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Internal multi-scale multi-physics coupled system for high fidelity simulation of light water reactors

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ABSTRACT

In order to increase the accuracy and the degree of spatial and energy resolution of core design studies, coupled 3D neutronic (multi-group deterministic and continuous energy Monte-Carlo) and 3D thermal–hydraulic (CFD and subchannel) codes are being developed worldwide. At KIT, both deterministic and Monte-Carlo codes were coupled with subchannel codes and applied to predict the safety-related design parameters such as minimal critical power ratio (MCPR), maximal cladding and fuel temperature, departure from nuclide boiling ratio (DNBR). These coupling approaches were revised and considerably improved. Innovative method of internal on-the-fly thermal feedback interchange between the codes was implemented. It no longer relies on explicit material definitions and allows the modeling of temperature and density distributions based on the cell coordinates. In contrast to all existing coupled schemes, this method uses only standard MCNP geometry input and requires only proper definition of the geometrical dimensions. The initial material definition is arbitrary and is determined on-the-fly during the neutron transport by the thermal–hydraulic feedback. Another key issue addressed is the optimal application of parallel computing and the implementation of less time consuming tally estimators. Using multi-processor computer architectures and implementing collision density flux estimator, it is possible to reduce the Monte-Carlo running time and obtain converged results within reasonable time limit. The coupled calculation was accelerated further, by implementing stochastic approximation-based relaxation technique. Further, it is shown that large fuel assemblies can be analyzed on subchannel level.

1. Introduction

High fidelity coupled solutions of neutron physics and thermal–hydraulic codes are being developed worldwide to increase the accuracy and the degree of spatial resolution of core design studies. For example coupled, Three-Dimensional (3D) neutronic (multi-group deterministic and continuous energy Monte-Carlo) and 3D thermal–hydraulic (CFD and subchannel) codes have been realized (Tippayakul et al., 2007; Watta et al., 2006; Puente-Espel et al., 2009, 2010). At the Karlsruhe Institute of Technology (KIT), both deterministic and Monte-Carlo codes have been coupled with subchannel codes and applied to predict the safety-related design parameters such as pin power, maximum cladding and fuel temperature of a PWR fuel assembly at nominal conditions (Sánchez et al., 2008; Sanchez and Al-Hamry, 2009).

The research done on the topic however, is mainly limited to small problems consisting of only few pins and based on external coupling of the involved codes. For such problems the stability of the coupled system is not effectively tested. In the case of large problems consisting of many thousands of cells, achieving convergence of the coupled calculation, convergence of the fission source and proper statistics poses a real challenge. The existing coupled schemes are affected by the inability of some Monte-Carlo codes, such as MCNP, to model three dimensional (3D) distributions of density and temperature. In practical terms, the definition of large numbers of cells with distinct material specifications is required, a serious drawback resulting in large input files. This approach seriously limits the flexible geometry definition of Monte-Carlo codes. The main application of such a coupled system is to provide reference solutions, to serve as numerical benchmark and to validate deterministic calculations of complex fuel assembly designs, where the homogenization theory requires reliable validation. Therefore, having this in mind one requires the ability to model large problems within a consistent coupled system.

In the current paper, the further development and improvement of the KIT coupling approaches will be presented. In addition the effects of the stochastic approximation method on the convergence of the coupled scheme will be presented. Using this new

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acceleration method, it is possible to achieve uniform convergence. In addition, it is shown how the degree of convergence depends only on the number of coupled iterations.

The innovative internal coupling scheme implemented recently in MCNP5/SUBCHANFLOW, enabling the cell-wise definition of density and temperature distributions, will be presented. Using this innovative coupling approach it is no longer necessary to define massive MCNP inputs, when distribution of densities and temperatures are required. The MCNP input is kept as simple as possible and it can be built by using only standard MCNP features. In the framework of the new internal coupling scheme the neutrons obtain their feedback information on the fly as they explore the geometry. This strategy is applied to both single differential and double differential data.

2. Codes used in the coupled calculations

The Monte-Carlo code MCNP5 and the thermal–hydraulic subchannel code SUBCHANFLOW are selected for these investigations. In addition, NJOY modules LEAPR, THERMR, ACER and BROADR are used to process the nuclear data.

2.1. The thermal–hydraulic subchannel code SUBCHANFLOW

For performing the subchannel analysis, SUBCHANFLOW (SCF), a code under development at the KIT, was employed (Śanchez et al., 2010; Imke and Sanchez, 2012). It is based on the COBRA code family and is able to treat hexagonal and square bundle geometries with axially varying cell size. SUBCHANFLOW is written in FORTRAN 95 language in a fully modular way. Global data structure as well as fluid and material properties are stored in separate modules. The code solves mass, axial momentum, lateral momentum and energy conservation equations for vertical flow conditions. SUBCHANFLOW supports water, lead, helium, lead–bismuth and sodium as working fluid. Using thermal–hydraulic modeling based on 3 equations approach. Recently, a boron transport model and a point kinetics model have been implemented.

2.2. The neutronic code MCNP5 and the nuclear data processing code NJOY

MCNP5 simulates neutron transport in three dimensions using the Monte-Carlo method (Brown, 2005; MCNP, 2004). In the coupled run MCNP5 is used to generate the power profile, which is then transferred to SUBCHANFLOW. In order to read the power profile the newly implemented collision density estimator for the cell tally (Fx:n) and mesh tally (FMESH4:n) are used. In addition, the nuclear data processing code NJOY99 was used. The module BROADR (NEA/NSC/DOC, 2006) was used for Doppler-broadening of the continuous energy cross sections. In addition to the BROADR module, the LEAPR-THERMR-ACER module sequence was used for preparing thermal scattering data at different temperatures.

3. Coupled Monte-Carlo – thermal–hydraulic calculations

3.1. Mathematical definition of the problem

The steady-state neutron transport equation with no external sources can be transformed into integral form (1), the complete derivation can be found in Spanier and Gelbart, (1969), Lewis and Miller, (1984).

$$\varphi(\zeta) = \iint_{\Gamma} K(\zeta,\zeta')\varphi(\zeta')d\zeta' \tag{1}$$

Here Γ denotes the integration domain of the phase space and ζ represents the phase space variables. This is a Fredholm integral equation. Being a fixed point problem the existence of solution is determined by the Banach fixed point theorem (Dunford and Schwartz,1958), (Kolmogorov and Fomin, 1963):

Theorem 1. *Let $\mathcal{M}$ be a complete metric space with distance between two points A and B given by $\rho(A,B)$. Moreover, let $\mathcal{L}:\mathcal{M}\to\mathcal{M}$ be a contraction operator, for which there exists $k\in(0,1)$ such that for all $A,B\in\mathcal{M}$, $\rho(\mathcal{L}(A),\mathcal{L}(B))\leqslant k\rho(A,B)$. Then, there exists a unique $A\in\mathcal{M}$ such that $\mathcal{L}(A)=A$. The point A, can be generated by the iteration $\mathcal{L}(A_{n-1})=A_n$, with A_0 being arbitrary.*

Here the distance is defined to have the following properties: For all $A,B,C\in\mathcal{M}, \rho(A,A)=0,\ \rho(A,B)\geqslant 0, \rho(A,B)=\rho(B,A)$ and $\rho(A,B)\leqslant\rho(A,C)+\rho(B,C)$.

These important properties of the space $\mathcal{M}$ allow us to define convergence. In fact, the proof of the theorem is based on showing that $\rho(A_n,A_m)$ for $A_n,A_m\in\mathcal{M}$ is a Cauchy sequence converging due to the metric space $\mathcal{M}$ being complete by definition. Therefore, the following limit exists (2)

$$\begin{aligned}&\lim_{n\to\infty}A_n=\lim_{n\to\infty}\mathcal{L}(A_{n-1})\\&A_*=\mathcal{L}(A_*).\end{aligned} \tag{2}$$

The Banach fixed point theorem gives important insight into the solutions of (1) and the space they reside on. It should be noted that to fulfill the conditions of a contraction operator, the kernel of the integral transport equation should be bounded and continuous (Dunford and Schwartz,1958).

As pointed out in Dufek and Gudowski, (2006), the estimation of the power profile distribution results in the solution of the following problem (3)

$$\varphi = G(T(\varphi),H(\varphi)), \tag{3}$$

where $H(\varphi)$ and $T(\varphi)$ are the density and temperature distributions and the value of $G(T(\varphi), H(\varphi))$ is estimated by the Monte Carlo codes with superimposed statistic noise ε. The Monte-Carlo estimate of the left hand side of (3) is defined as (4)

$$Y(\varphi) = G(T(\varphi),H(\varphi)) + \varepsilon \tag{4}$$

The problem as given by (3) can be in principle solved by an iterative scheme, consecutively updating $H(\varphi)$ and $T(\varphi)$. However, this is a very inefficient method. Moreover, the convergence will be limited by the magnitude of ε. Therefore, in order to achieve convergence one must run large number of iterations applying huge number of particle histories. Based on this, it is recommended to use an acceleration scheme. In the past relaxation scheme, acting on the thermal–hydraulic parameters only, has been used (Watta et al., 2006; Hoogenboom et al., 2011). The old relaxation scheme is described by the equation set (5), where "i" is the iteration step number.

$$\begin{aligned}T^{\text{weighted}}_{\text{fuel},i+1} &= (1-\omega)T_{\text{fuel},i-1} + \omega\left(T^{\text{actual}}_{\text{fuel},i}\right),\\ T^{\text{weighted}}_{\text{H}_2\text{O},i+1} &= (1-\omega)T^{\text{actual}}_{\text{H}_2\text{O},i-1} + \omega\left(T^{\text{actual}}_{\text{H}_2\text{O},i}\right),\\ \rho^{\text{weighted}}_{\text{H}_2\text{O},i+1} &= (1-\omega)\rho^{\text{actual}}_{\text{H}_2\text{O},i-1} + \omega\left(\rho^{\text{actual}}_{\text{H}_2\text{O},i}\right).\end{aligned} \tag{5}$$

This scheme accelerates the solution. Unfortunately the convergence rate is still correlated to the statistical noise. The natural method of acceleration for problem (3) is to use a stochastic approximation technique. Although the same method of acceleration as in Dufek and Gudowski, (2006) is used, different reasoning concerning its applicability is applied. The theorem of Robbins and Monro is to be stated hereafter. The formulation of the theorem as well as the proof can be found in Wasan, (1969). The basic idea is, that by observing random variables $Y(X_n)$ of an unknown distribution, roots of the unknown underlying distribution can be found. In the particular case this is the estimate of (4).