HIGH ACCURACY MODELING FOR ADVANCED NUCLEAR REACTOR CORE DESIGNS USING MONTE CARLO BASED COUPLED CALCULATIONS

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by
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ABSTRACT

The main objective of this PhD research is to develop a high accuracy modeling tool using a Monte Carlo based coupled system. The presented research comprises the development of models to include the thermal-hydraulic feedback to the Monte Carlo method and speed-up mechanisms to accelerate the Monte Carlo criticality calculation.

Presently, deterministic codes based on the diffusion approximation of the Boltzmann transport equation, coupled with channel-based (or sub-channel based) thermal-hydraulic codes, carry out the three-dimensional (3-D) reactor core calculations of the Light Water Reactors (LWRs). These deterministic codes utilize nuclear homogenized data (normally over large spatial zones, consisting of fuel assembly or parts of fuel assembly, and in the best case, over small spatial zones, consisting of pin cell), which is functionalized in terms of thermal-hydraulic feedback parameters (in the form of off-line pre-generated cross-section libraries). High accuracy modeling is required for advanced nuclear reactor core designs that present increased geometry complexity and material heterogeneity. Such high-fidelity methods take advantage of the recent progress in computation technology and coupled neutron transport solutions with thermal-hydraulic feedback models on pin or even on sub-pin level (in terms of spatial scale). The continuous energy Monte Carlo method is well suited for solving such core environments with the detailed representation of the complicated 3-D problem. The major advantages of the Monte Carlo method over the deterministic methods are the continuous energy treatment and the exact 3-D geometry modeling. However, the Monte Carlo method involves vast computational time. The interest in Monte Carlo methods has increased
thanks to the improvements of the capabilities of high performance computers. Coupled Monte-Carlo calculations can serve as reference solutions for verifying high-fidelity coupled deterministic neutron transport methods with detailed and accurate thermal-hydraulic models. The development of such reference high-fidelity coupled multi-physics scheme is described in this dissertation on the basis of MCNP5, NEM, NJOY and COBRA-TF (CTF) computer codes. This work presents results from studies performed and implemented at the Pennsylvania State University (PSU) on both accelerating Monte Carlo criticality calculations by using hybrid nodal diffusion Monte Carlo schemes and thermal-hydraulic feedback modeling in Monte Carlo core calculations.

The hybrid MCNP5/CTF/NEM/NJOY coupled code system is proposed and developed in this dissertation work. The hybrid coupled code system contains a special interface developed to update the required MCNP5 input changes to account for dimension and density changes provided by the thermal-hydraulics feedback module. The interface has also been developed to extract the flux and reaction rates calculated by MCNP5 to later transform the data into the power feedback needed by CTF (axial and radial peaking factors). The interface is contained in a master program that controls the flow of the calculations. Both feedback modules (thermal-hydraulic and power subroutines) use a common internal interface to further accelerate the data exchange.

One of the most important steps to correctly include the thermal hydraulic feedback into MCNP5 calculations begins with temperature dependent cross section libraries. If the cross sections used for the calculations are not at the correct temperature, the temperature feedback cannot be included into MCNP5 (referred to the effect of temperature on cross sections: Doppler boarding of resolve and unresolved resonances,
thermal scattering and elastic scattering). The only method of considering the temperature effects on cross sections is through the generation (or as introduced in this dissertation through a novel interpolation mechanism) of continuous energy temperature-dependent cross section libraries. An automated methodology for generation of continuous energy temperature-dependent cross section libraries has been developed as part of the hybrid Monte Carlo-based coupled core studies at PSU. This tool is used together with the automated cross-section temperature interpolation capability for intermediate points. The automated methodology, combined with the interpolation capability, has considerably reduced the cross section generation time.

A new methodology for generation and interpolation of temperature-dependent thermal scattering cross section libraries for MCNP5 is introduced as well. Using the interpolation methodology specially designed for thermal scattering cross sections, a thermal scattering grid at the desired temperature was generated. This gives the possibility of performing MCNP5 criticality calculations at the correct moderator temperature and improving the accuracy of the calculations. A cross section update methodology has been included, which efficiently reduces the time of the cross section libraries update.

Several acceleration strategies are introduced and implemented in the hybrid coupled code system. The computation process is greatly accelerated by calculating the 3-D distributions of fission source and thermal-hydraulics parameters with the coupled NEM/CTF code and then using coupled MCNP5/CTF code to fine tune the results to obtain an increased accuracy. The PSU NEM code employs cross-sections generated by MCNP5 for pin-cell based nodal compositions.
Finally, the hybrid coupled system is automated and enhanced in order to provide
the user with an efficient and easy to use high accuracy modeling tool.
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Chapter 1

Introduction

1.1 Background

The present trend in advanced and next generation nuclear reactor core designs is towards increased material heterogeneity and geometry complexity. The continuous energy Monte Carlo method [1] has the capability of modeling such core environments with high accuracy. Because of its statistical nature, Monte Carlo core calculations usually involve a considerable computer time to attain reliable converged results for both integral parameters and local distributions. This is especially true when coupling it with a thermal-hydraulics code to obtain three-dimensional (3-D) power and thermal-hydraulic solutions for a reactor core. Results from feasibility studies performed at the Pennsylvania State University (PSU) on both accelerating Monte Carlo criticality calculations by using hybrid nodal diffusion Monte Carlo schemes and thermal-hydraulic feedback modeling in Monte Carlo core calculations are first presented in this PhD dissertation. These results are followed by the discussion of the new developments of the hybrid Monte Carlo-based coupled core calculations at PSU and the results of applying the developed coupled hybrid system MCNP5/CTF/NEM/NJOY to a simplified 3-D 2x2 fuel-pin array from a BWR assembly.
1.2 Literature review

Currently, the Monte Carlo based methodology has increasingly been used for the nuclear reactor core and fuel lattice physics calculations and analysis [2, 3, 4, 33, 34, and 35]. This section summarizes and reviews the most relevant publicly available literature related to the utilization of the Monte Carlo based coupled methodology for a reference analysis.

1.2.1 Reactor simulation with coupled Monte Carlo and computational fluid dynamics

The paper was presented at M&C + SNA 2007, Monterey, California, USA, in April 2007 by Volkan Seker (Purdue University), Justin W. Thomas (Argonne National Laboratory), and Thomas J. Downar (University of California, Berkeley at the time of the publication).

Seker et al. have introduced an interesting methodology to couple the Monte Carlo code MCNP5 to the Computational Fluid Dynamics (CFD) code STAR-CD. The authors design a master code to control the flow of the calculations. Various results of simple PWR test problems were presented to support the new methodology. The authors demonstrated the feasibility of using Monte Carlo analysis to carry out nuclear reactor core simulations with thermal-hydraulic feedback from a CFD code. The Monte Carlo calculation is still not applicable for practical analysis of nuclear reactors, since the computational time is still too large. It can rather be used to generate reference solutions. This methodology is unique in that the thermal-hydraulic feedback is obtained from a
CFD code. Conversely, several deficiencies in the paper were noticed and are summarized below:

1) The authors failed to describe in more detail the codes and their capabilities. In addition, there was no information about which release of the MCNP5 code, and the ENDF/B version, were used in this study. This could have served to determine the available capabilities of the specific MCNP5 version, and to establish how new the nuclear data is and if it is consistent with data used for DeCART (a deterministic code in which the authors have been involved and wish to validate) cross-sections.

2) The general explanation of the three techniques for updating the cross section libraries was deficient in declaring the nuclides considered in the study, the range of temperatures of the calculations, the temperature variation in each material region, and a comparison of the second and third methods, against the cross sections generated by NJOY at the actual temperature. The first technique, which is described as the most accurate, would be to update the cross section libraries with NJOY, for each nuclide, in their corresponding region, at the temperature of that region. For the second technique, the cross sections library for each nuclide would be pre-generated, with small temperature increments (2 K - 5 K), within the range of temperatures of the calculation. The third technique would be to also use a pre-generated cross-section library with larger temperature increments (25 K - 50 K), and then, an interpolation method would be used to approximate the cross-sections at the provided by STAR-CD temperatures.

3) The description of the coupling scheme left numerous points uncovered that raised significant questions. It seemed that the first technique for updating the cross section libraries is used after the CFD calculation provides the thermal-hydraulic
feedback. In contrast, the coupling scheme states that either the second or the third techniques, to update the cross section libraries, are available in the coupled calculation. The method used to update the cross section libraries is not clear. The interpolation method could be linear, quadratic, or a square root of temperature.

4) The source distribution convergence was not analyzed in this work. There were no indications that the number of histories that the authors used made the source distribution to achieve the ‘exact’ equilibrium state. In other words, the accuracy of the technique might not be optimized. A larger number of histories in the criticality calculation step might have improved the accuracy of the new technique. Alternatively, if the criticality calculation step had already reached the converged equilibrium state, at a smaller number of histories than that used by the authors, the computational time could have been reduced further to attain the same accuracy as presented in the paper.

5) The two problems explained in the paper, lack the description of the type of materials, or more particularly, the isotopes of the fuel and the presence of boron in the moderator.

6) The results obtained from the McSTAR calculation of the two test models, were compared against the START-CD calculation coupled with the deterministic transport code DeCART. The DeCART code was not described. The results presented did not specify the number of coupled iterations needed to reach the calculated values nor the observed convergence ratio. These would have helped in understanding better the comparison and the proposed coupled methodology.

7) Although acceleration and convergence methods were mentioned in the introduction of the paper, as ongoing research, yet they were not described in the paper.
1.2.2 Development of a coupling scheme between MCNP and COBRA-TF for the prediction of pin power of a PWR fuel assembly

The paper has been submitted to the M&C 2009 in Saratoga Springs, New York, May 3-7, 2009 by V. Sanchez (Research Center at Karlsruhe GmbH) and A. Al-hamry (University of Applied Sciences FH Aachen)

This paper presents an interesting methodology to couple the Monte Carlo code MCNP5 to the COBRA-TF sub-channel code. The authors design a master code to control the flow of the calculations. A simple PWR fuel assembly is used for the calculations. (It is important to note that in the work presented in this dissertation COBRA-TF is also being used to provide the thermal-hydraulic feedback. Actually the critiqued paper in this section makes reference to one of the previous publications [5] carried out within the research of this dissertation). The most relevant points of this paper are:

1) The treatment of temperature dependence of the cross sections for MCNP5. The author mentioned the different ways to account for the thermal-hydraulic effects (online generation of cross section data using NJOY, pre-generation of nuclear data with NJOY for the whole range of state parameters, and the pseudo material approach). Then the authors state that they tested different interpolation methods for the coupling scheme. The authors failed to state the observation of the method and the reason why they use square root of temperature for a temperature weighting factor, which utilization is not explained.

2) The relaxation method implemented to speed-up the convergence behavior. A weighting factor is applied to “weight” the results of the actual simulation step with the
ones of the previous step. Since there are no studies available on this weighting factor, the value has to be selected from parametric studies on a case by case basis.

3) The authors lack to explain the update of the cross-section libraries and the utilization of the cross-section extensions.

1.2.3 An integrated thermal hydraulic feedback method for Monte Carlo reactor calculations

The paper was presented at International Conference on the Physics of Reactors “Nuclear Power: A Sustainable Resource” Casino-Kursaal Conference Center, Interlaken, Switzerland, September 14-19, 2008, by David P. Griesheimer (Bechtel Bettis, Inc., Pittsburgh, PA, USA), Daniel F. Gill, Jeffrey W. Lane, David L. Aumiller (Pennsylvania State University, Department of Nuclear Engineering, University Park, PA, USA).

Griesheimer et al. have proposed an integrated thermal hydraulic feedback method for use in Monte Carlo transport calculations. The methodology is tested using MC21, a Bechtel, continuous-energy Monte Carlo particle transport code. A pressurized water reactor (PWR) example problem is used for the tests. The authors presented an interesting and unique simplified approach to perform the thermal hydraulic feedback. On the other hand, the model is too simplified and may lack precise local parameters for the thermal-hydraulic data. The authors declare that the loss in accuracy is justified by the gain in computational speed. The lack of precise thermal-hydraulic feedback information is a concern for BWR calculations, because of the two-phase flow problem.
One of the most relevant drawbacks of this integrated thermal-hydraulic model is the lack of updating the cross-section libraries to take into account the “real” effect of the thermal-hydraulic feedback.

1.3 Statement of objectives

The main purpose of this dissertation is to develop a high accuracy Monte Carlo based coupled methodology useful for core analysis. The dissertation includes the new developments and the implementation of the research. The following activities are considered to be the major objectives of this research.

1.3.1 Thermal-hydraulic feedback modeling to Monte Carlo core calculations

The thermal-hydraulics feedback effects in Monte Carlo reactor core calculations include changes in the dimensions of the geometry, material density effects, and temperature effects on cross-section data. Input changes are required to account for dimension and density changes. Special routine/interface is developed, which updates the MCNP5 input deck to account for the material density changes as provided by the thermal-hydraulics feedback module, which in this case is COBRA-TF [6]. The temperature effects on continuous cross-section data include Doppler broadening of resolved resonances; Doppler broadening of unresolved resonances; changes in $S(\alpha, \beta)$ thermal scattering kernel; and elastic scattering, which is Doppler broadening over entire energy range. As a result, continuous temperature dependent cross-section libraries were
generated for MCNP5 at PSU along with automated cross-section temperature interpolation capability. The cross section generation methodology comprises the next objective.

1.3.2 Generation and interpolation methodologies for temperature dependent cross-section libraries

The behavior of the reactor and hence the multiplication factor and power distribution of the system are greatly affected by temperature. Hence, the temperature of the reactor must be considered for a proper modeling of the system. The temperature effect, and thus the temperature feedback, is accounted through the generation and utilization of the temperature dependent cross-section libraries.

The continuous energy treatment is one of the major advantages of the Monte Carlo method over the deterministic ones. These continuous or point-wise cross sections can be produced by a nuclear data processing code. The NJOY code [7] is the nuclear data processing system used in the present studies. The nuclear data is enclosed in the ENDF files. The code converts the evaluated nuclear data into libraries useful for applications in nuclear engineering problems. It has the capability to generate the required continuous energy MCNP5 cross sections.

The generation process for cross-section libraries is tedious and involves a lot of data manipulation. For this reason an automated tool has been developed (GEN-XS code) to process and manage all data requirements during the generation process.

The duration of the procedure has been significantly reduced. This automated tool performs the most time consuming tasks of the cross-sections generation process. This
The automated tool is used together with the automated cross-section temperature interpolation capability for intermediate points.

The most accurate technique to update the cross-section libraries, taking into account the temperature feedback, would be to update the libraries with NJOY, for each nuclide, in their corresponding region, at the temperature of that region. In particular, this technique would be the most accurate, but not practical because of the vast computational time that it would take. Investigations carried out at PSU have exemplified that the most appropriate and practical technique, with high accurate results, would be to use a pre-generated cross-section library with temperature increments of 50 K, and then, an interpolation method would be used to approximate the cross section values at the provided by COBRA-TF temperatures.

The temperature dependent modeling capability is included into the coupled code. Therefore it will automatically determine or interpolate the appropriate temperature dependent cross section library for the MCNP5 calculation according to the temperature feedback.

The automated tool is a program developed to generate temperature dependent MCNP5 continuous energy cross-section libraries and multi-group cross-section libraries for diffusion codes using MCNP5. Additionally, the possibility of generating/interpolating thermal scattering cross-section libraries has been included as well.

The methodology to generate temperature dependent continuous energy Monte Carlo cross section libraries to properly model the temperature feedback, the methodology used to generate multi-group cross section libraries for diffusion codes
using MCNP5 as well as the studies for generating/interpolating thermal scattering cross-section libraries are presented in the next chapters.

1.3.3 Acceleration schemes for Monte Carlo based coupled calculations

The continuous energy Monte Carlo method has the capability of modeling with high accuracy complicated reactor configurations. The main drawback is that Monte Carlo core calculations usually involve a considerable computer time to attain reliable converged results for both integral parameters and local distributions, due to its statistical nature. This is especially true when coupling it with a thermal-hydraulics code to obtain three-dimensional (3-D) power and thermal-hydraulic solutions for a reactor core.

In order to speed-up Monte-Carlo criticality calculations, which take the major part of the CPU time of coupled simulations, a combined strategy is investigated including parallel computing, accelerating techniques, and hybrid nodal diffusion/Monte Carlo approach.

The latest versions of coupled Monte Carlo based system (MCNP-CTF) present the possibility of executing the Monte-Carlo criticality calculation either in sequential or parallel mode. The OpenMP model [1] available in MCNP5, which is a shared-memory parallelism (threads) model, is used in the parallel execution mode.

Another strategy that is studied and implemented is to couple the codes in an internal manner. The internal coupling transfers the feedback data in a direct way avoiding any extra transfer action that will increase the time of the calculation. Internal coupling represents a faster and more efficient way of passing the feedback information.
In addition, the possibility of using the diffusion calculation to pre-generate the initial guess of the source distribution for the Monte Carlo calculation is studied and implemented. The fast nodal diffusion calculation is used to provide the fission source distribution as an initial source distribution for the Monte Carlo calculation. The fission source distribution simulated in the nodal diffusion calculation is practically closer to the true source distribution of the Monte Carlo calculation than the typical guess source distribution. Therefore, the coupled methodology avoids utilizing large number of inactive cycles in the Monte Carlo calculation.

1.3.4 Validation of the Monte Carlo based coupled calculations

The validation of the developed methodologies is as important as the implementation itself. In order to fulfill the specific objectives of the present work, a validation procedure is designed for each of the newly independent sections of the coupled system. Consequently, the methodologies for generation of continuous energy temperature dependent cross section libraries, of multi-group cross-section libraries for diffusion codes using MCNP5 code, and of thermal scattering cross-section libraries for MCNP5, as well as the for the multi-level MCNP5/CTF/NEM/NJOY scheme must are validated. Due to the lack of experimental data, the correctness of the methodology will be assessed for each individual new methodology against already “proven as correct” data. The detail descriptions of each validation procedure are included in the respective chapters.
1.3.5 Enhancements of the hybrid coupled Monte Carlo based code system

The hybrid coupled system is designed with a modular approach to facilitate the incorporation of new functions. The features of the code system are automated in order to provide the user with an efficient and easy to use high accuracy modeling tool. For instance, the automated coupled system includes post-processor subroutines that collect, summarize and print the results to a master output file. The main results are summarized in tables for: number of coupled iterations, number of COBRA-TF iterations per coupled iteration; axial fuel temperature distribution, moderator temperature distribution, moderator density distribution, and radial and axial peaking factors distribution.

One of the challenges for Monte Carlo methods is to devise more sophisticated tally analysis, which is needed to ensure numerical stability and true convergence when coupling to fluid and heat transfer algorithms. An approach for efficient accumulation of high-precision fluxes throughout the reactor core geometry on a specifically chosen grid of cells to support multi-physics coupling has been developed.
Chapter 2
Description of codes

2.1 Introduction

The following subsections described the codes used in the research studies presented in this dissertation work.

2.2 MCNP5 code

The MCNP code (Monte-Carlo N-Particle), MCNP5 [1], is an advanced version of a flexible 3-D Monte Carlo code with provision to compute accurate detailed analysis of complex reactor configurations. The publicly available MCNP5 and NJOY99 [7] codes have been utilized and modified at PSU for the purposes of this research. The basic version of MCNP used in the presented research was MCNP5 release 1.40.

The Monte Carlo method solves physical and mathematical problems in a statistical manner. Monte Carlo can be considered a numerical experiment; which reproduces in a theoretical way a statistical process. The process of interest (physical or mathematical) is described by the probability density function (pdf). The neutron transport is explicitly simulated in Monte Carlo with the pdf. The solution in Monte Carlo methods is obtained by simulating individual particle histories, a large number of times, and tracking specific aspects, which are named tallies, of the average behavior of the particles. The central limit theorem is used to obtain the average behavior of particles in
the system from the average behavior of the simulated particles. Moreover, the variance that represents the statistical error is calculated along with the average result. Because of its statistical nature (large amount of histories needed), Monte Carlo core calculations usually involve a considerable computer time to attain reliable converged results.

In broad terms, neutron transport theory can be analyzed by deterministic and Monte Carlo methods. Both, deterministic and probabilistic, methods are quite different. On the one hand, deterministic methods obtain the solutions of the approximated representation of the model (energy, spatial and angular discretizations). In this manner, deterministic methods solve the transport equation throughout the phase space of the problem (represented by discrete units). In contrast, Monte Carlo Methods solve the exact representation of the model statistically (approximately; with statistic deviations). The Monte Carlo method does not require writing the neutron balance equation. The Monte Carlo method finds the solution by simulating individual particle histories and tracking the average behavior of certain aspects (the ones of interest). The major advantages of the Monte Carlo method over the deterministic methods are, the continuous energy treatment, and the exact three-dimensional geometry modeling. However, the Monte Carlo method involves vast computational time compared to deterministic methods.

2.2.1 Monte Carlo criticality calculations

The Monte Carlo method can be used to simulate the interaction of nuclear particles with matter (which is a statistical process) and it is extremely useful for heterogeneous and complicated geometric problems, for which deterministic methods
cannot be applied precisely. The process is encompassed by individual probabilistic events that are simulated sequentially. The complete phenomenon is explained by statistically sampling the events dictated by the probability distributions. The random numbers comprise the base for the statistical sampling process. The actual process includes the follow up of each neutron particle from its emission from a neutron source throughout its life to its death. The neutron source can be fixed or fission source and its death can be caused by different events such as absorption, escape, etc. Firstly, the starting location in the source to emit the neutron is determined. Then, the energy, direction of flight and distance to the next collision are sampled. Subsequently, with the direction of flight and distance to next collision, the location of the next collision can be established. Next, a nuclide from the material is selected, following a criteria based on random numbers, for the neutron-nuclide interaction. Once the nuclide has been selected, the type of interaction (mainly absorption or scattering) is determined (also using random numbers). In the case where there is scattering, the new direction of flight and distance to collision are chosen, starting the process again. As previously mentioned the death of the neutron would be caused by absorption or leakage.

2.2.2 Neutron flux and reaction rates in Monte Carlo

In the work presented in this dissertation, the main interest focuses on coupled Monte Carlo criticality calculations. The effective multiplication factor is calculated directly by MCNP5. The feedback parameters for the thermal-hydraulic code, namely axial and radial power profiles, are obtained by the manipulation of the neutron flux and
fission reaction rates obtained from the MCNP5 tallies. The quantities of interest, neutron flux and reaction rates, are tallied during the neutron history. There are several methods for the tallying of particles. In this case, the track length estimate of the cell flux is used, where the average particle flux in a cell is as [1]:

\[
\bar{\phi}_r = \frac{1}{V} \int dE \int dt \int dV \int d\Omega \psi(\vec{r}, \Omega, E, t)
\]

\[
\bar{\phi}_r = \frac{1}{V} \int dE \int dt \int dV \int d\Omega n(\vec{r}, \Omega, E, t)
\]  \hspace{1cm} 2.1

\[
\bar{\phi}_r = \frac{1}{V} \int dE \int dV \int dt n(\vec{r}, E, t)
\]

Where \(N(\vec{r}, E, t) = \int d\Omega n(\vec{r}, \Omega, E, t)\) is the density of particles at a specific point, not considering their trajectories. The differential unit of track lengths, \(ds\), can be defined as \(ds = v dt\) so Eq. 2.1 can be written as,

\[
\bar{\phi}_r = \frac{1}{V} \int dE \int dV \int ds N(\vec{r}, E, t)
\]  \hspace{1cm} 2.2

Where \(\bar{\phi}_r\) is the average flux over the cell (neutrons/sec-cm²), \(E\) is the neutron energy (MeV), \(\Omega\) is the direction vector, \(V\) volume of the cell (cm³), \(t\) is the time (sec), \(v\) is the neutron velocity (cm/sec), \(N(\vec{r}, E, t)\) is the neutron density (neutron/cm³), and \(s\) is the traverse distance (cm). The tally process utilizes a weight for each neutron. If the real physical transport is simulated, the weight is equal to one. In the cases where other than the real simulations are performed, the weights would have other values (depending on the simulation technique). Accordingly, the neutron track length within the cell (TL) can be expressed as the neutron density \(N(\vec{r}, E, t)\), which is in turn expressed as the
summation of the neutron weight \( (W) \), per unit volume and the transverse distance, as in Eq. 2.3,

\[
\overline{\phi_v} = \frac{\int dE \int dV \sum_{i=1}^{N} W*TL_i^i(E)}{V} = \frac{\sum_{i=1}^{N} W*TL}{V}
\]  

Eq. 2.3

The summation only counts the particles, in this case the neutrons that cross the cell of interest. The reaction rate can be obtained by simply including in Eq. 2.3 the macroscopic cross section of interest (for instance the macroscopic fission cross section \( \Sigma_f \) or the absorption cross section \( \Sigma_a \)).

### 2.2.3 Multiplication factor

The criticality calculation in the Monte Carlo method is performed in many cycles, in which each cycle carries out a number of histories and at the end of the cycle the effective multiplication (\( k_{eff} \)) factor is determined. In general terms in reactor theory, \( k_{eff} \) is the ratio between the number of neutrons in consecutive generations. \( k_{eff} \) is estimated by calculating the average number of fission neutrons produced in one generation per fission neutron started. In this aspect, a generation is considered as the life of a neutron from its birth (caused by fission) to its death (caused by absorption or leakage).

In criticality calculations, the fission source changes from cycle to cycle. As explained and analyzed later in this dissertation, the \( k_{eff} \) and the fission source distribution converge differently. The \( k_{eff} \) converges more rapidly than the source
distribution and usually the contribution of the first cycles, where the source has not converged, is ignored.

The Monte Carlo method calculates the $k_{eff}$ using three different methods where the final result with its standard deviation is the combination of the methods. These three methods are the track length estimator, the absorption estimator and the collision estimator.

Track length estimator: 
\[
k_{eff}^{TL} = \frac{1}{N} \sum_i W_i \rho d \sum_k f_k \bar{V}_k \frac{\sigma}{\nu} \rho
\]

Collision estimator: 
\[
k_{eff}^C = \frac{1}{N} \sum_i W_i \left[ \frac{\sum f_k \bar{V}_k \frac{\sigma}{\nu} f_k}{\sum k f_k \sigma_{\nu}} \right]
\]

Absorption estimator: 
\[
k_{eff}^A = \frac{1}{N} \sum_i W_i \bar{V}_k \frac{\sigma_{f_k}}{\sigma_{c_k} + \sigma_{f_k}}
\]

Where $i$ refers to the $i^{th}$ collision in a cycle where fission is possible, $k$ is the $k^{th}$ nuclide of the material involved in the $i^{th}$ collision, $\sigma_{\nu}$ is the total microscopic cross section, $\sigma_{f_k}$ is the microscopic fission cross section, $\sigma_{c_k}$ is the capture microscopic cross section, $\bar{V}_k$ is the average number of neutrons produced per fission, $f_k$ is the atomic fraction for nuclide $k$, $N$ is the nominal source size for cycle, $W_i$ is the weight of particle entering collision, $\rho$ is the atomic density in the cell, and $d$ is the trajectory track length from the last event.
Because of its statistical nature, the Monte Carlo results must take into account the standard deviation. The combination of the standard deviation and the result form the interval of confidence. The $k_{eff}$ results are usually given for three confidence intervals [1]:

- 68% confidence interval; the average result plus or minus one standard deviation.
- 95% confidence interval; the average result plus or minus two standard deviations.
- 99% confidence interval; the average result plus or minus three standard deviations.

### 2.3 Nodal Expansion Method (NEM) diffusion code

The Nodal Expansion Method (NEM) diffusion code has been developed, maintained, and continuously enhanced at PSU. NEM [8] is a few-group (with up to 10 energy groups) 3-D steady-state and transient nodal core model with three geometry modeling options: Cartesian, Hexagonal-Z, and Cylindrical (R-0-Z). The code is based on transverse integration procedure and it was recently updated to utilize semi-analytical transverse-integrated flux representation and improved transverse leakage approximation. The nodal coupling relationships are expressed in a partial current formulation. NEM is using the Response Matrix technique for inner iterations to calculate (update) ongoing partial currents for each spatial node in the framework of each energy group solution. The coarse-mesh rebalance and asymptotic extrapolation methods are used to accelerate convergence of the outer iterative solution process.
2.4 Advanced thermal-hydraulic sub-channel code COBRA-TF

The PSU version of the advanced thermal-hydraulic sub-channel code COBRA-TF (CTF) [6] has been recently improved and applied for stand-alone and coupled Light Water Reactor (LWR) core calculations. COBRA-TF stands for COlant Boiling in Rod Arrays – Two Fluid. CTF is applicable to both Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR) analyses. The code features two-fluid, three-field representation of the two-phase flow. The three-fields are continuous vapor, continuous liquid, and entrained liquid drops in the annular flow region. For each space dimension, CTF solves three momentum conservation equations, four mass conservation equations, and two energy conservation equations. The code is able to handle both hot wall and normal flow regimes maps and it is capable of calculating reverse flow and cross flow situations. The conservation equations for each of the three fields and for heat transfer from and within the solid structure in contact with the fluid are solved using a semi-implicit, finite-difference numerical technique on an Eulerian mesh. The code features extremely flexible nodding for both the thermal-hydraulic and the heat-transfer solution. This flexibility provides a capability to model the wide variety of geometries encountered in vertical components of a nuclear power vessel.

2.5 NJOY99 nuclear data processing system

The NJOY nuclear data processing system [7] converts evaluated nuclear data in the ENDF (Evaluated Nuclear Data File) format into cross-section libraries for different applications including continuous-energy Monte Carlo (MCNP). NJOY 99 is the latest
release of the NJOY nuclear data processing system and this release is used for the present studies.

The ENDF format is a general accepted format used around the world, providing its users a broad selection of current nuclear data. Table 2-1 lists some examples of the Nuclear Data Libraries around the world.

Table 2-1: ENDFs libraries around the world.

<table>
<thead>
<tr>
<th>Library</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>American</td>
<td>ENDF/B-VII</td>
</tr>
<tr>
<td></td>
<td>ENDF/B-VI</td>
</tr>
<tr>
<td>European</td>
<td>JEFF-3.1.1</td>
</tr>
<tr>
<td></td>
<td>JEF 2.2</td>
</tr>
<tr>
<td>Japanese</td>
<td>JENDL 3.3</td>
</tr>
<tr>
<td></td>
<td>JENDL 3.2</td>
</tr>
<tr>
<td>Russian</td>
<td>BROND 2.2</td>
</tr>
<tr>
<td>Chinese</td>
<td>CENDL-2.1</td>
</tr>
</tbody>
</table>

The calculations and studies in this research used mainly the American and European ENDF libraries. Some calculations have also been performed with the Japanese ENDF library.

The NJOY system is capable of processing evaluated data for different applications like deterministic transport codes, reactor lattice codes and continuous energy Monte Carlo codes. An ample variety of nuclear effects can be process through NJOY, which include: resonances, Doppler broadening heating (KERMA), thermal scattering (for moderators), radiation damage, photo-atomic particles, self shielding, probability tables, photon production, gas production, neutrons and charged particles, and high-energy interactions.
The NJOY code designed is modular. Each module performs a well defined processing task. Actually, each module can be considered a separate program, which is linked to the other modules by input and output files.

For this research, the NJOY processing system is used for the generation of continuous energy and thermal scattering cross sections. The specific NJOY modules used to generate continuous energy and thermal scattering cross sections respectively, are described in detail in Chapter 4.
Chapter 3

MCOR as a reference tool for benchmarking spectral codes

3.1 Introduction

One of the main research studies in Monte Carlo based coupled systems at the Reactor Dynamics and Fuel Management Group (RDFMG) at Penn State has been carried out in cooperation with AREVA NP in the area of Monte Carlo depletion calculations. The design and development of the Monte Carlo depletion system MCOR, was carried out during the first stage of the cooperation between PSU and AREVA NP by Dr. Chanatip Tippayakul, while he was student at PSU, under the guidance of Dr. Stefan Misu and Prof. Kostadin Ivanov [9]. The enhancements of the code, as well as the introduction of the Monte Carlo depletion system as a reference tool for benchmarking spectral codes have been performed by the author of the present dissertation under the same above mentioned guidance [10]. Due to its relevance, gained experience, and the fact that in long-term the coupled calculations will be implemented within the framework of this Monte Carlo depletion system, a brief description follows in this chapter. In this way the Monte Carlo depletion system will be able to provide reference solutions not only at fixed temperature conditions but also for operating conditions with temperature spatial distribution.

The possibilities to assess spectral codes alone are limited. The number of critical experiments and spent fuel analysis is limited. Mostly, these experiments are at exposure
zero and the existent fuel samples available for spent fuel validation do not cover the
particular interests of modern assembly designs (burnup steps up to 70 GWD/MTU or
more, various void levels, 0 up to 80% void, different enrichments and gadolinium
content). Gamma scans pin by pin are even more uncommon than the critical
experiments, and the errors in the history of the samples can be significant. Some of the
experiments are proprietary. The reactivity changes with exposure cannot be assessed by
measurements unless a three-dimensional (3-D) core simulator is used, which is an
indirect way to prove the quality of the spent fuel analysis. Therefore, such "numerical
experiments" as performed by MCOR calculations are provided to bridge gaps where
measurements lack to make comparisons for specific fuel assemblies.

The MCOR (MCnp-kORigen) code is an interfacing code that provides depletion
capability to the LANL [1] Monte Carlo code by coupling two reference codes: MCNP5
with the AREVA NP depletion code KORIGEN [11]. The physics modeling quality of
both reference codes is unchanged.

The MCOR code system has been maintained and continuously enhanced since it
was developed and validated. The verification of the coupling was made by comparing
the MCOR code against similar sophisticated codes like MONTEBURNS [12] and
OCTOPUS [13].

The chapter describes the further developments of the MCOR code system and
evaluates the calculation methodology of the spectral codes APOLLO2-A [14] and
CASMO-4 [15] with one of higher physics modeling degree like the MCOR code. The
study introduces MCOR as a reference tool for benchmarking deterministic codes by
presenting a qualification of the spectral (lattice physics) codes.
3.2 MCOR code system description

The MCOR code system is a Monte Carlo based depletion system for reference fuel assembly and core calculations. The MCNP5 code has been often employed as reference calculations for many problems because it is capable of calculating explicitly three-dimensional geometries and also treating continuous energy. Although the MCNP5 code is powerful and capable of modeling complex problems, the current version of the MCNP5 still does not provide the depletion functionality. The KORIGEN code, which is a material depletion code at AREVA NP, is thus employed as the depletion module for the MCNP5 code. In general, the coupling between the MCNP5 and KORIGEN requires a great deal of data exchange; hence, manual coupling between the two codes is very tedious and error-prone. An interfacing code is therefore foreseen and developed as a comprehensive tool for the coupling work. The MCOR code is developed such that it automates the sequences needed between the MCNP5 and KORIGEN codes.

The following subsections describe the MCOR characteristics and capability enhancements.

3.3 Computer codes

The following computer codes have been used in the coupling scheme of MCOR code.

The MCNP code (Monte-Carlo N-Particle), version MCNP5, is an advanced version of a flexible 3-D Monte Carlo code with provision to compute accurate detailed analysis of complex reactor configurations. The publicly available MCNP5 code has been
utilized and modified at PSU for the purposes of this research. The basic versions of MCNP used in the presented research were MCNP5 releases 1.30 and 1.40.

KORIGEN is the standard code employed at AREVA NP for depletion analysis. KORIGEN was developed at the research center of Karlsruhe (Germany) as an extension of ORIGEN-S [16].

### 3.4 MCOR code capabilities

The MCOR code system is a Monte Carlo based depletion system for reference fuel assembly and core calculations. The MCOR code couples MCNP5 with KORIGEN in an automatic manner. The MCNP5 code calculates burnup dependent cross sections and fluxes for the KORIGEN code and the KORIGEN code provides material compositions after burnup for the MCNP5 code, all these is performed automatically by MCOR. The MCOR code is flexible enough to perform individual depletion calculation of each burnup zone. No burnup zone grouping is required.

Various improvements were performed at the first stage of the cooperation between PSU and AREVA NP. The major improvements are summarized as following.

### 3.4.1 Utilization of KORIGEN as the depletion module

The first major upgrade to the MCOR code system was to replace ORIGEN-S with KORIGEN as the depletion module since KORIGEN, as mentioned before, is the standard code employed at AREVA NP for depletion analysis. The KORIGEN depletion
code requires the thermal flux, not the total flux as in ORIGEN-S, to perform the burnup calculation. Moreover, the KORIGEN code requires three group neutron spectra; namely, THERM (for thermal group), RES (for resonance) and FAST (for fast). Therefore, the flux tallies utilized in the MCNP5 calculation should be energy-binned accordingly. In addition, KORIGEN contains specific cross-section libraries for representative fluxes of modern BWR and PWR assemblies.

3.4.2 Online burnup cross-section generation by the Monte Carlo calculation

The next improvement to the MCOR code was the implementation of on-line burnup cross section generation by the MCNP5 calculation, instead of using the burnup cross section library pre-generated by a transport code (TRITON [17]). The generation of the burnup cross sections based on Monte Carlo calculation reflects the most current conditions in the most accurate way.

The current AREVA-MCOR implementation determines the one-group burnup cross sections from the reaction rate tally of the MCNP5 calculation by Eq. 3.1

\[
\sigma_x = \frac{\text{Reaction } "x" \text{ rate tally value}}{\text{Total flux tally value}}
\]  

3.1

To compromise between the computational time and the accuracy of MCOR, eighty-eight isotopes, which one-group cross sections are updated by the Monte Carlo calculation, are selected from an importance ranking procedure performed by CASMO-4. The rest of the burnup cross sections, other than these eighty-eight isotopes, are taken
directly from the standard KORIGEN libraries pre-calculated for each fuel assembly type.

### 3.4.3 Predictor-Corrector depletion algorithm

Additionally, a predictor-corrector depletion algorithm was introduced in MCOR to account for the neutron spectrum changes during the depletion step. The stochastic error is reduced in MCOR by imposing for each step a high statistical accuracy in MCNP5 (less than 0.25 mk on the $k_{\text{inf}}$, 1 mk is 100 pcm) and by using a predictor-corrector depletion algorithm. The carefully selected burnup step and the predictor-corrector depletion algorithm avoid the propagation of the stochastic error. In order to further reduce possible errors small depletion time steps typically 0.5 MWd/t during Gd-burnout and 2.5 MWd/t otherwise are used.

### 3.4.4 Expansion of the maximum number of tallies

The maximum number of tallies of MCNP5 used with the MCOR code is expanded from 100 to 1000 so that MCOR can be used with a problem having a number of burnup zones larger than 100 which is typical for cases with Gd$_2$O$_3$ fuel pins. This allows the modeling of all individual Gd-pins with 10 burn-up rings.
3.4.5 New fission Q value used to include both prompt and delay energy released per fission

Since the fission Q value originally used in MCNP5 is only total prompt energy released per fission, the new fission Q value shall be used to include both prompt and delay energy released per fission, so the Q value are the same as those of CASMO-4.

3.5 MCOR code enhancements

The MCOR code presents several valuable capabilities over other coupled MCNP5-ORIGEN based code systems like: a) a predictor-corrector depletion algorithm, b) utilization of KORIGEN as the depletion module, c) individual depletion calculation of each burnup zone (no burnup zone grouping is required, which is particularly important for the modeling of gadolinium rings) and d) online burnup cross-section generation by the Monte Carlo calculation (to compromise between the computational time and the accuracy of AREVA-MCOR, eighty-eight isotopes, which one-group cross sections are updated by the Monte Carlo calculation, are selected from an importance ranking procedure performed by CASMO4. The burnup cross sections of other isotopes not in this list are taken directly from the standard KORIGEN libraries pre-calculated for each fuel assembly type.). Besides the just mentioned capabilities, the MCOR code enhancements are summarized in the following paragraphs.
3.5.1 Possibility of executing the MCNP5 calculation in sequential or parallel mode

The latest version of MCOR presents the possibility of executing the Monte-Carlo criticality calculation either in sequential or parallel mode. The OpenMP model available in MCNP5, shared-memory parallelism (threads) model, is used in the parallel execution mode. When the parallel mode is selected, the number of processors (depending on the available system) is specified in the correspondent MCOR input card. All the required parallel information is specified in the MCOR input file and controlled by the MCOR code.

3.5.2 Check input card subroutine

A further enhancement of MCOR assures that all input parameters of each input card are read properly. The new MCOR version is capable of capturing the errors if the entries of some cards are not complete and prompts the user to correct the input prior to starting the calculation.

3.5.3 User-friendly automatic restart capability

The latest version of MCOR incorporates an automatic restart capability. In this way the user does not have to perform any task manually. The new MCOR restart mode backups automatically the output files for reference and locates, or regenerates, if it is necessary, the composition file needed for the restart.
3.5.4 Modification of the burnup step size evaluation

Other improvement focused on the modification of the burnup step size evaluation to allow small burnup size steps to model a decay period between operating conditions.

3.5.5 MCOR post-processor and test-matrix

The MCOR post-processor summarizes the $k_{\text{inf}}$, isotopic content, and fission rates distribution results as a function of burnup steps. When the MCOR code performs reference calculations, the post-processor compares the different results (MCOR vs. APOLLO2-A for example) and prints the mean and standard deviation for the $k_{\text{inf}}$ results, the root mean square (RMS) and peak pin power for the fission rates distribution results, and the difference of the isotopic content results.

3.6 Verification and validation of MCOR

Different models, pins and assemblies, were used to assess the capabilities and correctness of the MCOR code. In addition, the calculations were executed using different cross-section libraries (ENDFB-VI release 8 [18-19], JEF2.2 [20] and JEF3.1 [20]). The results of the MCOR calculations were compared against the predictions of other commercial codes (APOLLO2-A and CASMO-4), but of more relevance, the MCOR calculations were validated against other reference codes (MONTEBURNS and OCTOPUS).
In the case of the pin cell tests, two cases (UO₂ and MOX) were selected to verify the proper modeling of the MCOR code. Both pin cell models were taken from the Benchmark, “Problem Suite for Reactor Physics Study for LWR Next Generation Fuels” [21]. The UO₂ pin cell model is run in MCOR with two different libraries, JEF2.2 and ENDF/B-VI, and compared against the calculations of the codes specified in the Benchmark. The \( k_{\text{inf}} \) results calculated by the HELIOS, CASMO4 and MCOR codes for the UO₂ Pin cell model are depicted in Figure 3-1.

![Figure 3-1: \( k_{\text{inf}} \) comparison of the UO₂ pin cell model](image)

The close comparison of the MCOR \( k_{\text{inf}} \) predictions against the reference Benchmark is illustrated by the mean and the standard deviation in mk shown in Table 3-1 below.
The isotopic concentration comparison of the UO₂ PIN cell model between MCOR and TRIPOLI-PEPIN [22] is illustrated in Table 3-2. As specified in this Benchmark, the discharged burnup is 70 (GWd/t).

<table>
<thead>
<tr>
<th></th>
<th>HELIOS(B6/KA) vs MCOR(JEF2.2)</th>
<th>HELIOS(B6/KA) vs MCOR(ENDFB-VI)</th>
<th>MCOR(JEF2.2) vs CASMO(B4/NF)</th>
<th>MCOR(ENDFB-VI) vs CASMO(B4/NF)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mean</strong></td>
<td>4.467</td>
<td>3.100</td>
<td>0.334</td>
<td>1.701</td>
</tr>
<tr>
<td><strong>Std. Dev.</strong></td>
<td>3.726</td>
<td>2.632</td>
<td>1.728</td>
<td>0.982</td>
</tr>
</tbody>
</table>

Table 3-1: \( k_{\text{inf}} \) comparison between the Benchmark and the MCOR codes
Table 3-2: Isotopic concentration comparison for the UO$_2$ pin cell model at 70 GWd/t Burnup between MCOR and Tripoli-Pepin.

<table>
<thead>
<tr>
<th>Isotopes</th>
<th>MCOR-ENDFB-VI / TRIPOLI PEPIN</th>
<th>MCOR-JEF2.2 / TRIPOLI PEPIN</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-235</td>
<td>0.99</td>
<td>1.00</td>
</tr>
<tr>
<td>U-236</td>
<td>1.05</td>
<td>1.04</td>
</tr>
<tr>
<td>U-238</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Np-237</td>
<td>1.11</td>
<td>1.17</td>
</tr>
<tr>
<td>Pu-238</td>
<td>1.10</td>
<td>1.17</td>
</tr>
<tr>
<td>Pu-239</td>
<td>1.01</td>
<td>1.00</td>
</tr>
<tr>
<td>Pu-240</td>
<td>0.99</td>
<td>1.01</td>
</tr>
<tr>
<td>Pu-241</td>
<td>1.01</td>
<td>1.00</td>
</tr>
<tr>
<td>Pu-242</td>
<td>0.99</td>
<td>1.02</td>
</tr>
<tr>
<td>Am-241</td>
<td>0.97</td>
<td>0.93</td>
</tr>
<tr>
<td>Am-242m</td>
<td>0.89</td>
<td>0.83</td>
</tr>
<tr>
<td>Am-243</td>
<td>1.09</td>
<td>1.00</td>
</tr>
<tr>
<td>Cm-242</td>
<td>1.05</td>
<td>1.06</td>
</tr>
<tr>
<td>Cm-243</td>
<td>0.60</td>
<td>0.63</td>
</tr>
<tr>
<td>Cm-244</td>
<td>1.10</td>
<td>0.99</td>
</tr>
<tr>
<td>Cm-245</td>
<td>1.02</td>
<td>0.99</td>
</tr>
<tr>
<td>Cm-246</td>
<td>0.97</td>
<td>0.99</td>
</tr>
<tr>
<td>Mo-95</td>
<td>0.98</td>
<td>0.98</td>
</tr>
<tr>
<td>Tc-99</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Rh-103</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>Cs-133</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>Sm-147</td>
<td>0.99</td>
<td>0.97</td>
</tr>
<tr>
<td>Sm-149</td>
<td>1.01</td>
<td>0.99</td>
</tr>
<tr>
<td>Sm-150</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>Sm-152</td>
<td>0.98</td>
<td>0.98</td>
</tr>
<tr>
<td>Nd-143</td>
<td>0.98</td>
<td>0.99</td>
</tr>
<tr>
<td>Nd-145</td>
<td>0.97</td>
<td>0.99</td>
</tr>
<tr>
<td>Eu-153</td>
<td>0.97</td>
<td>1.00</td>
</tr>
<tr>
<td>Gd-155</td>
<td>0.96</td>
<td>1.01</td>
</tr>
</tbody>
</table>

As illustrated by the figure and tables in this subsection, the $k_{inf}$ and the isotopic content results of MCOR and the ones presented in the Benchmark are within good agreement. Of particular interest is the comparison between MCOR and TRIPOLI-PEPIN Monte Carlo depletion code, both codes are considered superior or references codes.
(because of the physical quality of the modeling), and the isotopic content predictions of these two reference codes are very close, as it can be seen in Table 3-3 the difference is very close to one for all the isotopes. In a similar manner and to compile with the validation process, MCOR is tested with a different Pin cell model, MOX Pin Cell, and compared against a different “reference code”, MONTEBURNS (MCNP5-ORIGEN). The results of this comparison also agreed well with the ones presented in the Benchmark (since these results are very similar as the ones for the UO$_2$ Pin Cell model, the comparison is not presented in the current work to not be repetitive).

The MCOR code is capable of modeling both types of LWRs, BWRs and PWRs. The next test analyzes the MCOR code capabilities to model a PWR assembly model. The test is based on the PWR Benchmark by GRS [23]. The $k_{inf}$ comparison of the codes specified in the Benchmark and MCOR is illustrated in Figure 3-2. As in the case for the BWR models, the MCOR simulation of the PWR assembly showed good agreement compared to the codes specified in the Benchmark. The $k_{inf}$ differences are very small and the MCOR predictions of the PWR assembly agree well with the rest of the calculations.
Several MCOR calculations have been performed for modern assemblies (ATRIUM™ 10 UOX and MOX assemblies; ATRIUM is a trademark of AREVA NP), with different cross-section libraries (ENDFB-VI, JEF2.2 and JEF3.1), as summarized in the next section. In addition, the MCOR code has been used to study the design of innovative assembly concepts (with uncommon geometric characteristics, like the content of displaced pins for instance) showing very good results. These assemblies are propriety and cannot be published.

Figure 3-2: $k_{inf}$ comparison of the PWR assembly model by GRS Benchmark
3.7 Qualification of APOLLO2-A and CASMO-4

The major advantages of the Monte Carlo method over the deterministic methods are, the continuous energy treatment, correct treatment of resonances, and no specific groups collapsation. Additionally no geometric homogenization is needed. The stochastic error is reduced in MCOR with high statistical accuracy (less than 0.25 mk on the $k_{inf}$) and by using a predictor-corrector depletion algorithm. The carefully selected burnup step and the predictor-corrector depletion algorithm avoid the propagation of the stochastic error.

3.7.1 Description of the AREVA NP spectral code APOLLO2-A

The APOLLO2-A is a new generation spectral code of high accuracy for Pressurized and Boiling Water Reactor applications. The new APOLLO2-A code was developed by AREVA NP based on the APOLLO2 multi-group transport code developed by Commissariat a l’énergie atomique (CEA) [24]. The APOLLO2-A code presents a new calculation scheme for the self-shielding and different levels flux solvers. The multi-group cross section library is based on JEFF3.1. This multi-group cross section library uses the 281 energy group SHEM mesh [25]. This energy mesh presents a fine energy spacing, which implicitly describes the self shielding and resonance overlapping in the energy range from 0 to 23 eV. The isotopic inventory of the multi-group cross section library is as follows: 40 heavy nuclides, 93 fission products and about 200 further nuclides. It is intended in the future to have as alternative a cross section library with the same energy mesh based on ENDF/B-VII.
The APOLLO2-A code uses a three level scheme, referring to three separate flux calculations with different degrees of spectral and spatial accuracy.

The calculation scheme starts by performing a self shielding calculation in 281 energy groups on one-dimensional (1-D) geometries. This calculation is performed for structural materials, water regions and pins, and on two-dimensional (2-D) geometry for the pins, which are subdivided into rings.

Then, the first level flux solution is calculated. The first level flux is computed on simplified assembly geometry with 281 energy groups using the collision probability (Pij) method with interface-current approximation. The calculated first level flux is used to collapse the self-shielded cross sections to 44 energy groups for the calculation of the second level flux solver.

The second level flux calculation is a 2-D calculation carried out on a Cartesian grid with homogenized pin cells. Using a discrete ordinates (IDT-SN) solver the second flux solution is calculated in 44 energy groups. The second flux solution is combined with the first level flux in order to obtain the 281 energy group 2-D flux and then the cross sections are collapsed to 26 groups for the third level solver.

The third level flux calculation uses the Method of Characteristics (MOC) solver on a very fine unstructured spatial grid, which represents the real geometry, with the collapsed cross sections to calculate the flux in 26 energy groups. The third level flux solution is combined with the first level flux to obtain a final reconstructed 2-D flux in 281 energy groups.
The APOLLO2-A depletion module uses the predictor-corrector scheme and the quadratic extrapolation of the reaction rates to improve the description of cases with burnable absorbers.

### 3.7.2 Description of the CASMO-4 code

CASMO-4 [15] is a multi-group two-dimensional (2-D) transport code for burnup calculations of simple pin cells, 2-D arrays of pin cells, and BWR and PWR assemblies.

The library contains the nuclear data with the microscopic cross sections in 70 energy groups. The neutron energy range covered is from 0 to 10 MeV. A library containing data in 40 energy groups is also available.

CASMO-4 can simulate non symmetric fuel bundles of 75 by 75 rods, this restriction can be modified by changing the array dimensions. In general, most of the bundles are symmetric. The assembly allows absorber rods, circular or square, or water holes covering 1x1, 2x2, 3x3, or 4x4 pin cell positions.

Some of the characteristics of the multi-group 2-D transport code CASMO-4 can be summarized as follows: the code calculates individually for each fuel pin the effective resonance cross sections. The leakage effects are taken into account by performing a fundamental mode calculation. The 2-D transport calculation can be performed in any random group structure. The microscopic depletion is computed in each fuel and burnable absorber pin. The depletion calculation uses a predictor-corrector approach. Discontinuity factors are calculated at the boundary between bundles and for reflector
regions. Macro and micro cross sections can be generated for few-group diffusion or transport theory programs.

CASMO-4 has incorporated two new features in the main calculation. One of the new features is the microscopic depletion of burnable absorbers, as Gadolinia, and the other feature is a heterogeneous model for the two-dimensional calculation.

3.7.3 Description of the ATRIUM™ UOX and MOX assemblies

Two fuel lattices of AREVA ATRIUM™ 10 design, 10x10 BWR lattice with an asymmetrically positioned large internal water channel covering 3x3 positions, were calculated with APOLLO2-A, CASMO-4 and MCOR. The first one, a UO₂ highly enriched bundle – UOX -(mean lattice value of 4.6 w/o U-235), had five pin enrichment levels covering the range from 2.65 up to 4.95 w/o U-235 and 16 pins with 2.5 w/o Gd₂O₃. The second lattice contained pins with MOX fuel, wherein the content in fissile Plutonium isotopes was between 1.6 w/o and 6.3 w/o, leading to a mean lattice enrichment of 3.9 w/o Pu₉₃.

The fuel assemblies were modeled in half symmetry as illustrated in Figure 3-3. Each fuel pin represents a single fuel zone, except for the fuel pin with Gd₂O₃ which was divided into 10 equal-volume rings, each being a fuel zone.
3.8 Results

The results of APOLLO2-A and CASMO-4 calculations are compared against the MCOR predictions. The APOLLO2-A, CASMO-4 and MCOR calculations of the two fuel lattices are modeled at 40% void. Detailed comparisons are performed for two different libraries - JEF2.2 and JEFF3.1. The results of the k_{inf}, fission rate distribution and isotopic content as functions of burnup were compared indicating a good agreement between the spectral codes and MCOR. Figure 3-4 presents, as example, the comparison of the k_{inf} calculated by the APOLLO2-A and MCOR codes as a function of burnup for the ATRIUM 10 UOX and MOX lattices at 40% void using JEFF3.1. k_{inf} is given in mk, 1 mk is 100 pcm.
Figure 3-5 illustrates the isotopic densities at burnup 70 GWd/t for Atrium 10 (UOX 4.6 % / MOX 4.05 % mean enrichment, at 40% Void) between APOLLO2-A MCOR.
The comparison of the most important isotopes of the actinides is below 5% difference, indicating very good agreement. The rest of the actinides are within the 10% difference, which indicates an acceptable agreement. In the case of the fission products, the comparison is well inside the 20% difference range.

Figure 3-5: Ratios of isotopic densities at burnup 70 GWd/t for ATRIUM 10 (UOX 4.6 % / MOX 4.05 % mean enrichment, at 40% Void) between APOLLO2-A and MCOR

Figure 3-6 presents the comparison of the $k_{inf}$ calculated by the CASMO-4 and MCOR codes as a function of burnup for the ATRIUM 10 UOX and MOX lattices at 40% void using JEF2.2. The comparison between the MCOR code and the respective spectral code is carried out using the same cross-section library. In this way, any difference caused by the library is eliminated and the analysis is focused only on the nuclear physics.
3.9 Sensitivity Studies

The sensitivity studies present a comparison of the MCOR results at different void fractions (0%, 40%, and 80%) using the ATRIUM 10 MOX fuel lattice and ENDF/B-VI cross section library, as illustrated in Figure 3-7. The MCOR predictions reflect the expected physical trend of $k_{\text{inf}}$ as function of burnup at different void fraction conditions. Selected results support the comparative analysis of the behavior of differences (between MCOR as reference and APOLLO2-A, and CASMO-4) as function of void fraction and cross-section library.
3.10 Conclusions

The Monte Carlo depletion calculations have provided great understanding and experience in order to prepare the framework of the hybrid coupled Monte Carlo based code system. Also, one of the recommendations for future work of this dissertation is that in the long-term, the hybrid coupled MCNP5/CTF/NEM/NJOY calculations should be implemented within the framework of this Monte Carlo depletion system. In this way the Monte Carlo depletion system will be able to provide reference solutions not only at fixed temperature conditions but also for operating conditions with temperature spatial distribution.

Figure 3-7: ATRIUM 10 MOX lattice $k_{\text{eff}}$ comparisons as function of burnup for different void fractions.
Chapter 4

Automated methodologies for generation of temperature dependent MCNP5 cross-section libraries

4.1 Introduction

The neutron-nucleus interactions vary rapidly with the incident neutron energy, with the type of nucleus (from one nucleus to another - even with isotopes of the same element), and with the temperature of the target nucleus. The motion (energy) of the nucleus changes with temperature and this affects the range of relative energy between the interacting neutron and the target nucleus. The thermal energy behavior of the nucleus is assumed to be distributed according to the Maxwellian distribution function. Consequently, even in the case where the neutron is mono-energetic, the relative energy interaction would be represented by a range of energy. This event is known as the “Doppler nuclear effect” since it is corresponding to the Doppler Effect in waves [26].

In this way, due to the nuclear Doppler Effect, the width of the resonance region broadens (Doppler broadening) causing the peak to decrease when the temperature of the target nucleus increases. The relevance of the Doppler broadening is that the total resonance area under the peak remains constant, i.e. with increasing temperature, the width of the resonance region increases (broadens) while the height of the peak decreases. With the increase in the width of the resonance region caused by the increase in temperature, the neutron absorption will augment. Consequently, the multiplication factor of the system decreases.
As described in the previous paragraphs, the behavior of the reactor and hence the multiplication factor of the system is greatly affected by core temperature and must be considered for a proper modeling of the system. The temperature effect, and thus the temperature feedback, is accounted through the generation and utilization of the temperature dependent cross-section libraries.

4.2 Generation of temperature dependent MCNP5 continuous energy cross-section libraries

The continuous energy treatment is one of the major advantages of the Monte Carlo method over the deterministic ones. These continuous or point-wise cross sections can be produced by a nuclear data processing code. The NJOY code is the nuclear data processing system, used in the present dissertation, which produces point-wise and group-wise cross sections from the Evaluated Nuclear Data File (ENDF). The nuclear data is enclosed in the ENDF files. The code converts the evaluated nuclear data into libraries useful for applications in computer codes solving nuclear engineering problems. It has the capability to generate the required continuous energy MCNP5 cross sections.

The ENDF data is freely obtainable from various sources such as national laboratories and data banks. In this work, the ENDF data was downloaded from the Los Alamos National Laboratory website. There are a number of versions of ENDF available. For this project, ENDF/B-VI.8 and ENDF/B-VII.0 are used with the NJOY version 99.161.

The generation process for cross-section libraries is tedious and involves a lot of data manipulation. Figure 4-1 illustrates the NJOY cross-section generation process, the
The process is performed per isotope per temperature. In broad terms, the NJOY code requires two inputs: the ENDF file with the nuclear data of the corresponding isotope and the NJOY input file with the corresponding generation methodology. The NJOY code generates several output files that need further processing in order to have the final output files used for the nuclear calculations.

For this reason, an automated tool has been developed (GEN-XS code) to process and manage all data processing requirements during the generation process. This automated methodology has been developed as part of the hybrid Monte Carlo-based coupled core studies at PSU.

The duration of the procedure has been significantly reduced. This automated tool performs the most time consuming tasks of the cross-sections generation process. The automated cross-section generation process is shown in Figure 4-2. The GEN-XS code generates NJOY input files, calls NJOY to execute all specified cases, and processes all
output. The GEN-XS code automates the process for all required isotopes and all required temperatures. The final output of the automated tool is a cross-section library together with the corresponding directory of cross-section files needed by MCNP5. The generated libraries are readily useable by MCNP5.

Figure 4-2: Automated cross section generation process

This tool is used together with the automated cross-section temperature interpolation capability for intermediate points. The temperature dependent modeling capability is included into the coupled-code. In this way, it will automatically determine or interpolate the appropriate temperature dependent cross section library for the MCNP5 criticality calculation according to the temperature feedback.
4.2.1 NJOY modules for generation of continuous energy cross section libraries

The NJOY99 code is designed in a modular way; where each module performs a specific task. This feature makes possible to choose only the modules that are relevant to a specific problem. The modules are coupled by their input and output files and other general parameters.

The following methodology was used in processing of ENDF files for generation of MCNP5 cross section.

**RECONR (reconstructs pointwise (energy-dependent) cross sections from ENDF resonance parameters and interpolation schemes)**

The RECONR module reconstructs resonance cross sections, in the resonance energy range, from ENDF resonance parameters. It also reconstructs the cross sections from ENDF/B nonlinear interpolation schemes. It reads the ENDF-format tape and produces a common energy grid for all neutron reactions so that all cross sections can be obtained by interpolation (within a specified tolerance). The cross sections are subsequently liberalized after the generation of the common grid over all energy ranges. The common energy grid and linearization of cross sections is carefully performed so that no important energy structure or resonance is missed. The output of the module is written into a PENDF (point-wise) tape, where the cross sections between two energy grids can be obtained by liner interpolation. This PENDF tape is the input file or starting point for other modules.
BROADR (Doppler-broadens and thins point-wise cross sections)

The BROADR module reads the PENDF tape and then Doppler-broadens the data with the accurate point-kernel method. All resonance reactions are broadened simultaneously thanks to the common energy grid, which reduces the computational time. Once the broadening and thinning has finished, the cross sections are again reconstructed form their parts and the results are written into a new PENDF tape. The BROADR module is of great relevance for generating temperature dependent continuous energy cross sections because it adds the temperature dependence to the PENDF cross sections.

The effective cross section for a given material at temperature T is defined as the cross section that presents the same reaction rate for stationary target nuclei as the real cross section presents for moving nuclei. Thus, it can be expressed mathematically as Eq. 4.1 [7]:

\[ \rho v \bar{\sigma}(\nu, T) = \int d\nu' \rho |\nu - \nu'| \sigma(|\nu - \nu'|)P(\nu', T) \]  \hspace{1cm} 4.1

where \( \nu \) is the velocity of the incident particles, \( \nu' \) is the velocity of the target, \( \rho \) is the density of the target nuclei, \( \sigma \) is the cross section of the stationary nuclei, and \( P(\nu', T) \) is the distribution of target velocities in the laboratory system.

When the target motion is isotropic, which happens for many cases, the distribution of velocities can be written by the Maxwell-Boltzmann function as in Eq. 4.2

\[ P(\nu', T)d\nu' = \frac{\alpha^{3/2}}{\pi^{3/2}} \exp\left( -\alpha \nu'^2 \right)d\nu' \]  \hspace{1cm} 4.2

where \( \alpha = M/(2kT) \), \( k \) is Boltzmann’s constant, and \( M \) is the target mass.
The standard form of the Doppler-broadened cross sections used in the code is obtained by partially integrating equation Eq. 4.1 in terms of the relative speed $V$, as shown by Eq. 4.3

$$\sigma(v) = \frac{\alpha^{1/2}}{\phi^{1/2} v^2} \int dV \sigma(V) v^2 \left\{ e^{-\sigma(v-v)^2} - e^{-\sigma(v+v)^2} \right\}$$

Eq. 4.3 is the standard equation form for Doppler broadened cross-sections.

**UNRESR (computes effective self-shielded pointwise cross sections in the unresolved energy range)**

The UNRESR module is used to produce the effective cross sections in the unresolved region. The UNRESR module computes the effective self-shielded pointwise cross sections, versus energy and background cross section, for resonance reactions in the unresolved resonance region. This is done for each temperature produced by the BROADR module using the mean resonance parameters from the ENDF evaluation. The unresolved range begins at the energy where it is difficult to measure individual resonances. It extends to the energy where the effects of fluctuations in the resonance cross sections become unimportant. The UNRESR module averages the values of resonance widths and spacings together with distribution functions for the widths and spacings. This representation is converted into effective cross sections. The module uses the ENDF tape and the PENDF tape from BROADR as input. The computed effective cross sections are written onto a new PENDF tape.
The UNRESR module has become out of date for dealing out unresolved region since it is presently replaced by the later PURR module. Even so, the standard NJOY procedure requires the UNRESR module to be executed before the PURR module.

HEATR (generates pointwise heat production cross sections (KERMA factors) and radiation-damage-production cross sections)

The HEATR module generates point-wise heat and radiation-damage-production cross sections for specified reactions. Neutron heating arises from the kinetic energy of the charged products of a neutron-induced reaction. It is proportional to the local neutron flux. The heating can cause damage to the crystalline structure of the material. The module uses the ENDF tape and the PENDF tape from UNRESR as input. The output is written onto a new PENDF tape.

PURR (is used to prepare unresolved-region probability tables for the MCNP5 continuous-energy Monte Carlo code)

The PURR module produces probability tables to treat unresolved-resonance self-shielded for the continuous-energy MCNP5 code. The UNRESR module generates unresolved self-shielding data suitable for multi-group methods after being processed by GROUPR. The method used by this module (Bondarenko method) is not very useful for continuous-energy Monte Carlo methods. Instead, according to Levitt [7] the correct and natural approach for treating unresolved-resonance self-shielding for Monte Carlo codes is the so called Probability Table method. This method creates probability tables of the elastic, fission, capture and total cross sections. The Monte Carlo code would sample a
random number between 0 and 1 to determine the corresponding cross section in the appropriate probability table.

**GASPR (produces gas production cross sections)**

The GASPR module is used to produce the gas production cross sections for several useful applications. The total productions of protons (hydrogen), alphas (helium) and other light charged particles equation produced from the neutron flux are needed and thus produced by the GASPR module. The GASPR module evaluates all the reactions producing each particle and includes them into the existing PENDF format.

**THERMR (produces cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range)**

The THERMR module generates point-wise neutron scattering cross sections in the thermal energy range. The energy distribution and angle of the scattered neutrons are affected by the motion of the bounded target atoms in the thermal energy range. It produces inelastic cross sections and energy-to-energy matrices for free atoms or bound scatterers by means of the \( S(\alpha, \beta) \) model. The THERMR module uses the ENDF tape and the PENDF tape from UNRESR as input. The output is written onto a new PENDF tape.
ACER (prepares libraries in ACE format for the Los Alamos continuous-energy Monte Carlo code MCNP5)

The ACER module reformats cross section libraries into the ACE format required by the MCNP5 code. The output of ACER module is cross section libraries readable by MCNP5. Since NJOY produces these libraries for each individual nuclide (according to the NJOY input file), it is necessary for these libraries to be combined into one library together with relevant directories. This is where GEN-XS manages the data and produces the required libraries containing all specified material.

MODER (converts ENDF “tapes” back and forth between formatted (ASCII, EBCDIC, etc) and blocked binary modules)

The MODER module converts the data from formatted mode (e.g. ASCII) to blocked-binary mode, and vice versa (from blocked-binary to formatted mode). A formatted file has a positive unit number, while a binary file has a negative unit number.

Figure 4-3 depicts the use of the NJOY modules for continuous energy cross sections generation.
4.2.2 Continuous energy cross sections as a function of temperature

The automated methodology, using the just described NJOY modules, was applied to generate several continues energy cross section libraries at different temperatures. The effects of temperature on cross sections can be illustrated graphically. The resonance peak goes down with temperature, while the resonance broadens,
preserving the area under the resonance. To exemplify this temperature effect on cross sections, Figure 4-4 shows the total cross section of U-235 at four temperatures: 600 K, 1000 K, 1500 K and 1950 K. As the temperature increases, the cross section peaks drop. This can be observed on Figure 4-4 where the highest peak corresponds to the 600 K graph and the lowest to the 1950 K. The transition through the intermediate peaks, corresponding to the intermediate temperatures of 1000 K and 1500 K respectively, are also shown in Figure 4-4.

![Figure 4-4: Effect of temperature on the total cross section (SigmaT) of U-235](image)
The previous Figure 4-4 illustrates the more than 60,000 points that describe the total cross section (SigmaT) of U-235. This detailed representation requires a logarithmic scale and the differences seem quite small. To understand the temperature effect on cross sections, Figure 4-5 illustrates the close up of one of the resonances peaks in a linear scale.

As observed in Figure 4-5, as temperature increases, the resonance peak falls down, since the area under the resonance is the same, the resonance broadens. Appendix A contains the plots illustrating the effects of temperature for several cross sections of U-235 and U-238.
Prior to the implementation of the temperature dependent cross sections into the coupled system, the automated methodology for generation of continuous energy cross sections is further tested using a simple model. The model comprises a pin cell extracted from the 3-D BWR 2 by 2 array used to test the coupled code in further sections. The characteristics of this model are described in detail in Chapter 6.

In order to assess only the effect of fuel temperature on cross sections, the rest of the parameters, like the moderator density, are assumed constant. The cross sections of the fuel isotopes are generated at temperatures of 566 K, 615 K, 673 K, 711 K, 766 K, 832 K, 891 K, 935 K, and 1045 K. Then the MCNP5 criticality calculation of the pin cell model at each of these temperatures was performed. Table 4-1 shows the effective multiplication factor ($k_{eff}$) results corresponding to each temperature.

<table>
<thead>
<tr>
<th>Temperature [K]</th>
<th>$k_{eff}$</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>566</td>
<td>1.38669</td>
<td>0.00026</td>
</tr>
<tr>
<td>615</td>
<td>1.38471</td>
<td>0.00026</td>
</tr>
<tr>
<td>673</td>
<td>1.38264</td>
<td>0.00025</td>
</tr>
<tr>
<td>711</td>
<td>1.38101</td>
<td>0.00025</td>
</tr>
<tr>
<td>766</td>
<td>1.37881</td>
<td>0.00025</td>
</tr>
<tr>
<td>832</td>
<td>1.37635</td>
<td>0.00025</td>
</tr>
<tr>
<td>891</td>
<td>1.37449</td>
<td>0.00026</td>
</tr>
<tr>
<td>935</td>
<td>1.37254</td>
<td>0.00026</td>
</tr>
<tr>
<td>1045</td>
<td>1.36916</td>
<td>0.00027</td>
</tr>
</tbody>
</table>

The effect on the $k_{eff}$ as a function of the average fuel temperature can also be observed on Figure 4-6.
Figure 4-6: $k_{\text{eff}}$ of the pin cell model as a function of average fuel temperature

Figure 4-6 shows the rather linear decrease of $k_{\text{eff}}$ with increasing average fuel temperature as expected.

Figure 4-7 shows that the absorptions rate increases linearly with increasing average fuel temperature caused by the Doppler Effect.
4.3 Generation of thermal scattering cross-section libraries for MCNP5

The cross sections, as well as the angular and energy distributions of the scattered neutrons are affected, at thermal neutron energies, by the binding of the scattering nucleus. This is because the neutron can lose or gain energy in the interaction. These effects are taken into account in the ENDF files, particularly in the thermal sub-library.

The generation of thermal scattering cross-section libraries, in the particular purpose of this research, focus on H₂O, the moderator of LWRs. The cross-section libraries of the thermal scattering of water do not follow the same procedure as for the

![Figure 4-7: Absorption rate in the fuel pin cell model in the epithermal range as a function of temperature](image.png)
generation of the continuous energy cross sections. These differences required a more complex study.

The thermal neutron cross sections are enormously difficult to calculate due to their susceptible dependence on the temperature, as well as on the chemical state of the scattering material. In broad terms the thermal cross section data is calculated as follows. The differential scattering cross section \( \sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \) is expressed using a quantity known as the scattering law \( S(\alpha, \beta) \) for the respective material as Eq. 4.5:

\[
\sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{1}{4\pi kT} \left( \frac{E'}{E} \right)^{1/2} \exp\left( -\frac{\beta}{2} \right) \sigma_b S(\alpha, \beta)
\]  

where \( E \) and \( E' \) are the incident and secondary neutron energies, respectively in the laboratory systems, \( \sigma_b \) is the bound scattering cross section, \( kT \) is the temperature in eV and \( S(\alpha, \beta) \) is the symmetric form of the thermal scattering law, which depends on two variables: the momentum transfer \( \alpha \) and the energy transfer \( \beta \) (which are defined in the following page).

The scattering law \( S(\alpha, \beta) \) depends on the dynamics and on the detailed of the scattering material. Several approximations are needed in order to be able to calculate \( S(\alpha, \beta) \); only incoherent scattering is considered, then the incoherent part of the scattering law is calculated with the Gaussian approximation. In such a way that the neutron scattering dependence on the motion of the atoms of the moderator is enclosed in a frequency distribution function. In the case of a harmonica solid, this function is known as the phonon frequency distribution. For the case of liquid moderators like in the case of
water, the model must include vibrations, hindered rotations and translations of the water molecule.

Most of the work performed in thermal neutron scattering was in the 1950s and 1960s. Later, General Atomic developed the GASKET methodology to generate data libraries. In the 1990s, the scattering law module LEAPR, which is based on the British code LEAP jointly with the original General Atomic physics model, was implemented in the nuclear data processing system NJOY. The LEAPR module can process the newer ENDF files that have a better accuracy over a wider energy range.

In NJOY, the LEAPR module is used to prepare the scattering law $S(\alpha, \beta)$ and related quantities that describe thermal neutron scattering from bound moderators, into the ENDF-6 format used by the THERMR module [27, 28].

The LEAPR module requires a uniform grid for the continuous frequency distribution. The specific points in the $\alpha$ and $\beta$ grid have to be carefully chosen for the dynamical modes. Subsequently the rho–energy corresponding to the frequency distribution at each temperature is used. As an example, Figure 4-8 shows the rho-energy distributions for different temperatures taken from the IKE model [28].
The thermal neutron scattering cross section theory, contained in the LEAPR module, can be broadly divided into three different parts:

**Inelastic**

It is important for all materials, incoherent as well as coherent fall in this class and is described by the scattering law $S(\alpha, \beta)$.

Figure 4-8: IKE model: rho-energy distributions for different temperatures. The data used to construct this graph was obtained from [28]
As expressed in the LEAPR documentation [28], the double differential scattering cross section for thermal neutrons for gases, liquids, or solids consisting of principal scatterer, randomly ordered, molecules is written as Eq. 4.5

$$\sigma(E \rightarrow E', \mu) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} S(\alpha, \beta)$$  

where $E$ and $E'$ are the incident and secondary neutron energies, respectively in the laboratory systems, $\mu$ is the cosine of the scattering angle in the laboratory system, $\sigma_b$ is the bound scattering cross section for the material (sum of $\sigma_b^{inc} + \sigma_b^{coh}$), $kT$ is the temperature in eV and $S(\alpha, \beta)$ is the symmetric form of the thermal scattering law, which depends on two variables:

- the momentum transfer $\alpha = \frac{E' + E - 2\sqrt{E'E} \mu}{AkT}$, where $A$ is the ratio of the scatter mass to the neutron mass, and

- the energy transfer $\beta = \frac{E' - E}{kT}$, $\beta$ is positive for energy gain and negative for energy loss.

**Coherent and Incoherent scattering**

The scattering of neutrons from a system with a certain number of particles with a random distribution of spins or isotope types can be expressed as the sum of a coherent and incoherent part. The properties of the materials state the cross sections for the coherent and incoherent scattering. The coherent and incoherent scatterings include both elastic and inelastic parts. There is no energy change in the elastic scattering. Thermal
elatic scattering can be considered to be scattering from the entire lattice, therefore the effective mass of the target is very large and in this way during the scattering process, the neutron does not lose energy. On the other hand, thermal inelastic scattering results in an energy loss or gain for the neutron with an excitation or deexcitation of the target respectively.

**Incoherent elastic**

It is important for hydrogenous solids like zirconium hydride and polyethylene or light water ice. It depends on the sum of noninterfering waves from all the particles of the system. Considering the properties of the materials, the scattering from hydrogen is almost completely incoherent.

**Coherent elastic**

It is important for crystalline solids such as graphite, beryllium or UO$_2$. It includes the effects from waves that are able to interfere with each other. Considering the properties of the materials, the scattering from carbon and oxygen is almost completely coherent.

**Short-Collision-Time Approximation (SCT)**

When the incident energy is high, the required values for $\alpha$ and $\beta$ might be outside the tabulated $S(\alpha, \beta)$. In such cases, the SCT approximation should be used for deep inelastic scattering of thermal neutrons as Eq. 4.6 [28]
where the effective temperature $T_{\text{eff}}(T)$ is correlated to the generalized frequency distribution.

NJOY modules for generation of thermal neutron scattering data

The LEAPR module is used to prepare the scattering law $S(\alpha, \beta)$ and related quantities that describe thermal neutron scattering from bound moderators, into the ENDF-6 format used by the THERMR module. In general, the NJOY module scheme is illustrated in Figure 4-9.

$$S^{\text{SCT}}(\alpha, \beta, T) = e^{\left[\left(\frac{\alpha - |A|}{4\pi T_{\text{eff}}(T)}\right)^2 + \left(\frac{\beta}{T_{\text{eff}}(T)}\right)^2\right]}$$  \hspace{1cm} \text{(4.6)}$$

$$T_{\text{eff}}(T) = \frac{4\pi\alpha}{T}$$

The process starts by the LEAPR module that generates the scattering data in ENDF-6 format file 7 for various temperatures (depending on the grid for the temperatures of interest). It contains the coherent or incoherent elastic data, or incoherent
inelastic with the tabulated $S(\alpha, \beta)$ and $T_{\text{eff}}(T)$. Then, the module THERMR calculates the pointwise thermal scattering cross sections in PENDF format. Finally the ACER module generates the thermal scattering data for MCNP code in ACE format [28].

The ENDF model for water includes the assumption that the scattering law for the primary scatter (H-1) is well represented by the hindered rotations, which are given as a solid-type frequency distribution, with two discrete oscillators (0.205 and 0.408 eV) in order to represent the molecular vibrations, and a free-gas translational mode using atomic weight 18. In the case of the oxygen, the scattering is represented using a free-gas law for mass 16. These choices are given in the input cards of the LEAPR module.

4.4 Multi-group cross-section libraries for diffusion codes generated by MCNP5

The cross-sections used in Monte Carlo and the nodal diffusion calculations need to be consistent. The Monte Carlo method is a transport calculation and can be used to produce the diffusion cross-section libraries for the diffusion calculations [29, 30]. The most consistent cross-section data to be used in the hybrid nodal diffusion/Monte Carlo calculation would be obtained by generating with the Monte Carlo method the diffusion cross-section library.

The reaction rate and the neutron flux can be calculated directly by the Monte Carlo method. The MCNP5 code has the capabilities to calculate several types of reaction rates (fission, absorption or total reaction rate). As a result, the fission cross-section, the production (nu-fission) cross-section and absorption cross-section can be directly obtained using the spatial and energy collapsation scheme, as well as the Assembly
Discontinuity Factors (ADFs). Regardless of that, the group-to-group scattering reaction rate cannot be calculated directly by MCNP5. Only the group scattering reaction rate can be calculated by MCNP5. The transport reaction rate, which is used to determine the diffusion coefficient, cannot be calculated by MCNP5 directly either. A methodology to generate the group-to-group scattering cross-section and the diffusion coefficient by the Monte Carlo method was developed at PSU. The MCNP5 was modified at PSU by adding routines calculating few-group node-wise homogenized diffusion parameters [30].

The detailed description of the theoretical model, as well as calculation of the group-to-group scattering and the diffusion coefficient by the Monte Carlo method is described in [30]. The design of a flexible collapsation script to extract the multi-group parameters and group constants is developed as part of this research. This strengthens the consistency of the hybrid nodal diffusion/Monte Carlo calculation process and further accelerates the MCNP5 calculation.

In broad terms, MCNP5 is modified to track (as part of the tallying method) the outgoing energy and scattering angle that result from a scattering event. So as to obtain the group-to-group scattering cross section, the group-to-group transfer function must be calculated for each possible scattering event in which group-to-group scattering is related.

The typical scattering laws for a typical Monte Carlo calculation are given in Figure 4-10.
The thermal scattering law is divided into elastic and inelastic scattering. Each of the scattering laws illustrated in Figure 4-10, requires a particular treatment in order to obtain the group to group fraction.

**Elastic scattering**

The analysis of the elastic scattering can be divided into two cases: the first case being when the target is at rest and the second when the target is in motion. It is important to note, that the elastic scattering target at rest is a special case of the elastic scattering target in motion since the target velocity is equal to zero, from the relative velocity.

The elastic scattering target at rest corresponds to the cases for which the energy of the incoming neutron is larger than 400 kT and the target is not H-1. If not, the case of the elastic scattering target in motion is used. The target velocity must be considered in
the case of the elastic scattering target in motion. MCNP5 uses the relative velocity for the kinematics of the system. The relative velocity is determined by sampling the target velocity and subtracting it from the velocity of the incoming neutron.

**S(α,β) scattering**

The neutron scattering to the bounded target nucleus (like H in H₂O) is described by the \( S(α, β) \) law. As for the case of elastic scattering of \( S(α, β) \) cross section, the neutron does not lose energy in the collision, so the outgoing energy is the same as the incoming energy of the neutron.

For the inelastic scattering of the \( S(α, β) \) law, the outgoing energy is identified from one of the likewise energy bins that are tabulated as a function of incoming energy. In a similar manner, the collision angle is identified from one of the likewise discrete cosine bins.

**Inelastic scattering**

The event of inelastic scattering contains processes like \((n,n')\), \((n,2n')\), \((n,3n')\), etc. Most of these reactions occur at high energy range (in the MeV range) and their corresponding cross sections are comparatively low to the ones of elastic scattering. Besides this, the neutron diffusion equation takes into account the scattering by considering one neutron release from the collision. For that reason, the \((n,n')\) reaction is considered for the cross section generation process. Depending on the different excited states, the ENDF designates card numbers to \((n,n')\). These numbers are specified in the
MT cards 51 - 91, depending on the excited state. For these cards, the MT reaction undergoes the discrete scattering law 3 here the center of mass is calculated as Eq. 4.7 [30]

\[ E_{cm}^{out} = A_2 (E' - A_1) \quad 4.7 \]

\[ A_1 \text{ and } A_2 \text{ are constant values obtained from the cross section library and the center of mass energy is related to the laboratory energy by Eq. 4.8} \]

\[ E_{lab}^{out} = E_{cm}^{out} + \frac{E' + 2 \mu_c \sqrt{E' E_{cm}^{out}}}{(A + 1)^2} \quad 4.8 \]

By the above equations the outgoing angle and the scattering can be connected. Next, a similar method as the one used to obtain the fraction of outgoing energy group as in the elastic scattering law can be used.

**Diffusion coefficient**

The diffusion coefficient is related to the transport cross section Eq. 4.9 [26]

\[ D = \frac{1}{3 \Sigma_{sr}} \quad 4.9 \]

In which the transport cross section is given by \( \Sigma_{sr} = \Sigma_s - \bar{\mu}_L \Sigma_s \) and \( \bar{\mu}_L \) is the average cosine of the neutron scattering angle for collisions in the laboratory system. The methodology [30] followed in this study modified the MCNP5 code to obtain the \( \bar{\mu}_L \). Essentially, during the tally process, the average cosine (\( \bar{\mu}_L \)) is multiplied by the cross section (\( \Sigma_s \)) and the flux (\( \phi \)). Then, the transport cross section is first obtained in multi-group and it is then collapsed into one energy group. Each scattering law presents
different formulations to derive the average cosine of the neutron scattering angle in the laboratory frame.

**Collapsation script**

The collapsation script is developed to collapse the cross sections and parameters generated by MCNP5 into multi-group format for nodal diffusion codes and applications.

For each important cell that is tallied, the collapsation script extracts and collapses the transport by Eq. 4.10 and group to group scattering cross sections as exemplified by Eq. 4.11,

\[
\frac{1}{\Sigma_{tr}} = \frac{1}{\sum_{g} \phi_{g}} = \sum_{g} \left( \frac{1}{\phi_{g}} \right) \Sigma_{tr}, \quad \tilde{g} = 1, ..., \tilde{G}
\]

\[
\Sigma_{mat}^{s,g' \rightarrow g} = \left( \sum_{s,g' \rightarrow g}^{mat} \phi_{s}^{mat} + ... + \sum_{s,g' \rightarrow g-N}^{mat} \phi_{s}^{mat} \right) + ... + \left( \sum_{s,g' \rightarrow g-N'}^{mat} \phi_{s}^{mat} + ... + \sum_{s,g' \rightarrow g-N'}^{mat} \phi_{s}^{mat} \right) \phi_{g}^{mat}
\]

\[
\tilde{g}, \tilde{g'} = 1, ..., \tilde{G}
\]

The fission and absorption cross sections as Eq. 4.12,

\[
\Sigma_{g}^{mat} = \frac{\sum_{g}^{mat} \phi_{g}^{mat} + ... + \sum_{g-N}^{mat} \phi_{g}^{mat}}{\phi_{g}^{mat} + ... + \phi_{g-N}^{mat}}, \quad \tilde{g} = 1, ..., \tilde{G}
\]

and the number of neutrons release per fission. Initially, the MCNP5 input specifies the energy group boundaries (G groups; G – 1 entries; assuming upper boundary as cutoff energy). Using these energy group boundaries, the collapsation script first obtains the averaged flux over the group per cell and then collapses it to the desired few-
group structure. Any structure can be specified; typically the final group constants are given for two groups: fast and thermal group respectively.

4.5 Summary

The first step to correctly include the thermal hydraulic feedback into MCNP5 calculations begins with temperature dependent cross section libraries. If the cross sections used for the calculations are not at the correct temperature, the temperature feedback cannot be included into MCNP5. The only method of considering the temperature effects on cross sections is through temperature-dependent generation; or by a novel approach as explained in the next Chapter 5. The temperature effects on continuous cross-section data include Doppler broadening of resolved resonances; Doppler broadening of unresolved resonances; changes in $S(\alpha, \beta)$ thermal scattering kernel; and elastic scattering, which is Doppler broadening over the entire energy range.

This chapter presents the theory and developed methodology to generate: 1) continuous energy temperature-dependent cross-section libraries, and 2) thermal scattering cross-section libraries. Bothe methodologies are required to properly model the temperature feedback. In addition, this chapter also described the methodology implemented to extract multi-group cross-sections and multi-group parameters generated by MCNP5 for diffusion codes when the theory and methodology [30] is applied.

The automated tool GEN-XS is a program developed to generate temperature dependent MCNP5 continuous energy cross-section libraries. This automated tool
processes and manages all data processing requirements during the generation process. The duration of the procedure has been significantly reduced.

The methodology for generating thermal scattering cross-section libraries has been studied and included as well. The research purposes on this area focus on generating thermal scattering cross-section libraries for H₂O, the moderator of LWRs. The possibility of having thermal libraries at the correct moderator temperature improves the accuracy of the modeling.

The methodology to generate multi-group cross-section libraries for diffusion codes using MCNP5 was used for the PSU NEM code. In this way, the NEM code employs cross sections generated by MCNP5 for pin-cell based nodal compositions in order to be consistent with the MCNP5 model.

In the case of the continuous energy cross sections methodology, there are several ways of using the different NJOY modules. This creates the necessity of verifying the implemented methodology by comparing MCNP5 new generated continuous energy cross-section by different methods. The comparison is carried out by using the same nuclear data files (ENDF/B-VI). In this way, any difference caused by the nuclear data file is eliminated and the analysis is focused only on the methodology. The generation of the thermal scattering cross section libraries follows the same verification and validation methodology. The verification process is performed using global sensitivity analysis as described in Chapter 8. It is a new and an especially appealing approach that allows us to study the interaction of different parameters and the individual and overall effects of the inputs in the output.
As for the methodology for generation of multi-group cross-section libraries for diffusion codes by MCNP5, the verification is contained in [30], but its implementation is verified by comparing the calculations of the diffusion code using the MCNP5 generated cross-sections against the current cross-sections of the diffusion code.
Chapter 5

Pre-generation of cross-section libraries and interpolation method using temperature feedback

5.1 Introduction

The most accurate technique to update the cross-section libraries, taking into account the temperature feedback, would be to update the libraries with NJOY, for each nuclide, in their corresponding region, at the temperature of that region. In particular, this technique would be the most accurate, but not practical because of the vast computational time that it would take.

In another approach, the cross sections libraries for each nuclide would be pre-generated, with small temperature increments, within the range of possible temperatures of the calculation. However, the pre-generation of the cross section libraries of this second approach, can also be very tedious and time consuming, depending on the number of nuclides considered and the temperature interval selected for the generation of the cross section libraries, as well as the temperature variation considered in each material region. Furthermore, the time spent by MCNP5 to read the cross section libraries, would also increase considerably. It is also important to mention that this second method would have an inherent error depending on the size of the temperature increment.

Investigations carried out at PSU have found that the most appropriate and practical technique, with high accurate results, would be to use a pre-generated cross-
section library with temperature increments of 50 K, and then, an interpolation method would be used to approximate the cross sections at the provided by CTF temperatures [31].

5.2 Temperature interpolation methodology

Potential interpolation methods are be linear, quadratic, or a square root of temperature. The traditional linear interpolation scheme is inaccurate since the Doppler broadening of cross-sections is not linear. The theory, literature review [5, 32], and investigations of continuous cross-section behavior over the whole energy interval of interest in nuclear reactors showed that an interpolation scheme using $\sqrt{T}$ functional behavior can be used.

The square root of temperature, $\sqrt{T}$, interpolation method is used in the studies presented in this research. This $\sqrt{T}$ interpolation method has demonstrated the correct trend and excellent agreement with the actual cross-sections [5, 32]. In addition, considerable amount of computational time is saved by not having to re-generate the cross section libraries for each isotope, of each region, at the specified feedback temperature of that region. The $\sqrt{T}$ interpolation approach can be described as follows, using any two continuous cross-sections at two different adjacent temperatures:

1) Unionize energy grids in order to generate the new energy grids.

2) Evaluate cross-sections at new energy grids (20 to 30 cross section types)
3) Interpolate between the two appropriate temperatures using the \( \sqrt{T} \) interpolation method

4) All data, including cross-section data, is then arranged and stored for future calculations

5) The cross-sections are written in ACE format ready to be used by MCNP5

The proposed cross section update methodology can be observed in Figure 5-1. The flow diagram starts by receiving the thermal-hydraulic (TH) feedback from CTF for each node of each pin. At this point, a selection criterion must be made for using the updated temperature information. On the one hand, if the cross section data exists for the received TH-feedback, the cross section libraries are obtained from the cross section database and used on the MCNP5 calculation. On the other hand, if there is no cross section data available for the received TH feedback, the cross section libraries will be updated using the interpolation method and these new libraries would be used in the MCNP5 calculation.

Once the cross section libraries are ready, obtained either from the cross section data base or from the interpolation methodology, the MCNP5 input deck is prepared. All thermal-hydraulic information is updated; fuel, clad and moderator temperatures, moderator densities, and cross section libraries for the corresponding temperatures. As mentioned previously the TH-feedback is updated per node. Finally, the MCNP5 criticality calculation is run.
Figure 5-1: Summarized cross section update methodology
Several relevant aspects must be considered for the proper update of the cross-section libraries and assimilation of the temperature feedback. Firstly, the interpolation process is carried out for each isotope of each region (since the cross section libraries are given per isotope at a given temperature) and this could represent a considerable amount of computational work depending on the axial meshing and number of nuclides of the material regions. To illustrate this, consider only the fuel region and assumed it is fresh fuel (which consists, depending on the type of fuel, of four isotopes: U-234, U-235, U-238, and O-16). Furthermore, the model of the fuel is divided in 50 regions in the axial direction. So, for each of the 50 axial nodes, the interpolation methodology would have to be applied, representing 200 interpolations per pin.

Secondly, at each interpolation time, new cross-section libraries would be generated and new cross-section extensions\(^1\) would have to be assigned. Currently, only two-digit cross-section extensions can be used, which considerably limits the possible numbers (because of the already existing extensions and the number of possible new extensions – for instance, each of the 50 axial nodes could have a different temperature, which would represent 50 new cross-section extensions, and this is just for one pin). This is explained more in detail in the section “5.4 Studies of the cross-section extensions methodology”.

Thirdly, which is directly related to the previous explained paragraph, the interpolation of cross-section libraries, just as the generation process, is tedious and involves a lot of data manipulation (and storage capacity), in this way an automated

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\(^1\) The cross-section extensions are included in the isotope identifiers in the MCNP5 input and their purpose is to identify the cross-section libraries to obtain the continuous energy data.
A subroutine is created to manage the existing and new libraries and all data processing needs.

Finally, the existence of the cross section database plays a quite significant role in the interpolation methodology. It serves as a source of cross section data, providing the necessary temperature grid for the interpolation methodology. Furthermore, the cross section data base is continuously updated with each calculation. Every time a new cross section library is generated via the interpolation method, the new cross section data is saved in the cross section data base for use in future calculations. The continuously updated cross section library represents an important acceleration mechanism for the hybrid coupled calculations, as shown in Figure 5-2. It first avoids the need to directly generate cross section libraries by using the interpolation mechanism and secondly, by saving all the interpolated cross section data, it avoids the interpolation mechanism for future calculations.
5.3 Interpolation of temperature-dependent thermal scattering cross section libraries for MCNP5

Depending on the available information, the thermal neutron scattering data is processed in NJOY using different modules. If the thermal neutron scattering data is available for the moderator of interest in the ENDF/B files (in the thermal data files), the files can be processed in NJOY using the THERMR module, at the temperatures specified on the file, for the generation of the thermal scattering cross sections. If the thermal neutron scattering data is not available in the ENDF/B thermal data files for the
desired temperature, the scattering law $S(\alpha, \beta)$ and related quantities that describe thermal neutron scattering from bound moderators must be prepared in advance by the LEAPR module of NJOY to be further processed by the THERMR and finally generate the thermal scattering cross sections. The scattering law $S(\alpha, \beta)$ is also available only for certain temperatures [19, 27, 28].

For this study, thermal scattering cross sections were processed using NJOY for both, starting directly from the available thermal data in ENDF/B files and using the THERMR module of NJOY, and the second method using the LEAPR module of NJOY to process the scattering law $S(\alpha, \beta)$ and related thermal quantities. Both methods required further processing with NJOY to generate the thermal scattering data for the MCNP5 code. These two methods lead to a series of thermal scattering cross sections data available only for certain temperatures, the ones at which the data is available. It is important to mention that the temperatures, at which these thermal scattering cross sections are generated including both methods, are not at the desired operating range of temperature for the calculations ($\Delta T = 10$ K approx. for BWRs $\approx 550$ K to 560 K). These generated temperatures are at a much higher or lower temperatures than the desire one.

When the THERMR module is used to process the thermal scattering data, the specified temperature must be contained in the ENDF thermal file or within a small number of degrees. In case the $\alpha$ or $\beta$ needed is not in the range specified in File 7, the THERMR module uses the short-collision-time approximation to obtain the differential scattering cross section.
The intermediate points of interest for the thermal scattering grid are to be obtained by using a novel interpolation automated tool, based on the square root of temperature interpolation method. The interpolation is performed between cross section files and not between the scattering law values [28]. The automated methodology checks the number of existing inelastic energies and angle distributions as well as number of existing elastic energies. In addition it checks for coincident energy grids and applies the interpolation scheme to related parameters. As a result, a thermal scattering grid at the desired temperature range ($\Delta T = 10$ K approx. for BWRs $\approx 550$ K to 560 K) is obtained. Figure 5-3 illustrates the $\sqrt{T}$ interpolation of the elastic cross section of H$_2$O for several temperatures.

Figure 5-3: Interpolation methodology applied to the elastic cross section of H$_2$O
In a similar manner Figure 5-4 shows the $\sqrt{T}$ interpolation of the inelastic cross section of H$_2$O for several temperatures.

This gives the possibility of performing MCNP5 criticality calculations at the correct moderator temperature and improving the accuracy of the calculation. When this thermal scattering grid is applied to the hybrid coupled system, each simulated axial node uses the correct moderator thermal scattering cross section, providing a correct axial distribution of thermal scattering data based on the moderator temperature.
A simple test case is used to initially test the new thermal scattering cross section library. The model corresponds to a simple pin cell surrounded by water. This pin cell model is extracted from the 3-D BWR 2 by 2 pin array model used in the hybrid Monte Carlo based coupled system. The material and geometrical details are explained in detail in the Chapter 6.

The MCNP5 calculation of the pin cell model is executed using four different thermal cross section libraries corresponding to 550 K, 560 K, 573 K, and 600 K. The interpolated thermal scattering cross section library is the one at 560 K. The results of the MCNP5 calculation are depicted in Table 5-1.

<table>
<thead>
<tr>
<th>Thermal Library Temperature [K]</th>
<th>k_{eff}</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>550</td>
<td>1.36617</td>
<td>0.00026</td>
</tr>
<tr>
<td>560</td>
<td>1.36571</td>
<td>0.00025</td>
</tr>
<tr>
<td>573</td>
<td>1.36553</td>
<td>0.00025</td>
</tr>
<tr>
<td>600</td>
<td>1.36489</td>
<td>0.00026</td>
</tr>
</tbody>
</table>

As observed from Table 5-1, when the MCNP5 calculation uses a thermal scattering cross section library at higher temperature, the value of the k_{eff} decreases. This improves the modeling of the moderator behavior by using a more accurate physical model; lower moderator temperature represents higher moderator density and more neutron moderation, increasing the power. In addition, at lower thermal energies there is less up-scattering; in this manner more fission is produced. The complete 3-D BWR 2 by
2 array model is tested in Chapter 9 with different thermal scattering libraries in a more complex and detailed test.

5.4 Studies of the cross-section extensions methodology

For each interpolation step, new cross-section libraries would be generated and new cross-section extensions would be needed. Currently, only two-digit cross-section extensions can be used, which considerably limits the possible numbers (because of the already existing extensions and the number of possible new extensions – for instance, each of the 50 axial nodes could have a different temperature, which would represent 50 new cross-section extensions, and this is just for one pin). There are only 49 possible 2-digit combinations in the existent cross-section directory of the MCNP5 1.40 release. Several tests were performed with 3-digit combinations, but it was not possible to use them. Neither MCNP5 nor NJOY accepts them. In order to resolve this limitation, the file management tool organizes the cross-section files and extensions after being used in another directory, so the same numbers can be used for cross-section extensions in different libraries. This adjustment resolves the limitation with the available numbers of cross sections extensions.

The interpolation of cross-section libraries, just as the generation process, is tedious and involves a lot of data manipulation (and storage capacity), so the automated program is created to manage the existing and new libraries and all data processing needs.
5.5 Summary

This chapter has discussed the pre-generation of cross-section libraries and interpolation methodology using temperature feedback. An automated tool is developed to manage the existing and new libraries and all data processing needs since the interpolation of cross-section libraries and the pre-generation generation process are tedious and involve a lot of data manipulation. The relevant aspects to be considered for the proper update of the cross-section libraries have been introduced and are managed by the automated tool.

The investigations carried have exemplified that the most appropriate and practical technique, with high accurate results, would be to use a pre-generated cross-section library with temperature increments of 50 K, and then, an interpolation method would be used to approximate the cross sections at the provided by CTF temperatures.

The $\sqrt{T}$ interpolation method has demonstrated the correct trend and excellent agreement with the actual cross-sections. In addition, considerable amount of computational time is saved by not having to re-generate the cross section libraries for each isotope, of each region, at the specified feedback temperature of that region.

The existence of the cross section database plays a quite significant role in the interpolation methodology. It serves as a source of cross section data, providing the necessary temperature grid for the interpolation methodology. Furthermore, the cross section data base is continuously updated with each calculation. It first avoids the need to directly generate cross section libraries by using the interpolation mechanism and
secondly, by saving all the interpolated cross section data, it avoids the interpolation mechanism for future calculations.

Using the interpolation methodology specially designed for thermal scattering cross sections, a thermal scattering grid at the desired temperature range ($\Delta T = 10$ K approx. for BWRs $\approx 550$ to $560$ K) was generated. This gives the possibility of performing MCNP5 criticality calculations at the correct moderator temperature and improving the accuracy of the calculation. When this thermal scattering grid is applied to the hybrid coupled system, each simulated axial node uses the correct moderator thermal scattering cross section, providing a correct axial distribution of thermal scattering data based on the moderator temperature.
Chapter 6
Monte Carlo based coupled calculations

6.1 Introduction

The development of the scheme and methodologies for the design of the hybrid coupled Monte Carlo based system is presented in this chapter. The developed methodology comprises the core of the coupled system, which controls the flow of the calculations and passing of information. The coupled methodology focuses on the multi-level MCNP5/CTF/NEM/NJOY scheme together with convergence diagnostic of the coupled calculations.

Before initializing the coupled calculations, it is necessary to assure that the stand alone MCNP5 calculation has reach convergence. The diagnostic of this convergence is presented in the first sub-section of this chapter. While the last sections of the chapter contain the implemented mesh that is applied to the coupled model and the acceleration schemes for the Monte Carlo criticality calculations. The speed-up study comprises different strategies that will be combined in the final automated hybrid coupled Monte Carlo based system to accelerate the calculations.

6.2 Multi-level MCNP5/CTF/NEM/NJOY scheme

The developed scheme and methodologies of the hybrid coupled Monte Carlo based system are presented in this section. The developed coupled methodology utilizes a
multi-level MCNP/CTF/NEM/NJOY scheme together with a convergence diagnostic of the coupled calculations, and controls the flow of the calculations and passing of information. The main objectives of this coupled methodology are focused on the thermal-hydraulic feedback modeling to Monte Carlo core calculations, the generation and interpolation methodologies for temperature dependent cross-section libraries and the acceleration schemes for Monte Carlo based coupled calculations. Figure 4-9 illustrates the components that comprise the multi-level coupling scheme.

![Diagram of Multi-level MCNP5/CTF/NEM/NJOY coupling scheme](image)

**Figure 6-1:** Multi-level MCNP5/CTF/NEM/NJOY coupling scheme

### 6.2.1 Thermal-hydraulics feedback modeling in Monte Carlo calculations

The thermal-hydraulics feedback effects in Monte Carlo reactor core calculations include changes in the dimensions for geometry, material density effects, and temperature effects on cross-section data. The thermal-hydraulic feedback information (densities and
temperatures) is provided by the CTF code and is transferred through the interfacing code. The dimension and density changes can be passed directly through the interfacing code to the MCNP5 input.

The temperature effects on continuous cross-section data include Doppler broadening of resolved resonances; Doppler broadening of unresolved resonances; changes in $S(\alpha, \beta)$ thermal scattering kernel; and elastic scattering, which is Doppler broadening over the entire energy range. In order to consider the above-mentioned effects, continuous temperature dependent cross-section libraries were developed for MCNP5 along with automated cross-section temperature interpolation capability (described in detail in Chapter 5).

### 6.2.2 Multi-level scheme

The coupling scheme presented in Figure 6-2 was devised at PSU [5], after reviewing the previously reported experience in coupling Monte Carlo core calculations with feedback models [33, 34] as well as in coupling CTF with neutron transport calculations on pin-by-pin basis [35].
The computation process can be greatly accelerated by calculating the 3D fission source distributions and the thermal-hydraulics parameters with the coupled NEM/CTF code and then using coupled MCNP5/CTF calculations to fine tune the results to obtain an increased accuracy. The PSU NEM code employs cross-sections generated by MCNP5 for pin-cell based nodal compositions. As mentioned above, the sub-channel code CTF is used for thermal-hydraulics analyses in individual flow channels of a fuel assembly. Initially, the nodal diffusion code NEM is utilized to calculate the complete solution of the core configuration and the fission source distribution in order to accelerate the MCNP5 calculations. NEM is coupled with CTF in serial integration manner to provide this solution (in fact NEM is incorporated as a subroutine in the CTF calculation flow). Once this is achieved, the results are transferred to the MCNP5 code to obtain final high-accuracy converged results. An interface code transforms and incorporates the NEM/CTF output into the MCNP5 modeling and vise versa. There are two options for the fine-
tuning calculations – the first one is to use only CTF to update the thermal-hydraulic feedback parameters and pass them to MCNP5 at each coupled iteration, while the second option passes to MCNP5 in addition the converged NEM pin-wise fission source distribution to speed-up MCNP5 calculations. The multilevel coupling scheme is shown in Figure 6-2.

The coupled iterations stop when the convergence criteria are satisfied after evaluating the feedback parameters and power distribution between coupled iterations. The coupled convergence criteria of $\varepsilon=10^{-4}$ are set up on feedback parameters and power distribution between coupled iterations as depicted in the convergence scheme of Figure 6-3.

---

**Figure 6-3: Convergence scheme for the coupled calculation**
In the case of a MCNP5/CTF calculation, CTF is first run in stand-alone mode (initialized) using flat power distribution assumption and after achieving equilibrium steady state conditions the coupled iterations with MCNP5 are started. Then the MCNP5 code is run until the number of stated cycles, for attaining small statistical errors, is reached and the power feedback is passed to CTF. Finally, the couple iterations stop when the convergence criteria are satisfied after evaluating the feedback parameters.

Another case is the hybrid multi-level coupled code system MCNP5/CTF/NEM simulations. In this case, again the first CTF is initialized with a flat power distribution, then the coupled NEM/CTF calculation is converged to provide initial distributions of fission source and feedback parameters to MCNP5, and finally coupled MCNP5/CTF iterations are carried out for accurate solutions.

### 6.2.3 Spatial mesh overlays

In the BWR type study, the coupled hybrid Monte Carlo based code system is applied to a simplified 3-D 2x2 fuel-pin array extracted from a representative advanced Boiling Water Reactor (BWR) assembly [36]. The selected BWR assembly is a 9x9 BWR fuel assembly type. The plane view of the fuel assembly and other detailed information is shown in Figure 6-4.
The assembly has been divided into six lattices along the axial direction. Each lattice has two water rods located at the center. While preserving the actual heated length, the extracted simplified 2x2 pin array model uses only one material composition for each pin cell over the axial length. Each pin cell contains fresh fuel with different enrichment. In radial plane reflective boundary conditions are used, while in axial direction at the end of bottom and top reflectors vacuum boundary conditions are utilized. The detailed material specification of the model is given in Table 6-1.
The MCNP5, NEM and CTF models are consistent with each other. The axial direction over the heated length is divided into 50 equidistant nodes. The radial plane consists of four sub-channels in CTF, one node per pin cell in NEM and a lattice array in MCNP5. The radial and axial planes of the models are shown in Figure 6-5 below.

### Table 6-1: Material specifications of 2x2 pin array

<table>
<thead>
<tr>
<th>Pin</th>
<th>Density [g/cc]</th>
<th>Isotope</th>
<th>%wt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10.284</td>
<td>U-234</td>
<td>3.0999E-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-235</td>
<td>3.8789E+00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-238</td>
<td>8.4240E+01</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O-16</td>
<td>1.1850E+01</td>
</tr>
<tr>
<td>2</td>
<td>10.284</td>
<td>U-234</td>
<td>3.4999E-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-235</td>
<td>4.3189E+00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-238</td>
<td>8.3796E+01</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O-16</td>
<td>1.1850E+01</td>
</tr>
<tr>
<td>3</td>
<td>10.284</td>
<td>U-234</td>
<td>1.6999E-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-235</td>
<td>2.1159E+00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-238</td>
<td>8.6017E+01</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O-16</td>
<td>1.1850E+01</td>
</tr>
<tr>
<td>4</td>
<td>10.284</td>
<td>U-234</td>
<td>2.4999E-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-235</td>
<td>3.1739E+00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-238</td>
<td>8.4951E+01</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O-16</td>
<td>1.1850E+01</td>
</tr>
</tbody>
</table>
The NEM model is one node per pin cell in radial plane, the same 50 nodes as MCNP5 in axial direction over the heated length, plus 5 nodes of 10 cm each for bottom reflector and another 5 nodes of 10 cm each for the top reflector. The PSU NEM code employs cross sections generated by MCNP5 for pin-cell based nodal compositions in order to be consistent with the MCNP5 model.

The CTF model is consistent with the MCNP5 and NEM models. It consists of four sub-channels defined by the flow area of the fluid surrounding each fuel pin, as illustrated in the left side of Figure 6-5. The pins are modeled as UO₂ fuel rods with cladding material of Zircaloy-2. Only the heated length of the fuel pins is considered and it is divided into 50 equidistant nodes.

Figure 6-5: Spatial mesh overlays (general plane)
The feedback information, thermal-hydraulic data (moderator density and temperatures of the fuel, clad and moderator) as well as power data (axial and radial peaking factors), is transferred per node as depicted on the right side of Figure 6-5. The feedback transferred per node permits a detailed representation of the behavior of the modeled parameters.

One of the comparison studies, presented in detail in the next section of this research, refers to the comparison between two different CTF input models. The new CTF design input is based on the coolant centered approach (bottom model on the left side of Figure 6-5), which is compared against the model currently being used based on the rod centered sub-channel approach (top model on the left side of Figure 6-5).

6.2.4 Convergence diagnostic of Monte Carlo calculation

When MCNP5 is coupled, in this particular case with the CTF code, it is crucial that the solution provided by the MCNP5 code has converged. The effective multiplication factor ($k_{eff}$) and the fission source distribution, must both converge in order to start tallying when running criticality calculations. The $k_{eff}$ and the fission source distribution converge differently; $k_{eff}$ converges more rapidly than the source distribution. So the $k_{eff}$ alone cannot be used to assess the solution convergence.

Two methodologies have been proposed to measure the convergence of the fission source distribution. These two methods are the Shannon Entropy [37] and the Relative Entropy [30]. Since in the MCNP5 release 1.14 code version (this version was used in the first feasibility studies performed at PSU) a diagnostic feature to track the
fission source convergence in MCNP5 criticality calculations is not available, such feature were developed at PSU based on the Relative Entropy calculations. This feature was applied to the Monte Carlo method as posterior graphical stationary diagnostic tool to measure the convergence of the fission source distribution. In the most recent studies performed at PSU, the MCNP5 release 1.40 has been used. This latest release incorporates a vital tool to assess convergence.

The convergence of both, the $k_{eff}$ and fission source distribution, are illustrated in Figure 6-6 and close up of the region of interest in Figure 6-7. The calculations were performed for a 3-D $2 \times 2$ fuel-pin array extracted from the representative advanced BWR assembly described more in detail in the previous section.

\[ \text{This new tool is based on the Shannon Entropy of the fission source distribution [1].} \]
Figure 6-6: $k_{eff}$ and Shannon entropy convergence
In addition, the analysis of the source convergence helps to assess the initial fission source distribution from the nodal diffusion calculation. The Shannon Entropy convergence is used to observe the improvement in the reduction of cycles by using the fission source distribution simulated in the nodal diffusion calculation since it is practically closer to the true source distribution of the Monte Carlo calculation than the typical initial guess. Moreover, the convergence analysis is used to evaluate any bias in the source.

In a similar way, as when assessing the solution convergence, the number of histories used to make the source distribution to achieve the ‘exact’ equilibrium state must be analyzed. In other words, the accuracy of the technique must be optimized. A

Figure 6-7: $k_{eff}$ and Shannon entropy convergence, over the region of interest
larger number of histories in the criticality calculation step might improve the accuracy of the study. Alternatively, if the criticality calculation step had already reached the converged equilibrium state, at a smaller number of histories than that used previously, the computational time could be reduced further to attain the same accuracy.

6.3 Acceleration strategies for the coupled hybrid system

In order to speed-up Monte Carlo criticality calculations, which take the major part of the CPU time of the simulations, a combined strategy is investigated including hybrid nodal diffusion/Monte Carlo approach, accelerating techniques (like internal coupling), and parallel computing. The following subsections describe the studies and implementation of these strategies.

6.3.1 Hybrid nodal diffusion/Monte Carlo calculations

A new methodology to speed up the Monte Carlo criticality calculations was devised as part of the development of the Monte Carlo based coupled calculations [5]. The algorithm utilizes a hybrid nodal diffusion/Monte Carlo calculation scheme. The primary concept of this methodology is to pre-generate an initial source distribution of the Monte Carlo method by a nodal diffusion method. Typically, the Monte Carlo criticality calculation requires obtaining the converged fission source distribution before it begins tallying the final results. Some early neutron histories of the Monte Carlo calculation are just simulated as “inactive cycles” only to obtain the converged fission
source distribution. In the coupled nodal diffusion/Monte Carlo calculation scheme, the fast nodal diffusion calculation is used to provide the fission source distribution as an initial source distribution for the Monte Carlo calculation. The fission source distribution simulated in the nodal diffusion calculation is practically closer to the true source distribution of the Monte Carlo calculation than the typical guess source distribution. Therefore, the coupled methodology avoids utilizing large number of inactive cycles in the Monte Carlo calculation. The implementation of this hybrid methodology employs NEM as a nodal diffusion solver. In addition, when this approach is applied for coupled calculations it provides better initial guesses for thermal-hydraulic feedback distributions by first running NEM/CTF.

### 6.3.2 Internal coupling

The coupling between the MCNP5, CTF and NEM codes requires a great deal of data exchange; hence, manual coupling between the codes is very tedious and error-prone. An interfacing code has been developed as a comprehensive tool for the coupling work. The MCNP-CTF code is developed such that it automates the sequences needed between the MCNP5, NEM and CTF codes.

In general, codes can be coupled in an external manner (creating an automated tool to read/write/manage the feedback files) or in an internal (integrated) manner (creating an automated tool to control the flow of actions directly in the source files of the coupled codes). The external coupling is, typically, easier to perform, but slower because of the time it takes to transmit the feedback data between the codes. On the other hand,
the internal coupling transfers the feedback data in a direct way avoiding any extra transfer action that will increase the time of the calculation. Internal coupling represents a faster and more efficient way of passing the feedback information.

Essentially, the MCNP5/CTF/NEM code system includes an interfacing code that provides thermal-hydraulic feedback with hybrid nodal diffusion capabilities to the LANL Monte Carlo code, MCNP5 by coupling in an internal manner (where possible) with the thermal-hydraulic sub-channel code CTF and the NEM diffusion code. The MCNP5/CTF/NEM code is developed such that it automates the sequences needed between the MCNP5, CTF and NEM codes. The interfacing code system is entirely written in standard Fortran 90/95 language, like the latest versions of MCNP5 and CTF.

6.3.3 Parallel Monte Carlo calculations

The MCNP5 code is optimum to use the parallel capability due to the fact that each particle history can be run independently. In this way the total numbers of histories is divided in groups and send to different machines where the calculations are performed. The machines must be synchronized at the end of each cycle so as to calculate the $k_{eff}$ before starting the following cycle [37].

The MCNP-CTF code presents the possibility of executing the Monte-Carlo criticality calculation either in sequential or parallel mode. The execution mode depends on the number of processors available. The OpenMP model available in MCNP5 (release 1.40), shared-memory parallelism (threads) model, is used in the parallel execution mode [1].
The parallel analysis was performed using the Monte Carlo depletion system MCOR described in Chapter 3. The parallel capability was implemented in MCOR and MCNP-CTF, so that the new MCOR and MCNP-CTF versions present the possibility of executing the Monte-Carlo criticality calculation either in sequential or parallel mode. If parallel, the user will then specify in another input card the number of tasks (processors) for the MCNP5 calculation. The number of processor will depend on the available system.

Parallel calculations were run with 1, 2, 3 up to 8 processors (Threads) in the Challenge and Amquad machines at AREVA NP in Erlangen, Germany. The parallel MCOR calculations used different models, like a simple pin cell model and a much more complicated assembly models. The general observations are shown in Figure 6-8 for the decrease of the walk-clock time, in Figure 6-9 for the speed up ratio and in Figure 6-10 for the parallel efficiency.
Figure 6-8: Comparison of the wall clock time as a number of threads for the Challenge and Amdquad machines
Figure 6-9: Comparison of the parallel speedup ratio for the Challenge and Amdquad machines
Where the speed up ratio and the efficiency are calculated as shown in Eq. 6.1 and Eq. 6.2 respectively [38],

\[
\text{Speedup}(\text{# of processors} = n) = \frac{\text{Wall clock time used by one processor}}{\text{Wall clock time used by } n \text{ processors}}
\]

\[
\text{Efficiency}(n) = \frac{\text{speedup}}{n} \times 100\%
\]

The time of the MCOR depletion calculations has been considerably reduced using the parallel capability. A regular calculation of an assembly normally that takes around 6 to 7 months in sequential mode (depending on the computer, burnup steps, etc), this same calculation has been executed in just 2 weeks in parallel mode. The parallel calculations that were performed using two different machines (Challenge and Amdquad)
showed different results in the analyzed parameters. The Challenge machines showed a better performance than the Amdquad, which have to do mainly with the architecture of the machine and the options used for the compilation of the executable. Despite of this outcome, the main purpose of these calculations was to show the increase in performance using the parallel capability.

The hybrid coupled code system is intended to be used together with MCOR in the future to combine thermal-hydraulic feedback and depletion analysis in order to complete nuclear reference calculations.

6.4 Summary

The methodology to perform hybrid Monte Carlo based coupled calculations has been described in this chapter. Several relevant aspects must be considered in the coupled system for the proper modeling of all parameters. Firstly, in order to perform a deeper, more complete, nuclear analysis, a multi-level code system is designed and developed. One of the main objectives of the coupled system scheme is to incorporate the thermal-hydraulic feedback into MCNP5. The advanced sub-channel code CTF is used as the thermal-hydraulic module.

The thermal-hydraulic feedback modeling in MCNP5 requires a great attention on different details. As described in previous chapters, one of the most important aspects is the generation of temperature dependent cross section libraries to properly include the effects on cross sections. Another aspect of great relevance is that the codes in the coupled system must be consistent with the physical representation of the model. All
codes were designed using a different approach and they all have their unique spatial representation. When coupling these codes (MCNP5, CTF and NEM), it is important to develop a consistent interface for the proper exchange of the feedback parameters through a spatial mesh overlay.

Of great relevance as well, is the transfer of the correct converged results of each code independently prior starting the coupled calculation. If the incorrect results are transferred, the final coupled calculation would not reach convergence and would yield wrong results. With the purpose of avoiding this, the convergence of the solution provided by the MCNP5 code is checked to ensure the accuracy of the transferred information. The Shannon Entropy tool is used to check the convergence of both $k_{\text{eff}}$ and the fission source distribution of the MCNP5 criticality solution. The accuracy of the methodology is optimized by assuring that the correct number of cycles in the MCNP5 calculation is used. This diagnostic tool is also used to improve and reduce the number of skipped cycles needed to start tallying.

The Monte Carlo method can be considered a “numerical experiment” and provides the great possibility of generating reference solutions for verification and validation of commercial codes. The incorporation of the thermal-hydraulic feedback is of great interest and very appealing. On the other hand, Monte Carlo calculations required a great deal of computer resources and are quite “expensive” in computational time. Although the great amount of time required by the MCNP5 calculations, they are used to bridge the gap between fast diffusion calculations and the availability of experimental data. One of the objectives of this research is to present a combination of strategies to accelerate the coupled hybrid system, and in particular the MCNP5
calculation that takes the most amount of time. This Chapter presented and discussed the acceleration strategies based on a combined internal/external coupling approach, parallel Monte Carlo calculations and the introduction of a novel hybrid nodal diffusion/Monte Carlo approach. The acceleration techniques are evaluated by assessing the speed-up calculation performance and decrease in computational time. A considerably reduced in time has been observed and is presented in Chapter 9.
Chapter 7

Enhancements of the MCNP5/CTF/NEM/NJOY code system

7.1 Introduction

The methodology to perform hybrid Monte Carlo based coupled calculations has been described in previous chapters. The MCNP5/CTF/NEM/NJOY code system performs the hybrid coupled calculation for LWR analysis using several sophisticated and novel algorithms. Even so, additional functions were foreseen to improve the coupled code system and convert it into a user-friendly and effective practical fuel management tool. This chapter describes the ameliorations and new implementations made to enhance the capabilities of the MCNP5/CTF/NEM/NJOY code system.

7.2 User friendly automatic restart capability

Reference coupled calculations required a substantial amount of time, which is particularly true when the criticality part of the calculation is performed by MCNP5. During the total computational time, it is quite possible that the calculation is interrupted by an electricity shutdown, a computer problem, etc. So as to handle these unexpected interruptions, it is crucial to have an automatic restart capability.

The MCNP5/CTF/NEM/NJOY code system incorporates a user friendly automatic restart capability. In this way the user does not have to perform any task
manually and is able to restart the coupled computation from the last calculated point when it has been interrupted, as illustrated in Figure 7-1.

The two codes that form the main structure from the code system and that take the longest amount of computational time are MCNP5 and CTF. Figure 7-1 exemplifies the
considerable quantity of time that can be saved with the restart capability when the calculation has been interrupted during an advanced calculated point.

For example, if the calculation is interrupted during the MCNP5 section of the third coupled point, indicated in Figure 7-1 by the right bottom third bullet under the MCNP5 column. The restart module identifies the last calculated point; that in this case belongs to CTF as marked by the third bullet on the left bottom section on the CTF side. Once it has identified the last calculated point, the restart module obtains the necessary information and restarts the coupled calculation. This is illustrated by the dash line in Figure 7-1, which represents the restarted calculation.

The user friendly restart capability controls all the required actions automatically. First, all the output files are backup for reference and moved from the working directory to avoid that the restart calculation over-writes any old output file. Then the restart point is located; the calculation could either be restarted from CTF or MCNP5. Once the restart point has been identified, all the restart data as well as the data from previous calculation points is extracted. The data from previous calculation is used at the end for the analysis of the feedback parameters. Finally, the restart calculation is executed.

7.3 Implementation of a relaxation method for iterative systems

As an additional strategy to accelerate the calculation process, a relaxation method for iterative systems was implemented in the coupled code system. This relaxation method utilizes the feedback information of previous iterations in order to improve the convergence speed and avoids feedback oscillations (typical of iterative
systems). The relaxation method is applied to all feedback parameters as listed in Table 7-1.

<table>
<thead>
<tr>
<th>Power Distributions</th>
<th>Thermal-hydraulic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial Power Distribution</td>
<td>( T_{Fuel} )</td>
</tr>
<tr>
<td>Radial Power Distribution</td>
<td>( T_{mod}, \rho_{mod} )</td>
</tr>
<tr>
<td></td>
<td>( T_{clad} )</td>
</tr>
</tbody>
</table>

As an example of the relaxation scheme, the following equation shows the weighting of the current and previous calculations to obtain the current value,

\[
T_{Fuel}^{i}(i,k) = T_{Fuel}^{i}(i,k) \cdot DP + T_{Fuel}^{i-1}(i,k) \cdot (1 - DP)
\]  

7.1

In this example the fuel temperature is used as the relaxed parameter and DP stands for the dumping factor.

The relaxation system is used together with a convergence criterion on the coupled iteration that stops the Monte Carlo and CTF calculations once they are within the desirable confidence interval and pass the feedback, as illustrated in Figure 7-2.
The first coupled iterations are run using the convergence criteria, simultaneously interrupting MCNP/CTF calculations, respectively. The final calculations are run using the desirable number of cycles to fine-tune the coupled results.

### 7.4 Implementation of a post-processor module

The MCNP5/CTF/NEM/NJOY code system post-processor summarizes and compares the thermal-hydraulic and neutronics results. The post-processor prints all results for all corresponding pins/sub-channels for a specific coupled iteration. It also prints the results for a specific pin/sub-channel for all coupled iterations, which is particularly useful to analyze the effect of the feedback parameters.

The post-processor module comprises two sections; one that organizes all output data into files and a second section that prints the results. The first section, that manages the output data, prints a Master output file with the most important data for comparison and several secondary files, one for each feedback parameter \( T_{\text{Fuel}}, T_{\text{mod}}, \rho_{\text{mod}}, T_{\text{clad}} \) and
the power distributions), with the detail output data for each pin/sub-channel and coupled 
iteration.

The second section of the post-processor subroutine plots the results and 
compares then against a previous or reference solution if available.

7.5 Implementation of a complete-input-control module

As any other code system, the MCNP5/CTF/NEM/NJOY code system contains 
many variables that are machine dependant. These variables have to be set-up prior 
starting the calculation or the calculation would not run or run with errors. In order to 
 improve the portability of the MCNP5/CTF/NEM/NJOY code system and control all the 
variables in an easy manner, a complete-input-control-subroutine was created. This new 
subroutine contains in a simple list the variables that code needs to run. The variables are 
located in the input instead of inside the source code, which does not require a new 
compilation when the variables change. The complete-control-input also contains the 
information of the mode of the calculation (normal or restart) and model used in the 
desire calculation (rod or coolant centered approach).

7.6 Summary

The new features incorporated to the MCNP5/CTF/NEM/NJOY code system so 
as to enhance its capabilities were introduced in this chapter. These new features include
a user friendly restart capability, a relaxation method for iterative systems, a postprocessor module, and a complete-input-control module.
Chapter 8

Application of Global Sensitivity Analysis to nuclear reactor calculations

8.1 Introduction

Uncertainty and sensitivity analysis techniques can be used to carry out the study of uncertainty in model predictions occurring from inaccurately-known processes and input data. Specifically, sensitivity analysis is useful to establish the contribution of individual inputs to the uncertainty in model predictions. In this fashion, global sensitivity analysis facilitates the identification of high-order interactions among inputs in determining the uncertainty in the output of interest. Global sensitivity analysis deals with uncertainty sources spanning over finite or infinite ranges of uncertainties and with the simultaneous variation of such sources.

In this section, global sensitivity analysis is applied to the modeling of nuclear reactor calculations for better model understanding. Particularly, it is investigated how much criticality conditions are affected by uncertainties in various inputs, including nuclear cross-sections, at different energies, from several isotopes in the fuel, the absorber, and the moderator. For such coupled code system based on Monte Carlo, it is important to have a tool to evaluate the uncertainty in continuous cross-sections as well as the impact of Nuclear Data Libraries.
In this study, the sensitivity analysis employs the Sobol’ and Jansen formulas, which allow us to estimate, for each uncertain input, its main effect and its total effect (i.e. the overall effect, which includes all the interactions, at any order, with all the other uncertain inputs). The sensitivity analysis consists of a number of model simulations, which are performed using MCNP5 calculations.

8.2 Effect of Nuclear Data Libraries

Prior to applying global sensitivity analysis to the modeling of nuclear simulations, the difference between the Nuclear Data Libraries (NDLs) is carried out. The developed GEN-XS code, described in Chapter 4, is used to generate temperature dependant cross-section libraries based on the different NDLs. Then, the differences in the infinity multiplication factor ($k_{inf}$) calculated by MCNP5 are compared. Thanks to use of the automated tool for generation of temperature dependent continuous energy cross section libraries (GEN-XS), reference solutions can be provided using the different available NDLs. The results of this exercise form part of the Organization for Economic Co-operation and Development (OECD) Uncertainty Analysis in Modelling (UAM) Benchmark. The MCNP5 calculations, using the different NDLs, provided the required flexibility to the participants of the OECD UAM Benchmark.

The test problems are 2-D assembly models with reflective boundary conditions representative of BWR Peach Bottom 2 (PB-2), PWR Three Mile Island 1 (TMI-1), and VVER-1000 (Kozloduy-6 and Kalinin-3 plants). The 2-D assembly model with reflective boundary conditions is used in LWR analysis as a standard model for fuel assembly
cross-section generation. The geometry specification of the test problems is obtained from [29]. The test problems of Exercise I-2 are consistent with the ones used on Exercise I-1, where pin-cell models representatives of the same three PWR, BWR, and VVER types were used. The test calculations are studied at Hot Zero Power (HZP) conditions [39].

The cross-section uncertainty data, within the framework of Exercise I-2, is processed as an input uncertainty. The uncertainty files (nuclear data uncertainties) in the evaluated nuclear data libraries (NDL) are obtained from the analysis of experimental differential data and from nuclear models. The NDL effect is assessed in this paper by running Monte Carlo simulations with these major libraries: ENDF/B-VI.8 [18-19], ENDF/B-VII.0 [18-19], JEFF-3.1.1 [20], and JENDL-3.3 [40].

In this sensitivity study, each of the test assembly problems is run with the different NDLs. Firstly, the assembly tests were simulated using cross-section libraries based on ENDF/B-VII.0 and JEFF-3.1.1. The first part of the tests was to run the assemblies using three different thermal scattering libraries (lwtr.62t [1], lwtr.04t [1], th552.68t). The comparisons between the three thermal cross section libraries serve as a base to assess the accuracy of the newly developed thermal library (th552.68t). Therefore, for subsequent runs only the latest libraries were used (lwtr62.t and th552.68t) to provide reference calculations using ENDF/B-VII.0, JEFF3.1.1 and JENDL3.1 as showed in Table 8-1.
Table 8-1: $k_{inf}$ values for the LWR types using different cross-section libraries

<table>
<thead>
<tr>
<th>Assembly</th>
<th>Nuclear Data Library</th>
<th>Thermal Scattering Library</th>
<th>PURR $k_{inf}$/Std.</th>
<th>GROUPR $k_{inf}$/Std.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TMI</td>
<td>ENDF/B-VII.0</td>
<td>lwtr.62t</td>
<td>1.05899 0.00016</td>
<td>1.05826 0.00015</td>
</tr>
<tr>
<td></td>
<td>lwtr.04t</td>
<td>1.05737 0.00016</td>
<td>1.05718 0.00016</td>
<td></td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>1.06239 0.00025</td>
<td>1.06212 0.00025</td>
<td></td>
</tr>
<tr>
<td></td>
<td>JEFF3.1.1</td>
<td>lwtr.62t</td>
<td>1.05490 0.00015</td>
<td>1.05409 0.00015</td>
</tr>
<tr>
<td></td>
<td>lwtr.04t</td>
<td>1.05359 0.00015</td>
<td>1.05253 0.00016</td>
<td></td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>1.05851 0.00023</td>
<td>1.05746 0.00025</td>
<td></td>
</tr>
<tr>
<td></td>
<td>JENDL3.1</td>
<td>lwtr.62t</td>
<td>1.05544 0.00025</td>
<td>1.05511 0.00025</td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>1.05924 0.00026</td>
<td>1.05849 0.00024</td>
<td></td>
</tr>
<tr>
<td>VVER</td>
<td>ENDF/B-VII.0</td>
<td>lwtr.62t</td>
<td>0.95752 0.00022</td>
<td>0.95692 0.00021</td>
</tr>
<tr>
<td></td>
<td>lwtr.04t</td>
<td>0.95619 0.00021</td>
<td>0.95548 0.00021</td>
<td></td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>0.96192 0.00024</td>
<td>0.96087 0.00023</td>
<td></td>
</tr>
<tr>
<td></td>
<td>JEFF3.1.1</td>
<td>lwtr.62t</td>
<td>0.97187 0.00022</td>
<td>0.97174 0.00021</td>
</tr>
<tr>
<td></td>
<td>lwtr.04t</td>
<td>0.97048 0.00021</td>
<td>0.97033 0.00022</td>
<td></td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>0.97574 0.00024</td>
<td>0.97565 0.00024</td>
<td></td>
</tr>
<tr>
<td></td>
<td>JENDL3.1</td>
<td>lwtr.62t</td>
<td>0.97246 0.00023</td>
<td>0.97131 0.00024</td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>0.97655 0.00023</td>
<td>0.97574 0.00025</td>
<td></td>
</tr>
<tr>
<td>PB-2</td>
<td>ENDF/B-VII.0</td>
<td>lwtr.62t</td>
<td>1.05940 0.00009</td>
<td>1.05918 0.00009</td>
</tr>
<tr>
<td></td>
<td>lwtr.04t</td>
<td>1.05982 0.00009</td>
<td>1.05927 0.00009</td>
<td></td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>1.06038 0.00006</td>
<td>1.06028 0.00014</td>
<td></td>
</tr>
<tr>
<td></td>
<td>JEFF3.1.1</td>
<td>lwtr.62t</td>
<td>1.06277 0.00009</td>
<td>1.06235 0.00009</td>
</tr>
<tr>
<td></td>
<td>lwtr.04t</td>
<td>1.06280 0.00009</td>
<td>1.06255 0.00009</td>
<td></td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>1.06328 0.00014</td>
<td>1.06326 0.00014</td>
<td></td>
</tr>
<tr>
<td></td>
<td>JENDL3.1</td>
<td>lwtr.62t</td>
<td>1.05951 0.00014</td>
<td>1.05907 0.00015</td>
</tr>
<tr>
<td></td>
<td>th552.68t</td>
<td>1.06025 0.00014</td>
<td>1.05962 0.00015</td>
<td></td>
</tr>
</tbody>
</table>
The new thermal scattering cross section library was compared with MCNP5 built in libraries (lwtr.04t and lwtr.62t) [1]. Both of these MCNP5 built in thermal scattering libraries are at 600 K, a much higher temperature than the desired at 552 K. The intermediate point of interest for the thermal scattering grid are obtained by using the novel interpolation automated tool, based on the square root of temperature interpolation method described in Chapter 5. As a result, a thermal scattering library at the desired temperature of 552 K is obtained.

This gives the possibility of performing MCNP5 criticality calculations at the correct moderator temperature and improving the accuracy of the calculation.

The difference in the infinite multiplication factor ($k_{inf}$) of the libraries is compared. The criticality calculations were performed using MCNP5 release 1.40. When using the new thermal scattering cross section library, which is at a lower temperature than the original library provided by MCNP5 at 600 K, a higher $k_{inf}$ is observed. The modeling is improved, the moderator behavior is simulated in a more accurate physical model; at lower thermal energies there is less up-scattering; in this manner more fission is produced.

The different possible ways of generating the cross-section libraries in NJOY adds sources of uncertainties to the overall study. In broad terms, the two possible approaches to generate temperature dependent continuous energy MCNP5 cross sections in NJOY are: with Probability Tables (using the PURR module) or with the Bondarenko method (using the GROUPR module) [7]. The PURR module produces probability tables to treat unresolved-resonance self-shielded for the continuous-energy MCNP5 code. The UNRESR module generates unresolved self-shielding data suitable for multi-group
methods after being processed by the GROUPR module. The method used by this module (Bondarenko method) is not very useful for continuous-energy Monte Carlo methods. Instead, according to Levitt [7] the correct and natural approach for treating unresolved-resonance self-shielding for Monte Carlo codes is to use the Probability Table method. This method creates probability tables of the elastic, fission, capture and total cross sections. The Monte Carlo code would sample a random number between 0 and 1 to determine the corresponding cross section in the appropriate probability table.

When comparing the calculations in Table 8-1, the PURR calculations produce higher $k_{\text{inf}}$ values than GROUPR.

Calculations with cross sections obtained from the different NDLs: ENDF/B-VII.0, JEFF-3.1.1 and JENDL3.1, have been performed for all LWR type test problems. Important differences were observed between the libraries when calculating the $k_{\text{inf}}$. This information points out that the choice of NDL used to perform the criticality calculation is of great relevance.

8.3 Global Sensitivity Analysis

Uncertainty Analysis (UA) focuses on the uncertainty quantification in a model output [41]. Furthermore, Sensitivity Analysis (SA), studies how this output uncertainty of a model can be apportioned to different sources of uncertainty in the model input. Together, UA and SA, should be run cyclically and this is usually performed in an iterative manner. SA can be further classified in two categories – Local Sensitivity Analysis (LSA) and Global Sensitivity Analysis (GSA).
GSA can be used in conjunction with the Monte Carlo method to generate the model outputs by sampling input factors’ values from their distributions. This can be done since the GSA approach explores the full space of input factors. While, LSA is based on derivatives and has to be implemented in the computer program of the model of interest and it is unwarranted for non-linear models. The derivatives are only informative at the base point where they are computed, and do not provide for an exploration of the rest of the space of the input factors.

8.3.1 Sensitivity Analysis

The uncertainty within the nuclear data files is difficult to assess. The uncertainty data, which is expressed in percentage with respect to the nominal value of a given cross section for a given energy, is available for few isotopes. Not all the nuclear data files include uncertainties. The current exercise focuses on the application of global sensitivity analysis to particular uncertainties found in cross-sections. It does not considered the engineering uncertainties found in geometrical models and material descriptions.

Among the available uncertainty data, the reactions that have cross section values larger than 100 barns were identified, considering that the uncertainty effect of less probable reactions is negligible on $k_{inf}$. The following assumption is taken in order to apply the uncertainty value: the cross section values are normally distributed with a mean value given by the nominal value (generally used in the computations) and a standard
deviation that is given by the product of the nominal cross section and the uncertainty value expressed in percentage points\textsuperscript{3}.

Preferably, the uncertainties of the cross sections should be modified within the nuclear data file. In order to do so, a computer code was developed to apply the sensitivity studies to the MCNP5 continuous energy cross-section libraries. This code is able to go directly into the continuous energy cross section libraries and modify them by applying the uncertainties to the specific cross sections at the selected energy value. The code is capable of modifying total, capture, scattering, absorption and fission cross sections, plus other type of reaction rates and parameters such as the neutrons released per fission. Given that continuous energy cross sections have point values instead of group values as in the multi-group cross sections, a specific energy point can be identified.

In order to apply global sensitivity analysis to the Monte Carlo method, the cross section values of several important isotopes of different regions were treated as uncertain quantities. Fuel, absorber and moderator are the three main regions selected for the presented global sensitivity analysis. For each of these regions, the most important isotopes, for which the uncertainty values exist, are selected and adjusted. The selected isotopes with their specific cross sections and their corresponding uncertainty values for the fuel [42], absorber [42] and moderator [43] regions are shown in Table 8-2, Table 8-3 and Table 8-4 respectively.

\textsuperscript{3} It is important to note that the isotopes used in this exercise were limited by the available uncertainty data. The isotopes contained in the fuel do not correspond to the ones listed in the OECD UAM Benchmark for Exercise 1 and certain important isotopes like U-238 could not be used because of the lack of uncertainty data. The main objective of this exercise is to apply global sensitivity analysis to cross section data using Monte Carlo continuous energy calculations in an innovative manner.
### Table 8-2: Fuel region: cross sections and uncertainty values as a function of energy

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Energy (MeV)</th>
<th>Fission XS (barns)</th>
<th>Uncertainty (%)</th>
<th>Capture XS (barns)</th>
<th>Uncertainty (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-235</td>
<td>2.53E-08</td>
<td>584.25</td>
<td>0.19</td>
<td>98.96</td>
<td>0.75</td>
</tr>
<tr>
<td>Pu-239</td>
<td>2.53E-08</td>
<td>747.99</td>
<td>0.25</td>
<td>271.43</td>
<td>0.79</td>
</tr>
<tr>
<td>Pu-241</td>
<td>2.53E-08</td>
<td>1012.68</td>
<td>0.65</td>
<td>361.29</td>
<td>1.37</td>
</tr>
</tbody>
</table>

### Table 8-3: Absorber region: cross sections and uncertainty values as a function of energy

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Energy (MeV)</th>
<th>Absorption XS (barns)</th>
<th>Sigma XS (barns)</th>
<th>Uncertainty (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B-10</td>
<td>2.53E-08</td>
<td>10B(n,a0)</td>
<td>241.2677</td>
<td>0.21</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10B(n,a1)</td>
<td>3598.228</td>
<td>0.16</td>
</tr>
<tr>
<td></td>
<td>9.40E-06</td>
<td>10B(n,a1)</td>
<td>186.435</td>
<td>0.16</td>
</tr>
</tbody>
</table>
As summarized in Table 8-5, the cross section values of the three regions are modified simultaneously (20 cross section values in total: 6 for the fuel, 3 for the absorber and 11 for the moderator). For the remaining isotopes the continuous energy nominal cross-section values were used (no uncertainties were attached). A 20-column sample matrix with 2816 rows (different cases) was generated to represent such uncertainties. Each row represents a case with 20 cross section values that are used to simulate continuous energy MCNP5 criticality calculation.

### Table 8-4: Moderator region: cross sections and uncertainty values as a function of energy

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>Uncertainty (%)</th>
<th>Elastic Scattering XS (barns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.53E-08</td>
<td>0.20</td>
<td>20.436330</td>
</tr>
<tr>
<td>2.0</td>
<td>0.22</td>
<td>2.903645</td>
</tr>
<tr>
<td>4.0</td>
<td>0.30</td>
<td>1.894349</td>
</tr>
<tr>
<td>6.0</td>
<td>0.36</td>
<td>1.418157</td>
</tr>
<tr>
<td>8.0</td>
<td>0.44</td>
<td>1.129564</td>
</tr>
<tr>
<td>10.0</td>
<td>0.50</td>
<td>0.934397</td>
</tr>
<tr>
<td>12.0</td>
<td>0.49</td>
<td>0.793504</td>
</tr>
<tr>
<td>14.0</td>
<td>0.46</td>
<td>0.687114</td>
</tr>
<tr>
<td>16.0</td>
<td>0.40</td>
<td>0.604026</td>
</tr>
<tr>
<td>18.0</td>
<td>0.35</td>
<td>0.537384</td>
</tr>
<tr>
<td>20.0</td>
<td>0.30</td>
<td>0.482746</td>
</tr>
</tbody>
</table>
A total of 2816 MCNP5 criticality runs are calculated. At the end of each calculation, the infinite multiplication factor is extracted and the process is repeated until all the runs have been executed. The whole process was automated into a code in order to facilitate the modification, execution and extraction of data for the analysis.

The methodology applied in this study for the sensitivity analysis is originally from Sobol’ and Jansen formulas [44], but it has been ameliorated by Saltelli et al [45]. The Sobol’s method is variance-based, which means that the variance of the model output can be decomposed into terms of increasing dimensionality, called partial variances, that represent the contribution of each single input (but even pairs, triplets, etc) to the overall uncertainty of the model output. This method allows the simultaneous exploration of the space of the uncertain inputs, which is carried out via pseudo-random or quasi-random sampling. Statistical estimators of partial variances are available to quantify the sensitivities of all the inputs and of groups of inputs through multi-dimensional integrals.

The computational cost required to estimate the sensitivities of higher-order interactions between inputs can be very high. With the intention of preventing this, the

<table>
<thead>
<tr>
<th>Values/Column</th>
<th>Cross Section Modified</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Fission U-235 Thermal</td>
</tr>
<tr>
<td>2</td>
<td>Fission Pu-239 Thermal</td>
</tr>
<tr>
<td>3</td>
<td>Fission Pu-241 Thermal</td>
</tr>
<tr>
<td>4</td>
<td>Capture U-235 Thermal</td>
</tr>
<tr>
<td>5</td>
<td>Capture Pu-239 Thermal</td>
</tr>
<tr>
<td>6</td>
<td>Capture Pu-241 Thermal</td>
</tr>
<tr>
<td>7</td>
<td>Absorption B-10 (n,a0) Thermal</td>
</tr>
<tr>
<td>8</td>
<td>Absorption B-10 (n,a1) Thermal</td>
</tr>
<tr>
<td>9</td>
<td>Absorption B-10 (n,a1) Fast</td>
</tr>
<tr>
<td>10 to 20</td>
<td>Elastic Scattering H-1 from 0 to 20 MeV</td>
</tr>
</tbody>
</table>
The concept of total sensitivity index has been introduced by [46], which requires much less computational effort. The total sensitivity index provides an indication of the overall effect of a given input, taking into account all possible interaction of that input with all the others. References are provided to the above mentioned literature for the technical details of the methods. In this exercise, both first order and total sensitivity indices are estimated.

The results for both, the first order and the total sensitivity indices, are illustrated in Figure 8-1 and Figure 8-2. These results yield very interesting findings. The highest indices were observed for the elastic scattering of H-1 at thermal energy. This result indicates that the uncertainties of this cross section have the major impact on the uncertainty of $k_{inf}$. It reflects how much the output changes with a variation of an input. The second highest sensitivity indices were found for the elastic scattering of H-1 at a middle energy point (8 MeV). Then, the next higher indices were for the fission cross sections (U-235, Pu-239 and Pu-241, for which the highest is for U-235, as expected) and the capture cross sections.
Figure 8-1: First order sensitivity indices (2816 MCNP5 calculations)
Quite the opposite, the sensitivity indices for the H-1 elastic scattering at the two highest energy groups indicate that these two cross sections have no effect on $k_{inf}$.

Figure 8-1 and Figure 8-2 show the sensitivity indices for the 20 parameters with their estimated 90% confidence intervals obtained by applying bootstrap [47]. With the purpose of reducing the obtained confidence intervals to make a clear ranking of the parameters, the number of calculations (and thus the number of cases-rows in the sample matrix) is extended. A total of 5110 cases are prepared and calculated. The new calculations are used to validate the obtained results. The sensitivity indices, with their corresponding bootstrap confidence intervals, for the 5110 sample matrix are shown in Figure 8-3 and Figure 8-4.
Figure 8-3: First order sensitivity indices (5110 MCNP5 calculations)
The previous analysis, the one made for the 2816 cases, is unchanged. The importance of certain parameters, refer to the variation of the output with regards to changes in certain inputs or combination of inputs, remains. The obtained confidence intervals with the 5110 cases are very similar with the 2816 one, with a slight reduction on the amplitude of the bounds.

The bootstrap analysis is very similar for both studies. Even that the number of cases/runs was increased considerably, from 2816 to 5110. It is important to note that these are MCNP5 calculations; with a high computational time cost. As the number of calculations increase, the amplitude of the confidence intervals will become smaller, as

Figure 8-4: Total order sensitivity indices (5110 MCNP5 calculations)
expected. The small variation on the bound’s amplitude illustrate the certain convergence has been reached. The results are stable and no unexpected changes should appear.

The obtained results are summarized. The first order indices, measuring the importance of individual parameters, illustrate that parameter 10 (thermal scattering cross section of H-1) is the most important (with the highest variation in the output). The other parameters present a smaller and equivalent influence on the output.

The total sensitivity indices, which measure the importance of one parameter considering all the interactions with the rest, help to identify the parameters that are not important and can be fixed; like parameters 7, 8, 9 and 20.

8.4 Summary

MCNP5 calculations with cross sections derived from, ENDF/B-VII.0, JEFF-3.1.1 and JENDL3.1 have been performed for all LWR type test problems from the OECD LWR UAM Benchmark. Important differences were observed between the libraries when calculating the $k_{\text{inf}}$. This information points out that the choice of NDL used to perform the criticality calculation is of great relevance.

The new thermal scattering cross section library was compared with MCNP5 built in libraries. As a result, a thermal scattering library at the desired temperature of 552 K is obtained. This gives the possibility of performing MCNP5 criticality calculations at the correct moderator temperature and improving the accuracy of the calculation.

Global sensitivity analysis is applied to the modeling of nuclear reactor physics for better model understanding. In particular, it is investigated how much criticality
conditions are affected by uncertainties in various inputs, including nuclear cross-sections, at different energies, from several isotopes in the fuel, the absorber and the moderator. The sensitivity analysis uses the Sobol’ and Jansen formulas, which allow us to estimate, for each uncertain input, its main effect and its total effect (i.e. the overall effect, which includes all the interactions, at any order, with all the other uncertain inputs). The highest indices were observed for the elastic scattering of H-1 at thermal energy. The second highest indices were found for the elastic scattering of H-1 at a middle energy point (8 MeV). Subsequently, the next higher indices were for the fission cross sections (U-235, Pu-239 and Pu-241, for which the highest is for U-235, as expected) and the capture cross sections.

The bootstrap analysis is very similar for both studies (for the 2816 and 5110 cases). The small variation on the bound’s amplitude illustrate the certain convergence has been reached. The results are stable and no unexpected changes should appear.
Chapter 9

Benchmark problems: results of the coupled hybrid system

9.1 Introduction

The results demonstrating the Monte Carlo based coupled calculations utilizing the described above multi-level scheme are given in this section. The developed coupled hybrid system MCNP5/CTF/NEM is applied to the simplified 3-D 2x2 fuel-pin array from a BWR assembly as mentioned in the previous chapter. Different cases and tests are performed to assess the capabilities of the hybrid coupled system.

9.2 BWR 3-D 2x2 pin array results

The simplified 3-D 2x2 fuel-pin array extracted from a representative BWR assembly is modeled with the coupled hybrid Monte Carlo based code system. Nominal operating conditions of a BWR are simulated in this model. The coupled convergence criteria were set up to satisfy the requirement that the maximum relative deviations in node-wise distributions of feedback parameters and power between two successive coupled iterations simultaneously to be less than 0.01%.

In order to demonstrate the functionality of MCNP5/CTF coping scheme the obtained results for two cases of the BWR 3D 2x2 pin array problem are presented and discussed. In Case 1 the inlet flow rate per a sub-channel is 0.16303 kg/s, while in Case 2 it is increased to 0.65212 kg/s. Table 9-1 and Table 9-2 show k_{eff} values and radial power
distributions for cases 1 and 2 respectively while Figure 9-1 through Figure 9-2 compare pin-array average axial power, fuel temperature and moderator density distributions for the two cases.

Table 9-1: Results for case 1

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
<th>$1.29626 \pm 0.00037$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2D$ Normalized Power</td>
<td>1.0664</td>
<td>1.0195</td>
</tr>
<tr>
<td></td>
<td>0.9402</td>
<td>0.9739</td>
</tr>
</tbody>
</table>

Table 9-2: Results for case 2

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
<th>$1.33868 \pm 0.00038$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2D$ Normalized Power</td>
<td>1.0863</td>
<td>1.0135</td>
</tr>
<tr>
<td></td>
<td>0.9329</td>
<td>0.9673</td>
</tr>
</tbody>
</table>

An initial cosine power distribution is assumed for the CTF calculation. Then, after several coupled iterations (these particular cases converged after three coupled iterations), the converged solutions are compared in the above-mentioned tables and figures. When increasing the flow rate (from case 1 to case 2) $k_{\text{eff}}$ is increasing also reflecting the physical fact that increased flow rate leads to higher moderator density and higher moderation resulting in higher $k_{\text{eff}}$. The axial power distributions depicted in Figure 9-1 reflect the thermal-hydraulic feedback effects and are consistent with the fact
that in the BWR 3D 2×2 problem the fresh fuel with the same enrichment is uniformly distributed axially (high power at the bottom - where there is a higher moderator density resulting in a higher moderation; and lower power at the top - where there is a lower moderator density resulting in a lower moderation). When increasing the flow rate (from case 1 to case 2) the axial moderator density distribution is shifting towards higher moderator density values (see Figure 9-1), which is shifting accordingly the axial power distribution (see Figure 9-1) and the fuel temperature distribution (see Figure 9-2) through the moderator and Doppler feedback mechanisms.

Figure 9-1: Comparison between cases 1 and 2 with different flow rates
9.3 Comparison between coolant centered and rod centered sub-channel approaches

In the first LWRs studies modeled with the coupled hybrid Monte Carlo based code system, a rod centered sub-channel approach was used as the thermal hydraulic input in CTF. In general, there are two sub-channel approaches to model the simplified 3-D 2x2 fuel-pin array in CTF: the rod and coolant centered sub-channel approaches. The sub-channel codes such as CTF are extensively validated based on the coolant centered sub-channel modeling. In order to provide a new validation scheme for comparison, a CTF input based on the coolant centered approach, as shown in Figure 9-3, was design to compare it against the model currently being used based on the rod centered model.
In this study, these two sub-channel approaches, namely rod centered and coolant centered as defined previously, are used to model the simplified BWR 3-D 2×2 fuel-pin array with the coupled hybrid Monte Carlo based code system. The rod centered sub-channel approach is the original model that was used in the previous LWR calculations of the MCNP/CTF/NEM system. The new CTF input based on the coolant centered sub-channel approach was designed, as mentioned earlier, to provide a new validation scheme for comparison. The CTF input based on the coolant centered approach represents a more complex model geometrically speaking. It divides the sub-channel and pins into more flow and heated regions respectively, increasing the number of calculation sections. The complexities appear when passing the feedback information. Since it has more channels, the feedback in the coolant requires special attention. A correct weighting of each sub-channel must be performed to average the parameters that will be passed.
An initial cosine power distribution is assumed for both cases. Subsequently, the converged solution is obtained after several coupled iterations and compared as depicted in the Figures below. Figure 9-4 compares axial peaking factors (illustrated by histograms) and moderator densities (shown as lines connecting the calculated points) for the two studied cases: rod centered (in pink or light color) and coolant centered (in blue or dark color) respectively.

Figure 9-4: Comparison between the rod and coolant centered sub-channel approaches
As exemplified by the above-mentioned figure, the rod centered approach calculates higher axial power factors (APF) before and during the bottom power peak\(^4\), in pink or light color, due to higher moderator density values. Both sub-channel models calculate the same total power, represented by the area under the axial peaking factors curve. In the case of the coolant centered approach, lower axial peaking factors are observed before and in the bottom power peak and higher APF values in the middle section (the same total power is preserved).

Figure 9-5 shows the radial power distributions for the coolant and rod centered cases in the four calculated pins respectively. As mentioned previously, each pin cell contains fresh fuel with different enrichment causing the difference in radial peaking factors between pins. In the comparison of the calculated radial peaking factors between sub-channel models, it can be observed that both cases are quite similar. The total array power is the same and the radial peaking factors are quite similar, the only difference is found in the axial distribution of the parameters caused by the different axial thermal hydraulic feedback from the sub-channel models.

\(^4\) The thermal-hydraulic feedback effects are consistent with the fact that in the BWR 3D 2×2 problem, the fresh fuel with the same enrichment is uniformly distributed axially (high power at the bottom - where there is higher neutron moderation resulting from higher moderator density; and lower power at the top - lower moderator density resulting in lower moderation).
9.4 Comparison between the standard and generated thermal scattering cross-sections using the rod model

In this comparison, the implementation of the new generated thermal scattering cross section for the H$_2$O moderator in MCNP5 is evaluated. Previously, the MCNP5 criticality calculations were executed using the standard provided thermal scattering cross section at 600 K for light water moderators, which was the closest temperature to the desired temperature range ($\Delta T = 10$ K approx. for BWRs $\approx 550$ K to 560 K). Using the
designed methodology, a new thermal scattering cross-section grid was generated and implemented in the MCNP5 criticality calculations. The grid containing the thermal scattering cross sections was generated for each degree in the desired temperature range. Once the thermal-hydraulic feedback is received, the automated cross section management system locates the thermal scattering cross section to be used for each of the 50 axial nodes. In this manner, the feedback transferred per node permits a detailed representation of the behavior of the modeled parameters.

The hybrid coupled code system modeled the two cases; the one with the original provided thermal scattering cross section at 600 K and the one using the new thermal scattering cross section grid in the desired temperature range. The comparison between the two mentioned calculations is illustrated in Figure 9-6.
When using the new thermal scattering cross section grid, this is at a lower temperature than the original provided by MCNP5 at 600 K, a higher axial power factor is obtained before and in the bottom power peak before the saturation conditions are reached. This improves the modeling of the moderator behavior by using a more accurate physical model; lower moderator temperature represents higher moderator density and more neutron moderation, increasing the power. In addition, at lower thermal energies there is less up-scattering; in this manner more fission is produced.

Figure 9-6: Comparison of the axial power distribution using the rod model between the standard and generated thermal scattering cross-sections
The same previous comparison performed with the rod sub-channel approach was carried out using the coolant centered based input model. The results showed similar behavior as can be seen in Table 9-3, which illustrates two comparisons between the radial power factors distribution. The comparisons illustrate the difference between the respective models, rod or coolant models, with and without the new thermal scattering cross section library.

<table>
<thead>
<tr>
<th>Case \ Pin #</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rod VS Rod TH</td>
<td>0.00077</td>
<td>0.00169</td>
<td>0.00116</td>
<td>0.00024</td>
</tr>
<tr>
<td>Coolant VS Coolant TH</td>
<td>0.00153</td>
<td>0.00051</td>
<td>0.00143</td>
<td>0.00061</td>
</tr>
</tbody>
</table>

A noticeable difference is observed in the comparisons between the respective models using the standard thermal scattering cross section data (provided in MCNP5) and the newly generated thermal scattering grid.

The $k_{\text{eff}}$ comparison was also carried out for the rod model with and without the new thermal scattering cross section grid. This $k_{\text{eff}}$ comparison is presented in Table 9-4. The rod centered case with the generated thermal scattering cross section library presents higher calculated $k_{\text{eff}}$, which is consistent with the higher power produced as shown in Figure 9-6 and illustrated quantitatively in Table 9-3 and Table 9-4. The higher $k_{\text{eff}}$ is the result of the thermal scattering cross section at the correct temperature, which is lower than 600 K. At lower thermal energies there is less up-scattering and more fission is produced.
9.5 Time reduction obtained with the implementation of the acceleration strategies

Reference coupled calculations required a substantial amount of time, which is particularly true when the criticality part of the calculation is performed by MCNP5. Several acceleration strategies are combined and implemented into the MCNP/CTF/NEM system in order to reduce the computational time of the complete calculation. Table 9-5 summarizes the acceleration strategies of the coupled hybrid system together with their corresponding timed reduction.

Table 9-4: $k_{\text{eff}}$ comparison the rod model and the same rod model using the generated thermal scattering cross-section

<table>
<thead>
<tr>
<th>Coupled Iteration</th>
<th>Rod Centered TH</th>
<th>Rod Centered No TH</th>
<th>$k_{\text{eff}}$ Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>#</td>
<td>$k_{\text{eff}}$</td>
<td>Std-Dev</td>
<td>$k_{\text{eff}}$</td>
</tr>
<tr>
<td>1</td>
<td>1.35039</td>
<td>0.00037</td>
<td>1.34914</td>
</tr>
<tr>
<td>2</td>
<td>1.33470</td>
<td>0.00038</td>
<td>1.33161</td>
</tr>
<tr>
<td>3</td>
<td>1.33502</td>
<td>0.00039</td>
<td>1.33266</td>
</tr>
<tr>
<td>4</td>
<td>1.33619</td>
<td>0.00034</td>
<td>1.33283</td>
</tr>
<tr>
<td>5</td>
<td>1.33574</td>
<td>0.00037</td>
<td>1.33298</td>
</tr>
</tbody>
</table>
The capabilities of the hybrid coupled system are analyzed in this chapter using different test cases. A 3-D 2 by 2 pin array model extracted from a representative BWR assembly is used as a model in the test cases. It is important to note that the BWR model is the most complicated, from a thermal hydraulic point of view, for nuclear reactor analysis of LWRs. The difficulties of a BWR model appear from the complex axial temperatures and moderator density changes, which are quite drastic. At the same time, the BWR model represents the perfect case to show the importance of the detailed

<table>
<thead>
<tr>
<th>Acceleration Strategies</th>
<th>Reduced/Affected Parameter</th>
<th>Estimated Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid System</td>
<td>Reduction on the # of MCNP5 cycles</td>
<td>Depends on the case. For 9 Coupled Iterations (CI) calculation, 739 cycles were skipped, approx 6 hrs reduction.</td>
</tr>
<tr>
<td>Parallel Criticality Calculations</td>
<td>Reduction on the wall clock time</td>
<td>Depends on the number of available processors (p). Using 2p, a 180 min reduction was observed. Speed up ratio of 1.61</td>
</tr>
<tr>
<td>Creation of a XS Database</td>
<td>No need to generate/interpolate XS for all cases</td>
<td>Depends on the computer, isotope, temperature, etc. It takes around 0.9 min per node. A 25 min or larger time reduction per CI has been observed.</td>
</tr>
<tr>
<td>Relaxation Method</td>
<td>Reduction on the total # of Coupled Iterations (CI)</td>
<td>Avoids oscillations. Depends on the case. A reduction of 1 CI has been observed. (Some cases show no reduction)</td>
</tr>
<tr>
<td>Internal Coupling</td>
<td>Avoid open/close/read/write files</td>
<td>Depends on the # of files &amp; CI. In the order of seconds, maybe few minutes for the total calculation.</td>
</tr>
</tbody>
</table>

9.6 Summary

The capabilities of the hybrid coupled system are analyzed in this chapter using different test cases. A 3-D 2 by 2 pin array model extracted from a representative BWR assembly is used as a model in the test cases. It is important to note that the BWR model is the most complicated, from a thermal hydraulic point of view, for nuclear reactor analysis of LWRs. The difficulties of a BWR model appear from the complex axial temperatures and moderator density changes, which are quite drastic. At the same time, the BWR model represents the perfect case to show the importance of the detailed
analysis per node performed by the hybrid couple system. It gives the opportunity to illustrate the drastic changes and effects of the feedback parameters.

The benchmark problems are selected to exemplify several different analyses using the hybrid coupled system. The first analysis presents the comparison of the BWR 3-D 2x2 pin array with two different mass flow rates. One of the mass flow rates is at normal BWR operating conditions, while the second is at a much reduced mass flow rate, representing a drastic case. This test reflects the effects of changing the flow rate on the moderator density, hence the axial power shape and finally the $k_{\text{eff}}$. All the distributions shifted accordingly. It was observed as well, the effects of the moderator and Doppler feedback mechanisms.

The second study, illustrates a comparison between the coolant centered and rod centered sub-channel approaches. These two different CTF sub-channels models can be used to represent fuel assemblies. The sub-channel codes such as CTF are extensively validated based on the coolant centered sub-channel modeling. In order to provide a new validation scheme for comparison, a CTF input based on the coolant centered approach. It can be observed that both cases are quite similar. The total array power is the same and the radial peaking factors are quite similar, the only difference is found in the axial distribution of the parameters caused by the different axial thermal hydraulic feedback from the sub-channel models. The CTF input based on the coolant centered approach represents a more complex model geometrically speaking.

The third analysis presented the importance of using the correct thermal scattering cross section library. Previously, the MCNP5 criticality calculations were executed using the standard provided thermal scattering cross section at 600 K for light water
moderators, which was the closest temperature to the desired temperature range (\(\Delta T = 10\) K approx. for BWRs \(\approx 550\) K to 560 K). Using the designed methodology, a new thermal scattering cross-section grid was generated and implemented in the MCNP5 criticality calculations. A noticeable difference is observed in the comparisons between the respective models using the standard thermal scattering cross section data (provided in MCNP5) and the newly generated thermal scattering grid.

Finally, the chapter summarizes the time reduction obtained with the implementation of the acceleration strategies into the coupled hybrid system.
Chapter 10

Conclusions and recommendations for future work

In this research project, a high accuracy modeling tool using a Monte Carlo based coupled system has been developed. The following sections summarize the unique contributions of this dissertation in the development of models to include the thermal-hydraulic feedback to the Monte Carlo method and speed-up mechanisms to accelerate the Monte Carlo criticality calculation.

10.1 Thermal-hydraulic feedback modeling to Monte Carlo core calculations

The thermal-hydraulics feedback effects in Monte Carlo reactor core calculations include changes in the dimensions of the geometry, material density effects, and temperature effects on cross-section data. A special interface has been developed to update the required MCNP5 input changes to account for dimension and density changes provided by the thermal-hydraulics feedback module, which in this case is CTF.

The interface has also been developed to extract the flux and reaction rates calculated by MCNP5 to later transform the data into the power feedback needed by CTF (axial and radial peaking factors). The interface is contained in a master program that controls the flow of the calculations. Both feedback modules (thermal-hydraulic and power subroutines) use a common internal interface to further accelerate the data exchange. The exchange interface requires several other functions and modules to
properly extract and convert the feedback data using the proper average and weighting of the parameters. The hybrid coupled system contains different codes, with different model representations. For instance, CTF has more axial nodes (on the top and at the bottom) than MCNP5. The coupling requires an axial meshing adaptation that adjusts the MCNP5 axial mesh to CTF axial mesh and vice versa when passing the information in the couple calculations.

All the feedback parameters need to be checked for convergence. The coupled convergence criteria are set up through the feedback parameters. The moderator temperature and density, as well as the fuel temperature are checked for convergence. The coupled convergence criteria were set up to satisfy the requirement that the maximum relative deviations in node-wise distributions of feedback parameters simultaneously to be less than $\varepsilon=10^{-4}$.

10.2 Generation methodology for temperature dependent cross-section libraries

The behavior of the reactor and hence the multiplication factor of the system is greatly affected by core temperature. Hence, the temperature of the reactor must be considered for a proper modeling of the system. The temperature effect, and thus the temperature feedback, is accounted through the generation and utilization of the temperature dependent cross-section libraries.

The first step to correctly include the thermal hydraulic feedback into MCNP5 calculations begins with temperature dependent cross section libraries. If the cross sections used for the calculations are not at the correct temperature, the temperature
feedback cannot be included into MCNP5. The only method of considering the
temperature effects on cross sections is through temperature-dependent generation. The
temperature effects on continuous cross-section data include Doppler broadening of
resolved resonances; Doppler broadening of unresolved resonances; changes in $S(\alpha,\beta)$
thermal scattering kernel; and elastic scattering, which is Doppler broadening over the
entire energy range.

The generation process for cross-section libraries is tedious and involves a lot of
data manipulation. An automated methodology has been developed as part of the hybrid
Monte Carlo-based coupled core studies at PSU. The duration of the procedure has been
significantly reduced. This automated tool performs the most time consuming tasks of the
cross-sections generation process. The GEN-XS code automates the process for all
required isotopes and all required temperatures. The final output of the automated tool is
a cross-section library together with the corresponding directory of cross-section files
needed by MCNP5.

The methodology for generating thermal scattering cross-section libraries has
been studied and included as well. The cross sections, as well as the angular and energy
distributions of the scattered neutrons are affected, at thermal neutron energies, by the
binding of the scattering nucleus. This is because the neutron can lose or gain energy in
the interaction. The thermal neutron cross sections are enormously difficult due to their
susceptible dependence on the temperature, as well as on the chemical state of the
scattering material. The research purposes on this area focus on generating thermal
scattering cross-section libraries for $H_2O$, the moderator of LWRs. The possibility of
having thermal libraries at the correct moderator temperature improves the accuracy of
the modeling.

This tool is used together with the automated cross-section temperature interpolation capability for intermediate points. The temperature dependent modeling capability is included into the coupled-code. In this way, it will automatically determine or interpolate the appropriate temperature dependent cross section library for the MCNP5 criticality calculation according to the temperature feedback.

10.3 Interpolation methodology for temperature dependent cross-section libraries

The most accurate technique to update the cross-section libraries, taking into account the temperature feedback, would be to update the libraries with NJOY, for each nuclide, in their corresponding region, at the temperature of that region. In particular, this technique would be the most accurate, but not practical because of the vast computational time that it would take.

Investigations carried out at PSU have exemplified that the most appropriate and practical technique, with high accurate results, would be to use a pre-generated cross-section library with temperature increments of 50 K, and then, an interpolation method would be used to approximate the cross sections at the provided by CTF temperatures.

The square root of temperature, $\sqrt{T}$, interpolation method is used in the studies presented in this research. This $\sqrt{T}$ interpolation method has demonstrated the correct trend and excellent agreement with the actual cross-sections. In addition, considerable amount of computational time is saved by not having to re-generate the cross section
libraries for each isotope, of each region, at the specified feedback temperature of that region.

A cross section update methodology has been proposed. The flow diagram starts by receiving the thermal-hydraulic (TH) feedback from COBRA-TF (CTF) for each node of each pin. At this point, a selection criterion must be stated as to the way of using the updated temperature information. On the one hand, if the cross section data exists for the received TH-feedback, the cross section libraries are obtained from the cross section database and used on the MCNP5 calculation. On the other hand, if there is no cross section data available for the received TH feedback, the cross section libraries will be updated using the interpolation method and these new libraries would be used in the MCNP5 calculation.

Once the cross section libraries are ready, obtained either from the cross section data base or from the interpolation methodology, the MCNP5 input deck is prepared. All thermal-hydraulic information is updated; fuel, clad and moderator temperatures, moderator densities, and cross section libraries for the corresponding temperatures. As mentioned previously the TH-feedback is updated per node. Finally, the MCNP5 criticality calculation is run.

The interpolation process is carried out for each isotope of each region (since the cross section libraries are given per isotope at a given temperature) and this could represent a considerable amount of computational work depending on the axial meshing and number of nuclides of the material regions.

The interpolation of cross-section libraries, just as the generation process, is tedious and involves a lot of data manipulation (and storage capacity), in this way an
automated subroutine is created to manage the existing and new libraries and all data processing needs.

The existence of the cross section database plays a quite significant role in the interpolation methodology. It serves as a source of cross section data, providing the necessary temperature grid for the interpolation methodology. Furthermore, the cross section data base is continuously updated with each calculation. Every time a new cross section library is generated via the interpolation method, the new cross section data is saved in the cross section data base for use in future calculations. The continuously updated cross section data base represents an important acceleration mechanism for the hybrid coupled calculations. It first avoids the need to directly generate cross section libraries by using the interpolation mechanism and secondly, by saving all the interpolated cross section data, it avoids the interpolation mechanism for future calculations.

Using the interpolation methodology specially designed for thermal scattering cross sections, a thermal scattering grid at the desired temperature range (ΔT = 10 K approx. for BWRs ≈ 550 K to 560 K) was generated.

This gives the possibility of performing MCNP5 criticality calculations at the correct moderator temperature and improving the accuracy of the calculation. When this thermal scattering grid is applied to the hybrid coupled system, each simulated axial node uses the correct moderator thermal scattering cross section, providing a correct axial distribution of thermal scattering data based on the moderator temperature.
10.4 Acceleration schemes for Monte Carlo based coupled calculations

The Monte Carlo method can be considered a “numerical experiment” and provides a great possibility of generating reference solutions for verification and validation of commercial codes. The incorporation of the thermal-hydraulic feedback is of great interest and very appealing. On the other hand, Monte Carlo calculations required a great deal of computer resources and are quite “expensive” in computational time. Although the great amount of time required by the MCNP5 calculations, they are used to bridge the gap between fast diffusion calculations and the availability of experimental data. One of the objectives of this research is to present a combination of strategies to accelerate the coupled hybrid system, and in particular the MCNP5 calculation that takes the most amount of time.

The acceleration strategies investigated were based on a combined internal/external coupling approach, parallel Monte Carlo calculations and the introduction of a novel hybrid nodal diffusion/Monte Carlos approach.

A new methodology to speed up the Monte Carlo criticality calculations was devised as part of the development of the Monte Carlo based coupled calculations. The algorithm utilizes a hybrid nodal diffusion/Monte Carlo calculation scheme. The primary concept of this methodology is to pre-generate an initial source distribution of the Monte Carlo method by a nodal diffusion method. In the coupled nodal diffusion/Monte Carlo calculation scheme, the fast nodal diffusion calculation is used to provide the fission source distribution as an initial source distribution for the Monte Carlo calculation. The fission source distribution simulated in the nodal diffusion calculation is practically
closer to the true source distribution of the Monte Carlo calculation than the typical guess source distribution. Therefore, the coupled methodology avoids utilizing large number of inactive cycles in the Monte Carlo calculation.

The MCNP5/CTF/NEM code system includes an interfacing code that provides thermal-hydraulic feedback with hybrid nodal diffusion capabilities to the LANL Monte Carlo code, MCNP5 by coupling in an internal manner (where possible) with the thermal-hydraulic sub-channel code CTF and the NEM diffusion code. The internal coupling transfers the feedback data in a direct way avoiding any extra transfer action that will increase the time of the calculation. Internal coupling represents a faster and more efficient way of passing the feedback information.

The MCNP5 code is optimum to use the parallel capability due to the fact that each particle history can be run independently. In this way the total numbers of histories is divided in groups and send to different machines where the calculations are performed. The MCNP-CTF code presents the possibility of executing the Monte-Carlo criticality calculation either in sequential or parallel mode. The execution mode depends on the number of processors available.

Also, as described in the previous point, the continuously updated cross section data base represents an important acceleration mechanism for the hybrid coupled calculations.

The acceleration techniques were evaluated by assessing the speed-up calculation performance and decrease in computational time.
10.5 Global Sensitivity Analysis using MCNP5 continuous energy calculations

Uncertainty and sensitivity analysis techniques can be used to carry out the study of uncertainty in model predictions occurring from inaccurately-known processes and input data. Global sensitivity analysis facilitates the identification of high-order interactions among inputs in determining the uncertainty in the output of interest. Global sensitivity analysis is applied to the modeling of nuclear reactor calculations for better model understanding. Particularly, it is investigated how much criticality conditions are affected by uncertainties in various inputs, including nuclear cross-sections, at different energies, from several isotopes in the fuel, the absorber, and the moderator. The sensitivity analysis consists of a number of model simulations, which are performed using MCNP5 calculations.

This exercise presented a novel and interesting way of applying global sensitivity analysis to nuclear applications using MCNP5 continuous energy criticality calculations. For such coupled code system based on Monte Carlo, is important to have a tool to evaluate the uncertainty in continuous cross-sections as well as the impact of NDL.

The cross sections were modified directly with the corresponding uncertainties. A sample matrix was generated to represent such uncertainties and the whole process was automated in a code. The first order and total sensitivity indices were obtained to assess the importance of certain parameters, refer to the variation of the output with regards to changes in certain inputs or combination of inputs. Finally the number of cases was considerably extended to reduce the amplitude of the confidence intervals.
10.6 Recommendations for future work

The current section summarizes several recommended research activities that can be carried out as a continuation of the present research. These suggestions are explained next.

10.6.1 Further validation with the measurement

One of the main objectives of this research is the implementation of the thermal-hydraulic feedback into MCNP5. The developed MCNP5/CTF/NEM/NJOY hybrid coupled system and later ameliorations were tested using a model based on LWRs, specifically on BWRs (since it was the most demanding model). Future work could continue with the application of the described studies and methodologies into research reactors; like the Pennsylvania State University Breazeale research reactor (PSBR). This future activity will further assess the accuracy of the modeling of the MCNP5/CTF/NEM/NJOY code system. The main advantage of using the PSBR, is the possibility of having reference data based on real measurements. Plus having the added advantage of illustrating the broad applicability of the studies described on the present research.

10.6.2 Further studies on accelerating the Monte Carlo criticality calculation

This dissertation proposed several acceleration strategies to reduce the computational time of the coupled calculation. Two of these acceleration strategies were
directed into the MCNP5 criticality calculations, which take the most time in the coupled
calculation. Besides the proposed techniques, there are more possibilities that can be
further investigated. Among the potential possibilities, one could look into the ALEPH
approach to further accelerate the tally processing, parallel calculations at higher levels,
and several other possibilities.

10.6.3 Design and development of a graphical user interface for the hybrid coupled
system

A graphical user interface would facilitate the utilization of the hybrid coupled
code system as a fuel management analysis tool. The graphical user interface could
comprise all the interfaces; from the input preparation (for cross section generation, for
coupled system inputs, for criticality and thermal hydraulic analysis), all the way to the
presentation and analysis of the results. In this way the graphical user interface will make
the code more user-friendly and accelerate the interaction between the user and the code.

10.6.4 Coupling between the MCNP5/CTF/NEM/NJOY code system and MCOR

Within the design of nuclear reactor assemblies and cores, one of the primary
responsibilities is the determination of the set of system parameters that will give in a
reliable and safe, while being economical, reactor operation; which should be at the rated
power level over the desired core lifetime. Indeed, the nuclear analysis of the core must
interact with other subjects of core design, such as thermal-hydraulic, economic
operation, etc. The nuclear design of the core would be restrained by considerations of such design aspects.

During the operating lifetime of the core, the core composition changes, affecting the core multiplication and power distribution. The study of the change of the core power distribution with the time-dependent depletion of the nuclei is known as burnup analysis. This is possibly, the most expensive, in terms of calculation time, and most important, in terms of economic behavior, study of the nuclear reactor analysis.

The MCOR code system, as described in Chapter 3, is a Monte Carlo based depletion system for reference fuel assembly and core calculations. In the long-term, the hybrid coupled MCNP5/CTF/NEM/NJOY calculations should be implemented within the framework of this Monte Carlo depletion system. In this way the Monte Carlo depletion system will be able to provide reference solutions not only at fixed temperature conditions but also for operating conditions with temperature spatial distribution.
Appendix A

Effect of temperature on cross section libraries

Figure A-1: Effect of temperature on the total cross section (SigmaT) of U-235
Figure A-2: Effect of temperature on the capture cross section (SigmaC) of U-235
Figure A-3: Effect of temperature on the elastic cross section (SigmaEl) of U-235
Figure A-4: Effect of temperature on the fission cross section (SigmaF) of U-235
Figure A-5: Effect of temperature on the total cross section ($\Sigma T$) of U-238
Figure A-6: Effect of temperature on the capture cross section (SigmaC) of U-238
Figure A-7: Effect of temperature on the elastic cross section (SigmaEl) of U-238
Figure A-8: Effect of temperature on the fission cross section (SigmaF) of U-238
Appendix B

NJOY input for generation of continuous energy cross section library of U-235

```
moder
20 -21
reconr
-21 -22
*pendf tape for U235 */
  9220 1 0 */
  0.005 0.7*/
*Uranium-235 */
0/
broadr
-21 -22 -23
  9228 1 0 0 0/
  0.005/
  552.15/
0/
unresr
-21 -23 -24
  9228 1 8 1/
  552.15/
1E+10 1E+3 1E+2 50 20 10 5 1/
0/
heatr
-21 -24 -25 47
  9228/
thermr
0 -25 -26
0 9228 3 1 1 0 1 221 0 /
  552.15/
  0.01 4.6/
groupr
-21 -26 0 -27
  9228 3 3 3 1 8 1/
*Uranium-235 at T- 552.15K*/
  552.15/
1E+10 1E+3 1E+2 50 20 10 5 1/
3/
0/
0/
acer
-21 -26 -27 35 36 /
1 1 1 14 0/
"U235 ENDF7 at 552.15K. F.Puente Espel"/
  9228 552.15 /
  1 1 /
stop
```

Figure B-1: NJOY input using groupr module
moder
20 -21
reconr
-21 -22
'pendf tape for 92-U-235 by njoy 99.81'/
9228 7 /
.001 /
'the following reaction types are added where available'/
'mt133 unresolved probability tables'/
'mt20x gas production'/
'mt221 free thermal scattering'/
'mt301 total heating kerma factor'/
'mt444 total damage energy production'/
0 /
broadr
-21 -22 -23
9228 1 0 1 /
.001 /
293.60 /
0 /
unreer
-21 -23 -24
9228 1 1 1
293.60 /
1e10 /
0 /
heatr
-21 -24 -25 /
9228 7 /
302 303 304 318 402 443 444 /
purr
-21 -25 -26
9228 1 1 20 64 /
293.60 /
1e10 /
0 /
gaspr
-21 -26 -27
aceous
-21 -27 0 28 29
1 0 1 0.99 /
'92-U-235 at 293.60K by njoy99.81'/
9228 293.60 /
/
/
stcp

Figure B-2: NJOY input using purr module
Appendix C

Hybrid coupled code system input
Appendix D

\( k_{\text{eff}} \) and source entropy convergence

Figure D-1: \( k_{\text{eff}} \) and source entropy convergence with the user defined initial source
Figure D-2: $k_{eff}$ and source entropy convergence with the previously calculated source.
Figure D-3: $k_{\text{eff}}$ and source entropy convergence


7. R. E. MacFarlane, “NJOY 99.0 Code system for producing pointwise and multigroup neutron and photon cross sections from ENDF/B data”, Los Alamos National Laboratory, 1999


VITA

Federico Puente Espel

Federico Puente Espel was born on the 4th of July, 1979, in Mexico City, Mexico. Being son of a Spanish mother and a Mexican father, he lived in Spain and Mexico during his early life. Later, he also lived in the United States. Federico completed a bachelor’s degree in mechanical engineering with a study major in energy engineering and a second bachelor’s degree in economics in Mexico City. Then he moved to Stockholm, Sweden, where he carried out his master of science in sustainable energy engineering with a study major in nuclear power technology. After his master studies, he worked two years in the nuclear industry in Sweden and Spain. It was then that he decided to continue his nuclear education through a PhD at The Pennsylvania State University.