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High-fidelity coupled Monte Carlo neutron transport and thermal-hydraulic simulations using Serpent 2/SUBCHANFLOW

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ABSTRACT

Efforts to develop high-fidelity, in silico or ab initio, high performance multi-physics tools are undertaken by many groups due to the availability of relatively cheap, large-scale parallel computers. To this end, an internal coupling between the Monte Carlo reactor physics code Serpent 2 and the sub-channel code SUBCHANFLOW has been developed. The coupled code system is intended to serve as reference for deterministic reactor dynamics code developments in the future. It exploits the fact that Serpent was conceived as a lattice code for such deterministic tools. The coupling utilizes Serpent's recently introduced universal multi-physics interface. With the multi-physics interface enabled, Serpent treats temperature dependence of nuclear data using the target motion sampling method. Since the target motion sampling methodology cannot be applied to thermal bound-atom scattering or unresolved resonances, a stochastic mixing fall back algorithm to enable the simulation of thermal reactors has been implemented. The developed coupled code is verified by code-to-code comparison with an external coupling of the Monte Carlo tool TRIPOLI4 and SUBCHANFLOW as well as the internally coupled code MCNP5/SUBCHANFLOW. Simulation results of all code systems were found to be in good agreement. Thereafter, the second exercise of the OECD/NEA and U.S. NRC PWR MOX/UO_2 core transient benchmark is studied to demonstrate that Serpent 2/SUBCHANFLOW may be employed to analyze realistic, industry-like cases such as a full PWR core under hot full power conditions in a reasonable amount of time. The obtained simulation results are compared to known benchmark solutions and the numerical performance of Serpent 2/SUBCHANFLOW is analyzed to assess the feasibility of routine application. While Serpent 2/SUBCHANFLOW's performance in terms of physics and numerical efficiency is found to be generally satisfactory, options to further improve the coupled tool concerning both aspects are discussed. Afterwards, first efforts to validate Serpent 2/SUBCHANFLOW using the hot zero power state of the cycle 1 of the BEAVRS benchmark are presented.

1. Introduction

Worldwide efforts to develop high-fidelity reactor simulation tools to be run on large-scale parallel computers for nuclear reactor design, optimization and safety analysis are undertaken. Developers intend to apply these tools instead of industrial standard Best-Estimate (BE) methods in the future. At the last International Conference on Mathematics and Computation (M&C), the large number of challenges one is facing developing such high-fidelity, in silico or ab initio tools has been summarized by Smith and Forget (2013). Most current efforts focus on pin-resolved neutron transport, thermal-hydraulics and mechanics simulations. Pin-resolved means here that all fuel rods are modeled explicitly without any significant simplifications in terms of geometry and materials. However, none of the tool prototypes known to the authors has yet reached a level of maturity as envisioned by Smith and Forget.

Groups working on high-fidelity reactor simulators employ both deterministic and Monte Carlo methods to solve the neutron transport problem. For example, the full core deterministic transport code nTRACER and the sub-channel code MATRA have been employed to perform core follow calculations for a Korean OPR1000 reactor (Jung et al., 2013). Furthermore, nTRACER has

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been used to study a simplified version of cycle 1 and 2 of the BEAVRS core (Ryu et al., 2014). Besides sub-channel thermal-hydraulic tools, computational fluid dynamics (CFD) codes have been used together with deterministic neutron transport codes to analyze a pressurized water reactor (PWR) core with quarter symmetry under steady-state conditions (Weber et al., 2007; Kochuas et al., 2012). Many groups couple Monte Carlo (MC) neutron transport methods to thermal-hydraulic tools (Espel et al., 2013; Li and Wang, 2012; Bernnat et al., 2012; Vazquez et al., 2012; Ivanov et al., 2013, 2014; Gill et al., 2014). Most of these coupling efforts utilize the MC code MCNP. The studied geometries vary from single fuel assemblies to full cores but so does the spatial resolution of the corresponding thermal-hydraulics model. The simulation of a hot full power (HFP) state of a full PWR core was performed by Bernnat et al. employing channel level thermal-hydraulics (Bernnat et al., 2012). Kelly et al. (2014) were the first to perform a core follow calculation for a simplified version of the first cycle of the PWR described in the BEAVRS benchmark.

The overall goal of this work is to obtain reference solutions to foster improving deterministic reactor dynamics codes, especially low order deterministic transport (SP_3 or diffusion) based ones such as the pin-homogenized simulator DYNSUB developed at KIT (Gomez-Torres et al., 2012a,b). As a first step, a coupled Monte Carlo neutron transport and thermal-hydraulics multi-physics tool is to be developed. Unlike MCNP, the Monte Carlo code Serpent developed by VTT Technical Research Center of Finland (Leppänen, 2013b) was originally designed and optimized to be used as a lattice code to generate effective few-group cross section libraries for such deterministic tools. While Serpent's current scope covers most reactor physics applications, it still offers the unique possibility to easily provide a reference solution and few-group cross section sets for a given problem to a deterministic reactor simulator eliminating the need to use a third tool, a classical deterministic lattice code. The latter would only introduce further sources of errors and complicate the performance analysis of the deterministic reactor simulator. Consequently, Serpent was chosen as stochastic neutron transport code in this work. Because of its superior functionality it was decided to use the Serpent 2 beta (SSS2) instead of the official Serpent 1 release. Though conceptually a high-fidelity, in silico or ab initio multi-physics tool should employ CFD as the thermal-hydraulics model with the least approximations, the authors feel that CFD in the nuclear engineering field is not yet mature enough and its computational cost is too high. To allow for simulating pressurized and boiling water reactors as well as Generation IV designs, in-house sub-channel thermal-hydraulics code SUBCHANFLOW (SCF) (Sanchez et al., 2010) is used for now.

In this paper, an internal coupling of Serpent 2 and SUBCHANFLOW is presented. It was preceded by a prototype external coupling based on Serpent 2's multi-physics interface (Daeubler et al., 2014). Thereafter, the solutions provided by Serpent 2/SUBCHANFLOW (SSS2/SCF) are verified by code-to-code benchmarking with internally coupled code MCNP5/SUBCHANFLOW (Ivanov et al., 2014) and the external coupling of TRIPOLI4 and SUBCHANFLOW (Sjenitzer, 2013; Sjenitzer et al., 2015). After the solution verification, Serpent 2/SUBCHANFLOW is employed to study a full PWR core under hot full power conditions, in particular the second exercise of the OECD/NEA and U.S. NRC PWR MOX/UO_2 core transient benchmark (Kozlowski and Downar, 2003). The obtained solutions are compared to the deterministic ones of the benchmark. The OECD/NEA and U.S. NRC PWR MOX/UO_2 core transient benchmark was selected as it includes the nuclide compositions of all fuel types loaded allowing for a Monte Carlo treatment. As the time-to-solution is considered to be important, the numerical performance of the new coupled code for the full core problem is looked at on a medium-sized parallel computer. Finally, the hot zero power state of the BEAVRS core cycle 1 (Horelik et al., 2013) is analyzed. It represents the starting point of the process of validating the coupled solutions provided by Serpent 2/SUBCHANFLOW with measured data.

2. Internal coupling of Serpent 2 and SUBCHANFLOW

In this section, the stand-alone tools Serpent 2 and SUBCHANFLOW are introduced briefly before outlining the coupling work done.

2.1. Monte Carlo code Serpent 2

Serpent 2 (Leppänen, 2013b) is a three-dimensional continuous-energy (CE) Monte Carlo neutron transport code. A new feature that has been recently introduced into Serpent 2 is a multi-physics interface (Leppänen et al., 2012). The interface may be utilized to exchange data with thermal-hydraulics and fuel performance codes. Currently, the universal multi-physics interface comprises four types of interfaces which differ in terms of the format used for passing data between the external solver in question and Serpent. One may employ piecewise constant distributions on regular meshes (type 1), weighted averages of point-wise values (type 2), a user-defined functional dependence (type 3) or unstructured three-dimensional meshes (type 4) (Leppänen, 2012, 2014).

Utilizing the multi-physics interface implies that Serpent uses the target motion sampling method to treat the temperature dependence of the continuous-energy cross sections (Leppänen et al., 2012). TMS has been implemented in Serpent in the recent past (Viitanen and Leppänen, 2012a,b). As of now, unresolved resonances and bound-atom scattering cannot yet be treated with TMS (Viitanen and Leppänen, 2012a, 2013) severely limiting the applicability of the method for nuclear engineering applications. An alternative method to treat the temperature dependence of nuclear data in case of thermal bound-atom scattering is discussed in Section 2.5.

In its original form the TMS method relies on 0 K continuous energy cross sections and does not require a Doppler Broadening Rejection Correction (DBRC) (Viitanen and Leppänen, 2012a; Becker et al., 2009). One measure to improve the numerical performance of TMS in Serpent is to use a basis library of continuous-energy cross sections for temperatures higher than absolute zero (Viitanen and Leppänen, 2013). However, in the latter case, one has to apply DBRC again. Unfortunately, up to now, the TMS implementation in Serpent 2 is incompatible with DBRC. In this paper, basis libraries of continuous-energy cross sections for temperatures higher than absolute zero are employed for reasons of computational efficiency but no resonance upscattering is considered.

2.2. Sub-channel code SUBCHANFLOW

The sub-channel code SUBCHANFLOW solves three mixture balance equations for mass, momentum and energy in axial direction as well as an additional lateral momentum equation at sub-channel or fuel assembly level (Sanchez et al., 2010). A fully implicit method is used to solve steady-state and transient problems. Three kinds of solvers are available: a direct Gauss elimination solver for small problems, a SOR and a BiCGStab iterative solver. Because of its solution method, SUBCHANFLOW is restricted only to sub-channel upward flow.

For water material properties and state functions, the IAPWS-IF97 formulations have been adopted (Cooper et al., 2007). The heat conduction in a fuel pin is solved with a standard finite volume method. The heat transfer coefficient between fuel pin and reactor coolant is determined by using empirical correlations