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DEVELOPMENT OF A COUPLING SCHEME BETWEEN MCNP5 AND SUBCHANFLOW FOR THE PIN- AND FUEL ASSEMBBLY-WISE SIMULATION OF LWR AND INNOVATIVE REACTORS

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ABSTRACT

In order to increase the accuracy and the degree of spatial resolution of core design studies, coupled 3D neutronic (deterministic and Monte Carlo) and 3D thermal hydraulics (CFD and subchannel) codes are being developed worldwide. At KIT both deterministic and Monte Carlo codes were coupled with subchannel codes and applied to predict the safety-related design parameters such as pin power, maximal cladding and fuel temperature, DNB. These coupling approaches were revised and improved based on the experience gained. One particular example is replacing COBRA-TF with SUBCHANFLOW ,in-house development subchannel code, in the COBRA-TF/MCNP coupling, accompanied with new way of radial mapping between the neutronic and thermal hydraulic domains. The new coupled system MCNP5/SUBCHANFLOW makes it possible to investigate variety of fuel assemblies types (BWR, PWR or SCFR). Key issues in such a coupled system are the way in which thermal-hydraulic/neutronic feedbacks, accuracy of the Monte Carlo solutions and observation of convergence during the iterative solution are handled. Another key issue might be considered optimal application of parallel computing. Using multi-processor computer architectures it is possible to reduce the Monte-Carlo running time and obtain converged results within reasonable time limit. In particular it is shown that by exploiting the capabilities of multi-processor calculation, it is possible to investigate large fuel assemblies in a pin-by-pin manner with a resolution at pin and subchannel level. One of the most important issues addressed in the current work is the temperature effects on nuclear data. For the particular studies pseudo material approach was used which produces interpolated results for Doppler broadened cross sections from NJOY pre-generated nuclear data.

Key Words: COUPLED CODES, MCNP5, SUBCHANFLOW, DESIGN, SAFETY, HPC.

1 INTRODUCTION

High fidelity coupled solutions of neutron physics and thermal hydraulics codes are being developed worldwide to increase the accuracy and the degree of spatial resolution of core design studies. For example coupled 3D neutronic (deterministic and Monte Carlo) and 3D thermal hydraulics (CFD and subchannel) codes were realized [1], [2], [3] and [4]. At Karlsruhe Institute of Technology (KIT) both deterministic and Monte Carlo codes have been coupled with subchannel codes and applied to predict the safety-related design parameters such as pin power, maximal cladding and fuel temperature of a PWR fuel assembly [5], [6].

In this paper, the further development and improvement of these coupling approaches will be presented. In particular COBRA-TF code was replaced by the in-house development SUBCHANFLOW code, a modern, modular fast running subchannel code written in Fortran 95 [7], in the already existing COBRATF-MCNP5 coupled code system. In addition, a more generic radial mapping between the neutronic and thermal hydraulic domain was realized and new data interchanging programs where written. The developed system MCNP5/SUBCHANFLOW makes it possible to investigate different types of fuel assemblies (BWR, PWR or SCFR) without modifying the interface which excanges data between thermal hydraulic and neutronic domains. Details of the coupling scheme as well as treatment of temperature dependency of the continuous energy cross sections will be explained in detail. Due to the statistical nature of MCNP, most of the computation time of the coupled calculation is spent in running it. However using parallel processors it is possible to reduce dramatically the computation time, and complete the coupled run in reasonable time. Hence the coupled approach was developed for a multiprocessor environment. By means of Portable-Batch-System scripts MCNP5 is run in parallel while SUBCHANFLOW is run consecutively in a single processor mode. The developed coupling scheme was applied to perform detailed 3D simulations of different problems representing PWR, BWR and a steam cooled fast reactor (SCFR) fuel pin clusters. Latter one was a whole hexagonal fuel assembly consisting of 271 pins while the PWR and BWR problems represented a 3x3 cluster of fuel pins.

2 CODES TO BE COUPLED

The Monte Carlo MCNP5 and the thermal hydraulic subchannel code SUBCHANFLOW are selected for these investigations.

2.1 The Thermal Hydraulic Subchannel Code SUBCHANFLOW

For performing the sub-channel analysis, SUBCHANFLOW [7], [8] a code developed at KIT former (FZK), was used. It is based on COBRA code family and is able to treat hexagonal and square bundle geometries with axially varying cell size. It is written in Fortran 95 language in fully modular way. Global data structure as wall as fluid and material properties are stored in separate modules. The code solves mass momentum and energy equations based on 3 equation approach for vertical flow conditions. In contrast to all COBRA-version, it is based on SI system of units. SUBCHANFLOW can investigate water, lead, lead-bismuth and sodium as working fluid. Using SUBCHANFLOW it is possible to run the 271 pins SCFR fuel assembly problem within 1.2 minuets, and by doing so significantly reduces the computation time.

2.2. The Neutronic Code MCNP5

MCNP5 solves the integral transport equation in 3 dimensions using Monte-Carlo simulation technique [9] and [10]. In the coupled run MCNP5 is used to generate power profile which is than transferred to SUBCHANFLOW. In order to read the power profile F7:n neutron tally and F4:n mesh tally are used. NJOY99 [11] code was used to generate Doppler-Broadened continuous energy cross sections which where subsequently used in the actual MCNP computation.

3 MCNP5/SUBCHANFLOW COUPLING SCHEME

In coupling codes describing different physical phenomenon in particular neutronics and thermal hydraulics, the spatial discretization of both domains has to be mapped to each other so that the exchange of information- in this case the feedback parameters – can be carried out in a consistent manner. In addition, how the iteration loop is initiated is also important. Furthermore, one has to make sure that a converged solution is obtained after running reasonable number of coupled iterations.

3.1 Radial mapping of neutronic and thermal hydraulic domains

The ideal case is to have a 1:1 mapping between the axial and radial nodalization of the two codes being involved in the coupling. This was the case for the investigations performed here. In order to transfer data between the codes, two PERL-scripts where developed for the automatic data interchange between the domains and to check the convergence. As shown in Figure 1 the MCNP-universe corresponds to the SUBCHANFLOW fuel rod in the radial nodalization scheme.

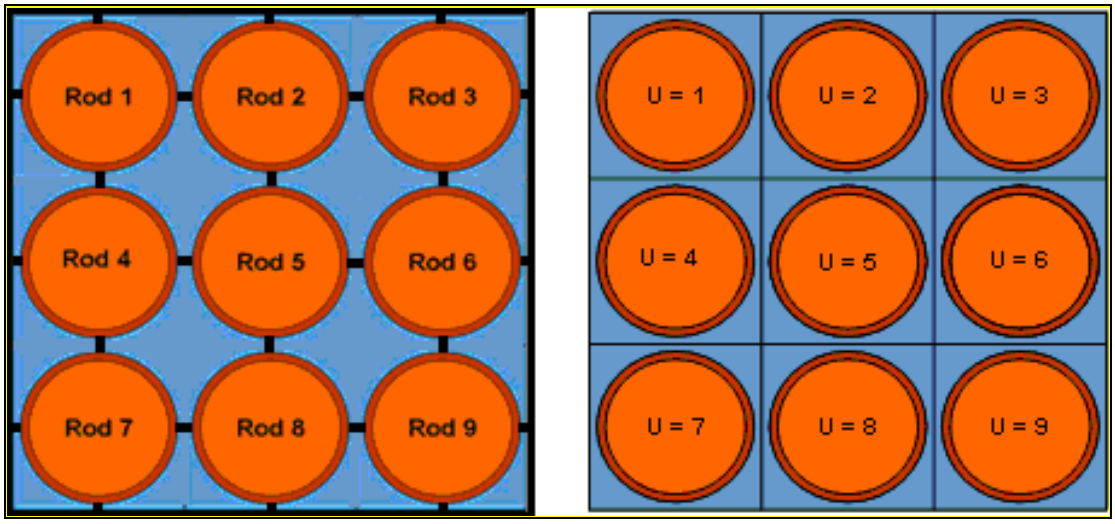


Figure 1 Radial nodalization in SUBCHANFLOW and MCNP

In order to read the axial power profile F4:n neutron mesh tally, together with MCNP5 tally multiplication card feature where used. Again the mesh tally should be chosen in coherence with the axial nodalization of the sub-channel code. Doing so, values in the middle of each axial cell are supplied and no interpolation is done on the side of SUBCHANFLOW. It is important to mention that nodal volume average of the fuel temperature of each pin is supplied to MCNP. For coolant density and coolant temperature values averaged over the sub channel area are used.

Each coupled calculation begins with SUBCHANFLOW run assuming a cosine axial profile and a flat radial pin power distribution. Following the previous work performed at KIT [6] the variation of the node averaged fuel temperature is used for checking the convergence. Convergence is met when the variation of the node averaged fuel temperature is less than 0.5 % In the following **Figure 2** scheme of the coupled system MCNP5/SUBCHANFLOW is shown

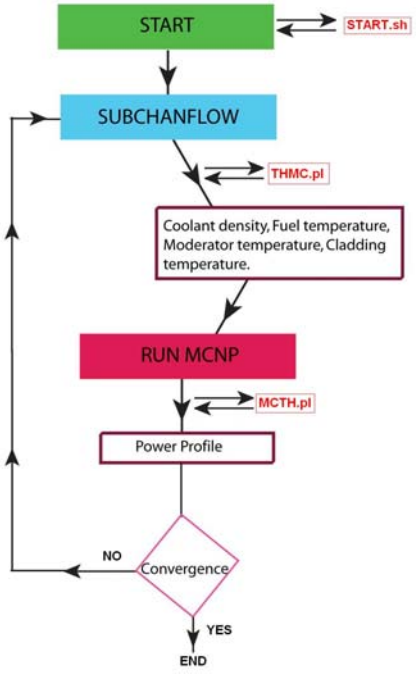


Figure 2 Coupled MCNP5/SUNCHANFLOW System

In order to avoid long waiting times in the queue, the coupled calculation is performed by single batch job. In this way once the number of processors required by the job is free, the calculation proceeds without delays. Computations were performed in parallel mode. The number of processors varies form 60 for the smaller MCNP inputs up to 120 for the whole fuel assembly of the SCFR.

It is worth to mention that this approach of coupling is flexible to treat variety of problem geometries providing the fact that specific formalism is observed when input files for the calculation are prepared, this flexibility is made possible by using keyword markers and the powerful pattern matching capabilities of PERL language.

3.2 Doppler broadening of nuclear cross sections

Since nuclear cross sections depend on relative velocity in the centre of mass system, temperature induced oscillations of the target atomic nuclei, which induce such changes, result in

Doppler effect on its side being one of the most important phenomenon in nuclear reactor safety. From thermal-hydraulics run different material temperatures are supplied. Hence the effect on the corresponding nuclear cross sections should be considered. MCNP is capable to make correction to nuclear data when they are used at temperatures different from those they are generated [2]. However this method is not precise enough, especially in cases when deviations from the default temperature are large. A possible solution is to adapt online nuclear data by running NJOY at each iteration step as has proposed in [12].
However in practical terms it may mean loss of large CPU time in running NJOY. In order to avoid this situation another more practical approach was followed here. After initial run of the thermal hydraulic code, intervals in which fuel and moderator temperature vary were determined. Later on, those intervals were divided into 50 K or 100 K increments. For the case of 50 K intervals NJOY 99 was used to generated the necessary broadened cross sections based on JEFF.3.1.1 library. On the other side for the case of 100 K increments nuclear data based on JEFF 3.1 already available on KIT computer cluster was used. NJOY was run by using automatic tool which enables the preparation of cross sections based on parameters defined by the user. In the actual MCNP calculation pseudo-material approach was used to interpolate the nuclear data already adapted with NJOY at fixed temperatures, where to each cell pseudo-material being mixture of two materials is assigned. The two materials used have temperatures being upper and lower bound of the particular interval in which the actual temperature obtained from SUBCHANFLOW is laying. For the atom fraction of the material obeying lower temperature we have

$$f_{low} = \frac{\sqrt{T_{high}} - \sqrt{T_{actual}}}{\sqrt{T_{high}} - \sqrt{T_{low}}}, \quad (1)$$

and for the higher temperature material in the mixture we have

$$f_{high} = 1 - f_{low}. \quad (2)$$

By using the pseudo material approach we obtain the following cross section

$$\Sigma_{pseudo}(T_{actual}) = f_{low}\Sigma_{low}(T_{low}) + f_{high}\Sigma_{high}(T_{high}). \quad (3)$$

In order to illustrate this method, two simultaneously plotted cross sections for the main resonance of U_{238}^{92} at 6.674 eV are shown in **Figure 3**. One cross section is obtained via NJOY at temperature of 650K and the other one is calculated by the pseudo material approach with materials at 700K and 600K.

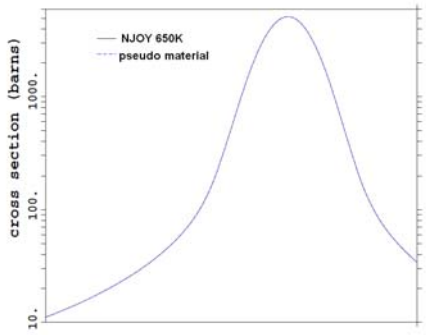


Figure 3 Comparison between NJOY generated nuclear cross section and pseudo material approach

3.3 Effect of temperature interpolation grid

The consistency of the interpolation scheme was tested for a simple one pin PWR problem. One calculation was run with the fuel temperature at 650 K with cross sections obtained at exact temperature via NJOY and 650 K interpolation between 600 K and 700 K. It should be taken into account that the same initial set of JEFF.3.1.1 cross sections were used as NJOY input. This is necessary in order to eliminate differences arising due to the application of different nuclear data. During the run TMP-card was also included in the MCNP input. Results are summarized in following **Table I**.

Table I k_∞ computed with exact NJOY processed data, and using the pseudo material approach.

Case	k_∞	Standard deviation	cycles	Histories per cycle	Skipped cycles
650K NJOY JEFF 3.1.1	1.38477	0.00005	250	500 k	30
650K Interpolation JEFF 3.1.1	1.38479	0.00005	250	500 k	30

This interpolation scheme was explored in [13] for benchmark problems and experimental data, and good agreement was found between for k_∞ calculated with NJOY processed data and the interpolation scheme.

3.4 Convergence of iterative coupled solution

Due to the iterative coupling approach between both domains, a large number of iteration may be needed to get a converged solution. Based on the previous work, the implementation of a relaxation method is helpful to speed-up the convergence behavior of the coupled system [6]. Since the local fuel temperature shows largest oscillations during the coupled runs, it was selected to be the convergence parameter. Plotting different cycles of a coupled run, it was observed that the axial power profile performs damped oscillations around the final converged value which results in oscillations of the node averaged fuel temperature. In this approach, the actual thermal hydraulic parameters will be mixed with the ones of the previous time step according to the following relation, written in particular for the pin cell fuel temperature

$$T_{fuel,i}^{weighted} = (1-x)T_{fuel,i-1} + x(T_{fuel,i}^{actual}), \quad (4)$$

where x is a parameter determined from parametric study. In [5] it was found out that a value of x = 0.5 leads to significant reduction of computation time. The remaining thermal hydraulic parameters were also mixed in the same manner as the fuel temperature. Using this approach [10] computation time and the number of iterations were also reduced.
As expected the application of relaxation scheme damped the axial power oscillation amplitude significantly, as can be seen in **Figure 4**. Using the relaxation method the number of coupled cycles needed to get converged results could be reduced from 15 to 7.

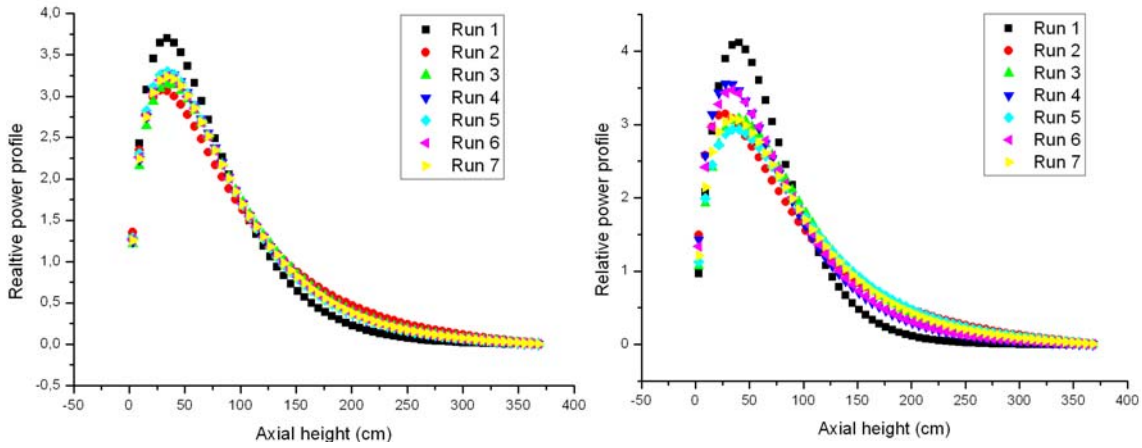


Figure 4 Evolution of the axial power profile over the first 6 iterations, with and without relaxation scheme applied, with relaxation parameter x = 0.5.

3.5 Refinement of temperature grid at which nuclear data is processed

Another important issue in thermal hydraulic / Monte Carlo coupled simulations is the temperature grid defined for the generation of nuclear data using NJOY on the basis of which the interpolation of cross sections is performed. In the frame of these investigations, a coarse (100 K) and a finer (50 K) temperature grid were used for the pre-generation of cross sections using

the JEFF.3.1 and JEFF.3.1.1 evaluated nuclear data. Then two runs were performed using the relaxation method (x = 0.5) to investigate a BWR pin cluster. It was found out that the simulation with the finer T-grid converged after seven iterations compared to eleven iterations for the run with 100 K T-grid. In **Table II**, the main parameters of both runs are compared to each other.

Table II Comparison between the coupled runs with cross sections prepared at 100K and 50K increments.

Case	Cycles Skipped	Cycles Total	Histories per Cycle	Processors	k_∞	Standard deviation	Coupled runs
100K JEFF 3.1	10	160	200k	60	1.10298	0.00010	11
50K JEFF3.1.1	10	160	200k	60	1.10257	0.00011	7

Both the k_∞ and the axial power profiles predicted by the two runs are very similar, for plot of the axial power profile see **Figure 5**.

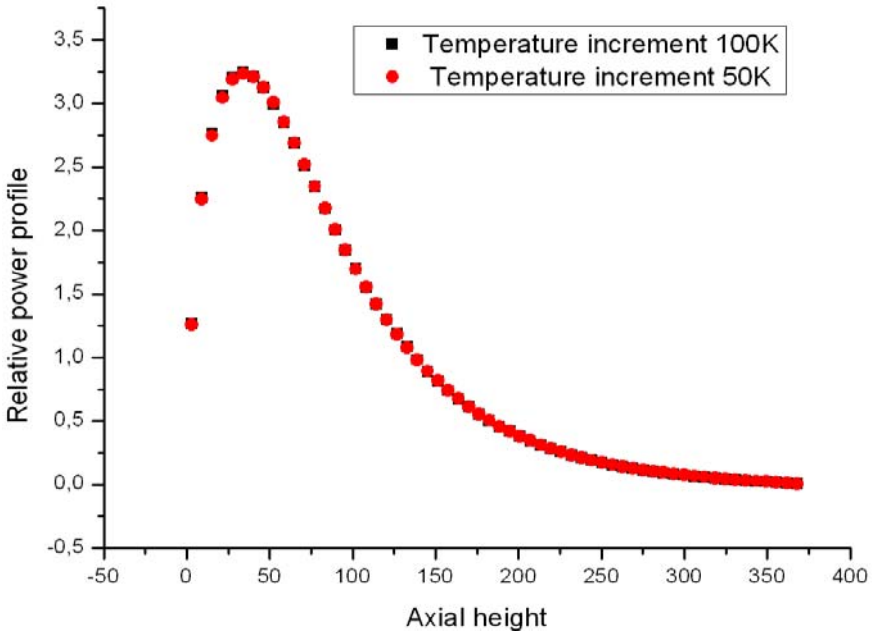


Figure 5 Axial power profile computed with cross section data having temperature increment of 100K and 50K.

3.6 Importance of checking the convergence of Monte Carlo solution

It is well know that the multiplication factor and the source have a different convergence behavior in Monte Carlo simulations. But it is very important to ensure that tally information computed by MCNP is reliable. In MCNP5 it is possible to check the convergence of the source Shannon entropy to make sure that tallying is done after the MC solution has really converged. In practice, an initial source distribution is calculated by TH/MC simulations using a homogeneous radial and cosine axial power profiles in the thermal hydraulic module. Than this source distribution is passed to the subsequent coupled simulation. Using this method it was possible to disregard fewer initial cycles and to obtain better values for both k_∞ and tallies. The values of Shannon entropy normalized with respect to the mean value for active cycles and k_∞ normalized with respect to the final value were plotted via MCNP RUNTPE file. In **Table III** the main parameters of two stand-alone MCNP5 simulations for a PWR and BWR 3x3 pin cluster are summarized.

Table III Summary of the standalone calculations

FA Type	Axial nodes/pins	Histories/ active cycles	Skipped cycles	Processors/time standalone run	k_∞	Standard deviation
PWR	10/8	200k/160	10	60/11min	1.32367	0.00011
BWR	60/9	200k/160	10	60/25min	1.10257	0.00011

It is evident from **Figure 6** that both k_∞ and Shannon entropy are converged over the active cycles. There can be observed that the multiplication factor as integral quantity converges much more uniform than the source. The initial source distribution is updated after each MCNP run and is used in the successive runs. It is evident that using the initial source distribution a low number of initial cycles skipped is needed. This leads to a reduction of the time for MCNP to run. In the companion paper [**15**], the geometry, material composition and boundary conditions for the PWR 3x3 pin problem together with calculation results are presented.

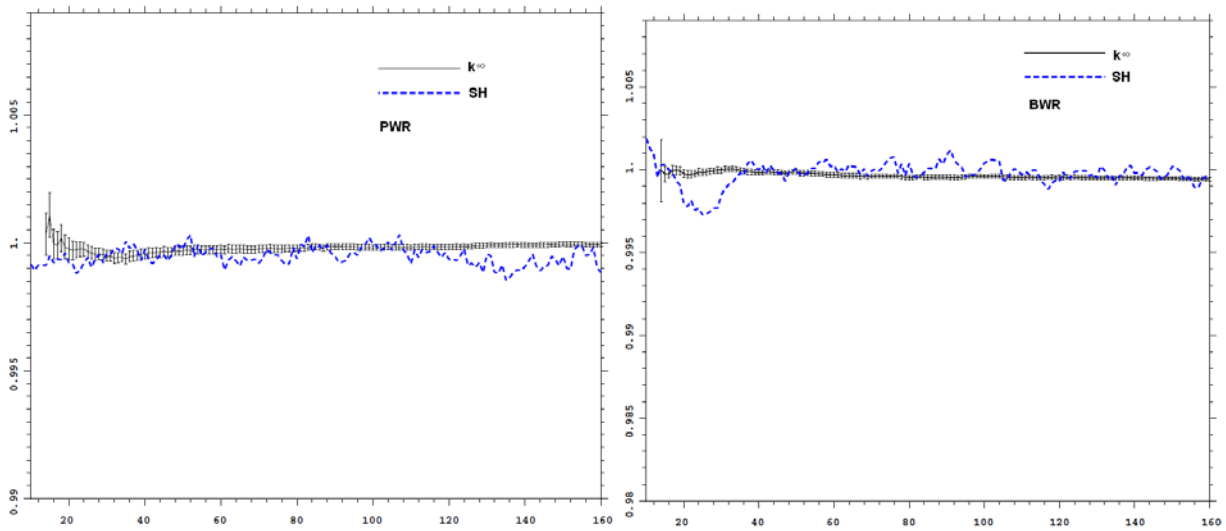


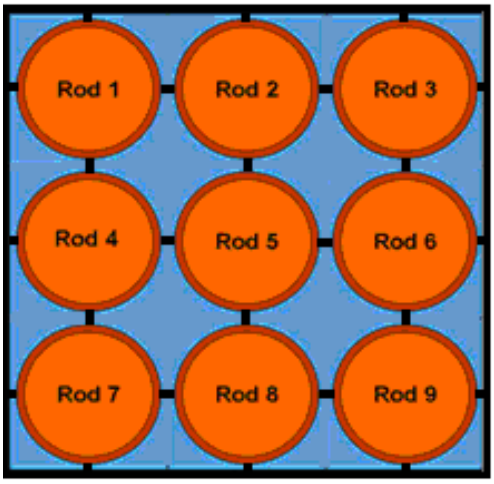
Figure 6 Plots of normalized k_∞ and Shannon entropy versus number of cycles for PWR/BWR lattices.

4 APPLICATION OF THE COUPLED SCHEME TO SPECIFIC PROBLEMS

The developed MC/TH coupling scheme will be applied for the pin-by pin simulation of both a BWR 3x3 pin cluster and of a large hexagonal fuel assembly of an innovative reactor concept, the steam cooled fast reactor (SCFR). A short description of the mentioned problems as well as the main results will be presented hereafter.

4.1 BWR 3x3 Pin Cluster Problem

The BWR 3x3 pin cluster consist of nine fuel rods with the dimensions and operation conditions as shown in **Figure 7**.



Total length	3.71m
Number of axial nodes	60
Inlet T	278.78°C
Mass flow rate	1.1205kg/s
Total power	0.551MW
Exit pressure	7.0MPa
Pin radius	0.5375cm
Pellet radius	0.45555cm

Figure 7 BWR 3x3 lattice and thermal hydraulics boundary conditions.

For the modeling of this pin cluster with MCNP5/SUBCHANFLOW 60 axial nodes were considered in the neutronic and thermal hydraulic models following the experience in [7], [8]. Considering that many axial nodes is advisory, doing the opposite will give very rude approximation of the boiling which occurs in the 3x3 lattice, and result into supplying coolant densities averaged over large moderator cells to the MCNP code.
In the radial direction, the MCNP5 model uses reflective boundary conditions while axially vacuum conditions are implemented. Giving vacuum boundary conditions on the axial planes is necessary in order to compute realistic axial power profile. In SUBCHANLOW sixteen subchannels are considered. In order to compute the cell averaged fuel temperature 6 radial nodes where considered in the fuel and one radial node in the cladding. The thermal hydraulic conditions specified in **Figure 7** are used for the subchannel code model. For the coupled simulations the MCNP5 parameters given in **Table IV** were used. The coupled solutions converged after seven iterations using 60 processors. It took 25 minutes in order to run one coupled step, where most of the time was spent in running MCNP code, in contrast to the fast running SUBCHANFLOW code which takes about 5 seconds computation time. In **Figure 8**, the axial power profile and the volume averaged fuel temperature is shown. It can be noticed that the highest fuel temperature corresponds to the highest axial power. Both are located in the lower part of the fuel rod, where the coolant is colder and hence denser compared with the upper part.

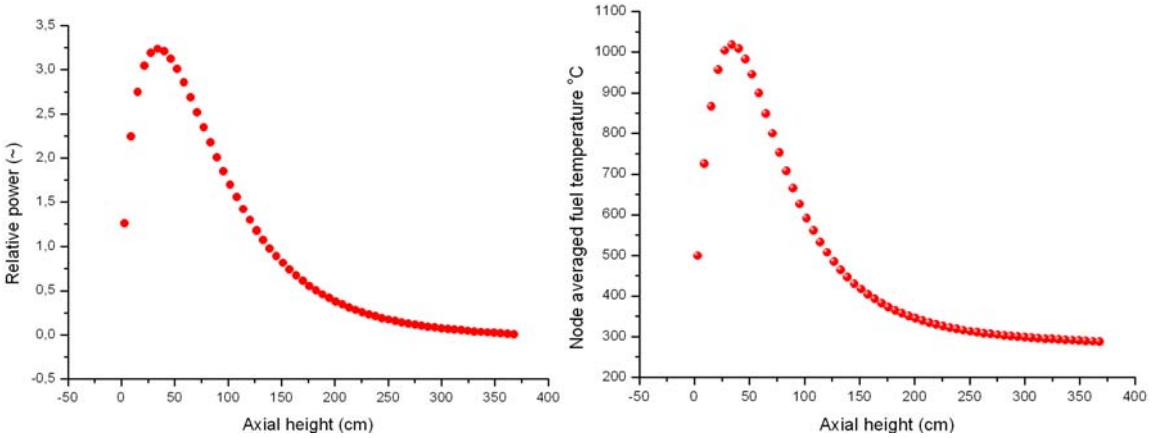


Figure 8 Axial power profile of the 3x3 BWR lattice and node averaged fuel temperature

Axial coolant temperature distribution and the coolant density are shown in **Figure 9**. The large density decrease is typical in BWR cores. It can be clearly seen that due to the large power peak in the bottom, fluid reaches boiling temperature already in the lower part of the lattice, which on its side leads to the shift in the axial power.

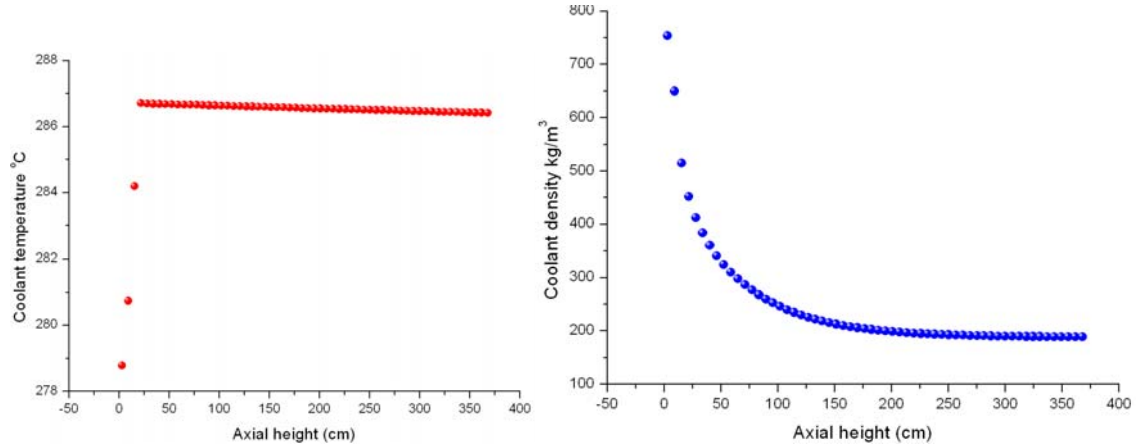


Figure 9 Coolant temperature and density along the axial height of the 3x3 BWR lattice

Finally, the predicted radial power profile is given in **Table IV** together with the computed value of k_∞ including the standard deviation which is observed to be small enough**.**

Table IV Radial power profile of the BWR lattice and calculation run summary

Pin7=1.00000583274251		**Pin8**=0.999818192174966			**Pin9**=1.00012199118908	
Pin4=1.00016443369841		**Pin5**=0.99984723178661			**Pin6**=1.00037329552062	
Pin1=1.00000583274251		**Pin2**=0.999818192174966			**Pin3**=0.999762346767959	
Parameter	k_∞	Standard deviation	Histories/Cycles	Skipped cycles	Processors/Cycle run time	Parallel run
Value	1.10257	0.00011	200k/160	10	60/25 min	**7**

4.2 Steam Cooled Fast Reactor (SCFR) Problem

The last problem investigated with MCNP5/SUBCHANFLOW was the innovative steam cooled fast reactor (SCFR) which main features are described in [14]. It is cooled by superheated steam and operates with MOX fuel at 12.5 MPa pressure. Since the density of superheated steam is small, the reactor core is characterized by a neutron flux spectrum similar to that of liquid metal cooled fast reactors. The fuel assembly obeys hexagonal lattice with active height of ca 1.5 m including two axial breeding blankets. In **Table V** the main parameters, and geometrical data of the SCFR are presented.

In **Figure 10** the radial models of SUBCHANFLOW and MCNP5 for the SCFR fuel assembly are shown. In MCNP5 reflective boundary conditions were imposed on the lateral walls and vacuum boundary conditions on the axial planes.

Table V Geometry and thermal hydraulic boundary conditions for the SCFR

Electrical output	1000MW	Control assemblies	25
Thermal power	2670 MW	Height of fission zone	85 cm
Thermal efficiency	37,4%	Height of axial reflector	2x35 cm
Outlet temperature	480 C	Radial reflector	34 cm
Core mass flow rate	4560 kg/s	Pin diameter	8 mm
Breeding ratio	1,17	Clad thickness	0.4 mm
Cooling medium	Water	Fuel pellet diameter	6.96 mm
Fuel assemblies	372	Fission gas plenum	60 cm
Reflector assemblies	198	Fuel type	MOX

From **Table VI** the presence of a large fission gas plenum can be observed, since it is situated above the upper reflector, is was neglected in the actual calculation. Taking it into the actual computation would mean that we shall loose computation time to track particles in region where no fission power is generated.

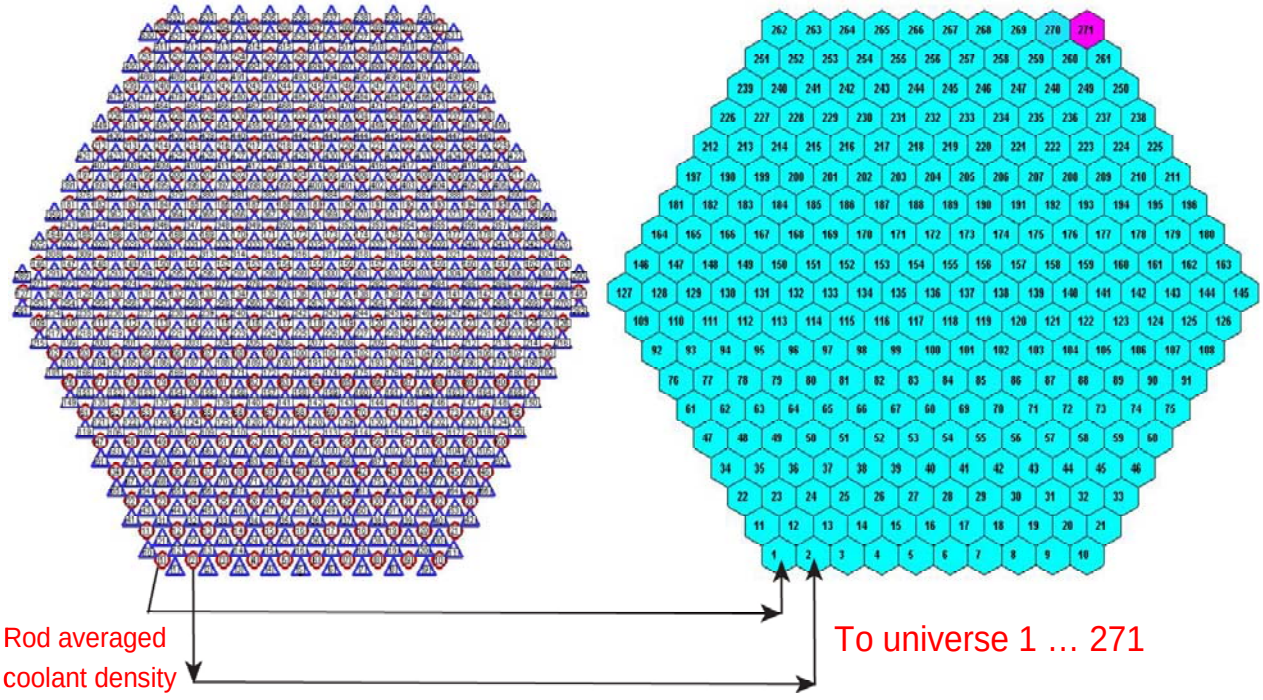


Figure 10 SUBCHANFLOW and MCNP5 Models of the SCFR fuel assembly (radial mapping)

Preliminary investigations were performed to assess the neutron spectrum of the SCFR fuel assembly using MCNP5. There the flux was computed with MCNP5 F4:n for homogenized coolant density. In **Figure 11** logarithmic plot of the so predicted neutron spectrum is given. Plotting the neutron flux clearly shows that the neutron energy distribution inside the SCFR fuel assembly is similar to that inside of a liquid metal cooled fast reactor fuel assembly.

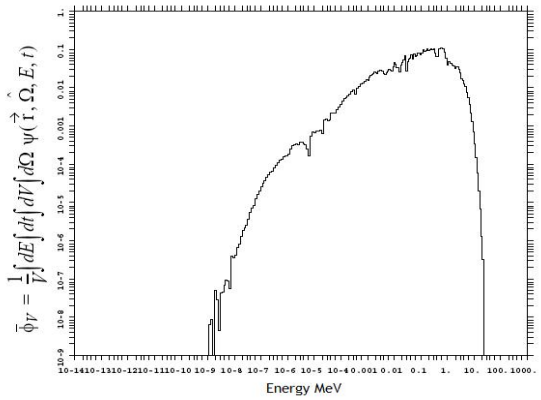


Figure 11 Neutron spectrum inside the SCFR fuel assembly for homogenized water density of 0.05 g/cm^3 plotted in logarithmic scale.

In addition, the energy distribution of neutrons causing fission for a PWR and BWR pin cluster and for the SCFR FA were compared to each other and summarized in **Table VII** as computed via MCNP. Taking both results into account it observed that the SCFR FA behaves like a fast breeder reactor.

Table VII Energies of neutrons causing fission for PWR,BWR,SCFR

Type	< 0.625 eV	0.625 eV - 100 keV	> 100 keV
BWR	55.44%	31.44%	13.11%
PWR	78.28%	15.19%	6.53%
SCFR	0.26%	45.36%	54.38%

Based on these investigations can be concluded that the reactions in the unresolved resonance range will play major role analyzing the SCFR FA. In order to take into account Doppler

broadening, BROADR module of NJOY was used. Unresolved resonance self shielding was treated with the PURR module based on "Probability table method".
Once the necessary nuclear cross sections were adapted a pin-by-pin simulation of the whole fuel assembly was performed with MCNP5/SUBCHANFLOW using 120 processors and the number of histories and cycles as given in **Table VIII**. In order to determine the number of processors and the efficiency of the coupled calculation few standalone runs where performed, and the figure of merit and standalone run time where observed. Doing so, it is possible to select the number of processors in optimal way. Those runs where performed with thermal hydraulic data taken form initial trial run of SUBCHANFLOW, and where used also to prepare initial source distribution, the figure of merit obtained was 6.13243E+02 .
In **Figure 12** the fuel temperature predicted with the coupled system MCNP5/SUBCHANLOW is shown for both the 12 iterations and for the last two ones. It can be observed there that the axial fuel temperature does not show as strong oscillations as in the case of the BWR. The axial power profile had slight distorted cosine shape with the maximum shifted towards lower coolant density, where a plot of the node averaged coolant density is shown in **Figure 13** (right side). A moderation decrease causes an increase of the averaged energy of neutrons causing fission in the MOX fuel and hence leading to an increase in the number of neutrons released per fission. The convergence behavior of the coupled simulations for the SCFR FA was not as good as in the cases of PWR and BWR. Problems which prohibited the uniform convergence behavior can be traced back to the specific physics of the SCFR, among which are large coolant velocities (31 m/s to 50 m/s) flow in close packed hexagonal lattice, which poses significant challenges to the thermal hydraulic computation. Another difference in comparison to conventional BWR rectors is the large averaged heat flux which when translated into the language of the coupled system means that small oscillations in the relative axial power profile computed with MCNP would results into significant changes of the fuel temperature.

In fact active length of the fuel assembly is only 85 centimeters and the averaged power per fuel assembly is 7.2 MW.

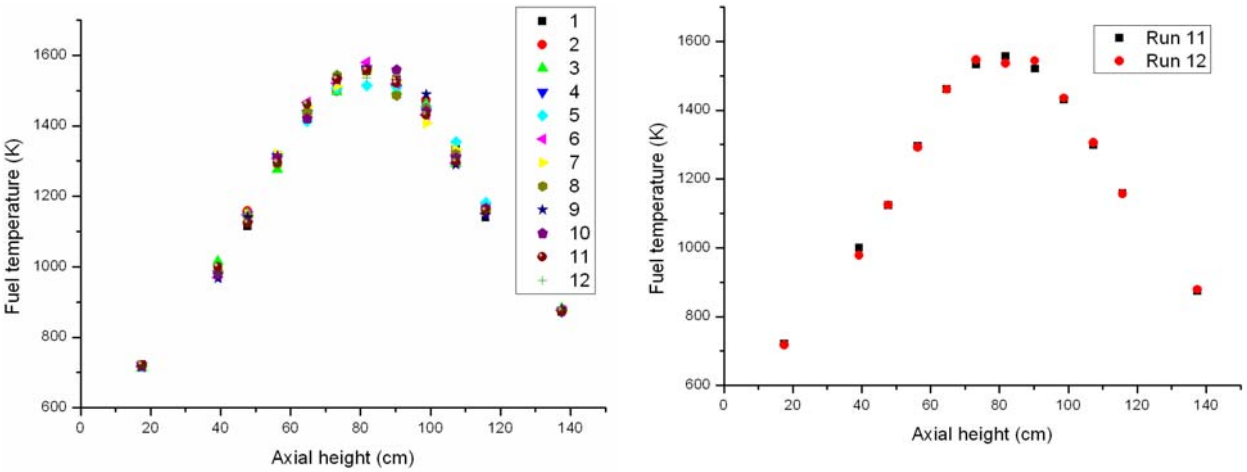


Figure 12 Axial distribution of fuel temperature SCFR

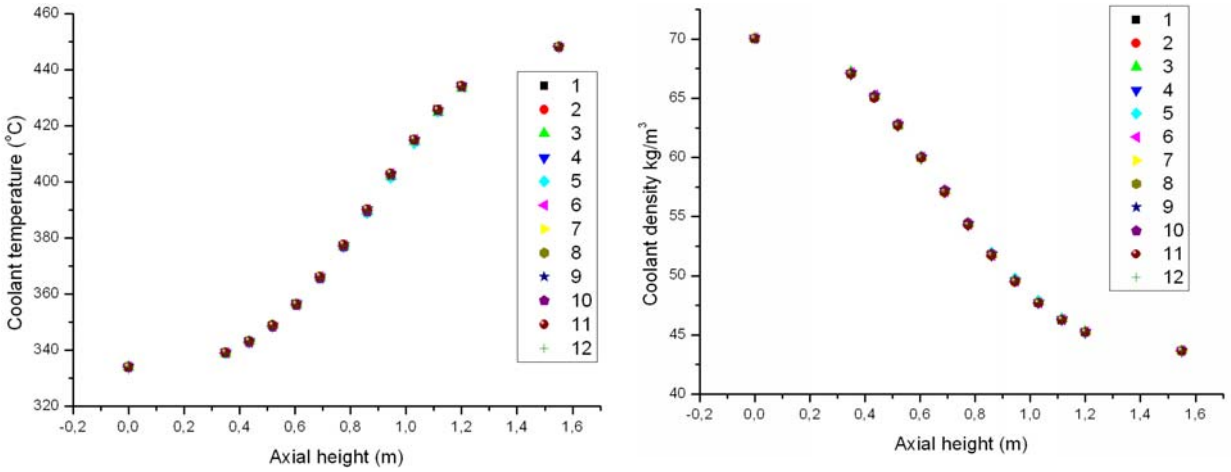


Figure 13 Axial distribution of coolant node averaged temperature and density in the SCFR fuel assembly

The relative pin power of the SCFR FA is exhibited in **Figure 14**. It can be noted that the pins staying at the outermost edge of the fuel assembly had a larger relative power than those located in the centre. However the difference is less than 2 percent.

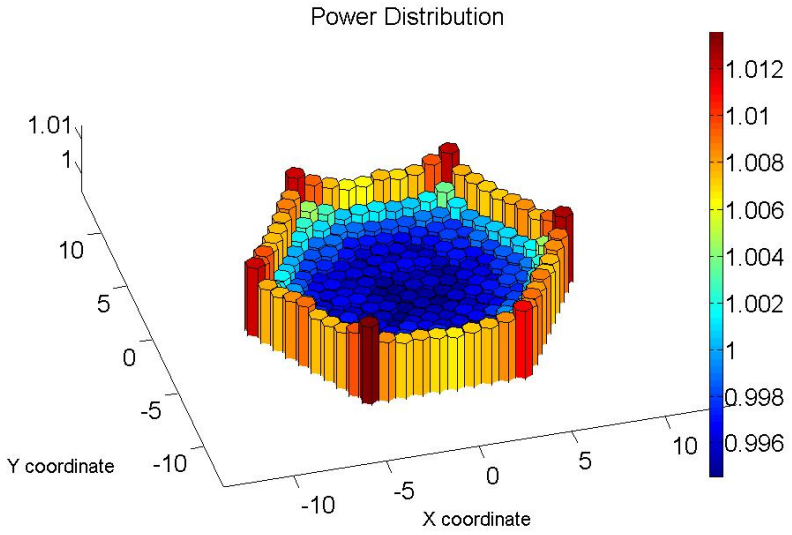


Figure 14 Radial relative power profile of SCFR

In **Table VIII** the calculation parameters of the investigation performed for the SCFR FA are summarized. The computation was performed on 120 parallel processors at the BWGrid Cluster. It took 37 hrs to reach convergence. It is evident that such computation is impossible if run in serial mode. Thank to the high performance computing (HPC) such kind of investigations are nowadays possible for detailed simulations of complex geometries including up to 8000 cells.

Table VIII Calculation run summary for the SCFR assembly.

Parameter	k_∞	Standard deviation	Histories/ cycles	Skipped cycles	Processors/Cycle run time	Iterations till convergence
Value	1.02603	0.00008	250k/160	15	120/185min	12

5 CONCLUSIONS AND OUTLOOK

The coupled Monte Carlo /SUBCHANFLOW solutions presented here are being developed at KIT/INR to improve the safety-related design investigation of pin clusters and fuel assemblies of LWR and innovative reactor concepts.
The parallel capabilities of MCNP5 facilitate detailed investigation of variety of fuel assemblies in a 3D sense coupled with thermal hydraulic solutions. Important issues such as treatment of the temperature dependence of the nuclear data, cross section interpolation, convergence of coupled iterative approach, etc. determining the accuracy of the obtained results with the coupled MCNP5/SUBCHANFLOW are listed and discussed.
The developed coupled system was applied to simple (pin cluster) and complex (fuel assembly) problems obtaining local parameters important to assess the safety parameters. All calculations were performed on parallel architectures achieving converged solutions within reasonable computation times. The general purpose coupling scheme is based on PERL pattern matching capabilities allowing the treatment of different types of fuel assemblies with the same coupling formalism. Despite the achieved progress, the coupling solutions needs to be further improved e.g. regarding the convergence criteria, the treatment of temperature dependency of the nuclear data, etc. In addition the coupled solutions need to be validated or at least benchmarked to other solutions including the ones of coupled deterministic/subchannel codes. Finally, the developed system MCNP5/SUBCHANFLOW will be applied for the analysis of whole cores at a fuel assembly basis.

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REFERENCES

1 C. Tippayakul, M. Avramova, F. Puente Espel, K. Ivanov, "Investigations on Monte Carlo Based Coupled Core Calculations", *Proceedings of ICAPP 2007*, Nice, France, May 13-18, 2007,Paper 7134.

2 C. Watta, T. Schulenburg, X. Cheng, *Coupling of MCNP With a Sub-Channel Code For Analysis of a HPLWR Fuel Assembly FZKA7233*, FZK, Karlsruhe Germany.

3 F. Puente Espel, M. Avramova, K. Ivanov, and St. Misu, "High Accuracy Modeling for Advance Nuclear Reactor Core Designs using Monte Carlo Based Coupled Calculations", *Invited paper for M&C 2009*, Saratoga Springs, New York, May 3-7, 2009.

4 F. Puente-Espel, M. Avramova, K. Ivanov, "New developments of the MCNP/CTF/NEM/NJOY Code system-Monte Carlo based coupled code for high accuracy modeling". *Proceedings of Advances in Reactor Physics to Power the Nuclear Renaissance (PHYSOR)*, Pittsburgh, Pennsylvania, USA, May 9-14.2010.

5 V. Sánchez, A. Al-Hamry, C.H. M. Broeders, "Development and Qualification of the Coupled Code System COBRA-TF/THREEDANT for the Pin-by-Pin Power Calculation", *Proceedings of ICAPP '08. Anaheim*, CA USA, June 8-12, 2008, Paper 8269.

6 V. Sanchez, A. Al-Hamry, "Development of a Coupling Scheme Between MCNP and COBRA-TF for the Prediction of the Pin Power of a PWR Fuel Assembly", *Proceedings of International Conference on Mathmatics, Computational Methods & Reactor Physics (M&C 2009)*, New York, USA.

7 U. Imke, *Input Instructions for SUBCHANFLOW* ,FZK, Karlsruhe, Germany, 1.6 July 28, 2010.

8 V. Sanchez, U. Imke, A. Ivanov, R. Gomez, "SUBCHANFLOW: A Thermal-Hydraulic Sub-Channel Program to Analyse Fuel Rod Bundles and Reactor Cores", *17th Pacific Basin Nuclear Conference*, Cancún, México, October 24-30, 2010.

9 F. Brown, "Fundamentals of Monte Carlo Particle Transport LA-UR-05—4983", Los Alamos National Laboratory, http://mcnp-green.lanl.gov/publication/pdf/LA-UR-05-4983_Monte_Carlo_Lectures.pdf (2005).

10 "MCNP - A General Monte Carlo N-Particle Transport Code, Version 5," Los Alamos National Laboratory (2004).

11 NEA/NSC/DOC(2006)18, "Processing of the JEFF-3.1 Cross Section Library into Continuous Energy Monte Carlo Radiation Transport and Criticality Data Library".

12 C. Jouanne, J. C: Trama, "Linux Binary of TRIPOLI-4 capable of producing point cross-sections at various temperatures", *NURISP Deliverable D.1.1.1.*, April 2010.

13 S. van der Marck, R. Meulekamp, A.Hogenbirk, "New Temperature Interpolation in MCNP", *Proceedings of M&C 2005 conference*, Avignon, France (2005).

14 A. Schaefer, *Technical Report KWU/RB 23 – 2998*, KWU, June 1974 (in German).

15 E. Hoogenboom, Ch. Diop, A. Ivanov, V. Sanchez, "Development of coupling methodologies for TRIPOLI and FLICA in the frame of NURISP Project", *The 2011 International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2011),* Rio de Janeiro, RJ, Brazil, May 8-12, 2011.