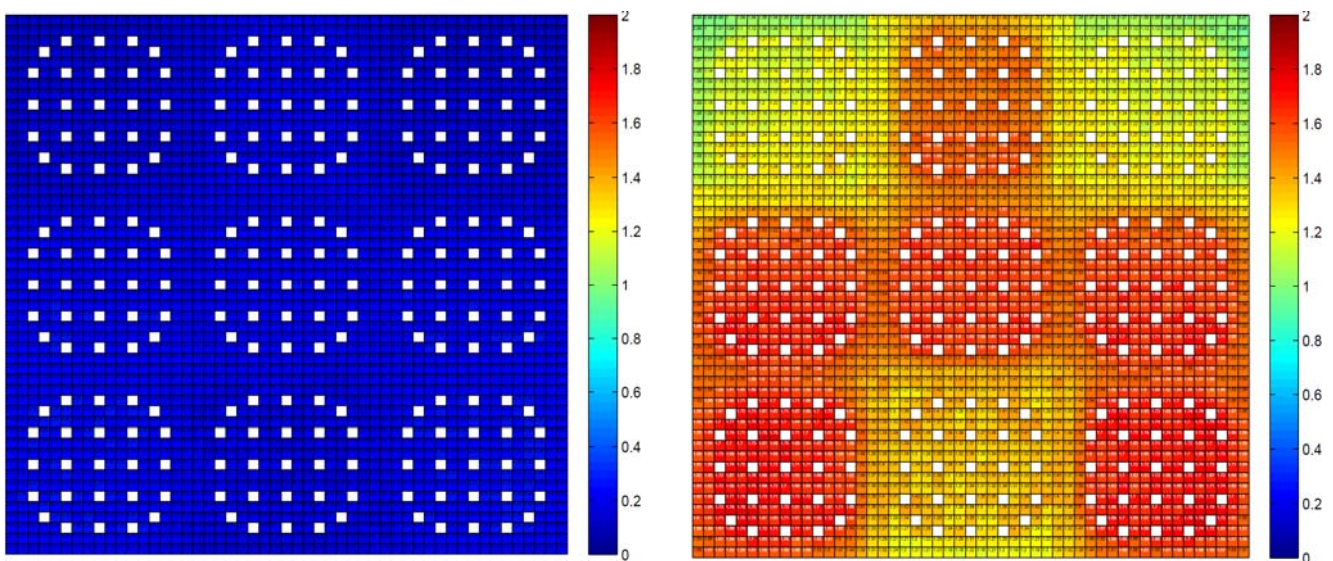


Figure 5: Fission rate distribution for two vertical cuts.

In addition to the radial fission rate distribution, axial distribution is shown in the following **Figure 6**. The indices showing the pin location have the following meaning. Each assembly is represented by a two-dimensional matrix with dimension offsets $|\text{INDEX}| \leq 17$ and the fuel assembly map is represented by a matrix having dimension offset $|\text{INDEX}| \leq 1$. The reader might right away see the effect of the WW technique used to reduce the variance. The power profile is smooth and has no unphysical tilts.

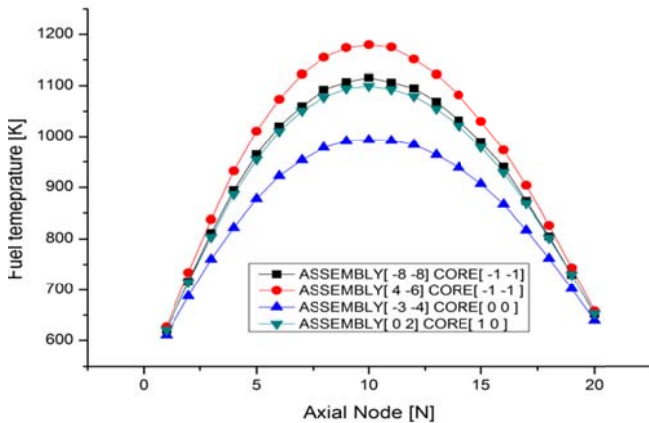


Figure 6: Axial distribution of the fission power deposition for selected pins.

VI. Conclusions and outlook

Using the internal coupling scheme has made a large coupled calculation between MCNP and the thermal-hydraulics code SUBCHANFLOW tractable. The convergence has been stabilized using a stochastic approximation technique. The efficiency of the power profile estimate has been improved by applying a flux based Weight Window scheme. All those innovations have resulted in a consistent calculation, capable of achieving the desired convergence. Currently the calculations scheme is under testing on a quarter core PWR model.

Acknowledgments

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References

- 1) X-5 Monte Carlo Team, *MCNP A General Monte Carlo-N-Particle Transport Code, Version 5, Volume I, MCNP Overview and Theory*, Los Alamos National Laboratory Report, LA-UR-03-1987, April 24, 2003 (Revised 10/3/05).
- 2) “PSG2 / Serpent Monte Carlo Reactor Physics Burnup Calculation Code,” <http://montecarlo.vtt.fi> (2011).
- 3) A. Ivanov, V. Sanchez, K. Ivanov, “Optimization of a Coupling Scheme Between MCNP5 and SUBCHANFLOW for High Fidelity Modeling of LWR Reactors”, *PHYSOR 2012 – Advances in Reactor Physics – Linking Research, Industry, and Education Knoxville, Tennessee, USA, April 15-20, 2012*
- 4) van Wijk A., Van den Eynde G., Hoogenboom E. “An easy to implement global variance reduction procedure for MCNP”, *Annals of Nuclear Energy*, 38:11(2011), p. 2496-2503.- ISSN 0306-4549
- 5) J. Dufek and W. Gudowski: Stochastic Approximation for Monte Carlo Calculation of Steady-State Conditions in Thermal Reactors, *Nuclear Science and Engineering*: Vol. 152, pp. 274–283, (2006)
- 6) A. Ivanov, V. Sanchez, R. Stiglitz, K. Ivanov: Internal Multi-Scale Multi-Physics Coupled System for High Fidelity Simulation of Light Water Reactors, *Accepted for publication Annals of Nuclear Energy*.
- 7) M.T. Wasan, *Stochastic approximation*, Cambridge University Press, 1969
- 8) PWR MOX/UO₂ Core Transient Benchmark, T. Kozłowski, T. Downar, <http://www.oecd-nea.org/science/wprs/MOX-UOX-transients/>