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Coupling of system thermal–hydraulics and Monte-Carlo code: Convergence criteria and quantification of correlation between statistical uncertainty and coupled error

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ABSTRACT

Coupled multi-physics approach plays an important role in improving computational accuracy. Compared with deterministic neutronics codes, Monte Carlo codes have the advantage of a higher resolution level. In the present paper, a three-dimensional continuous-energy Monte Carlo reactor physics burnup calculation code, Serpent, is coupled with a thermal–hydraulics safety analysis code, RELAP5. The coupled Serpent/RELAP5 code capability is demonstrated by the improved axial power distribution of UO_2 and MOX single assembly models, based on the OECD-NEA/NRC PWR MOX/UO_2 Core Transient Benchmark.

Comparisons of calculation results using the coupled code with those from the deterministic methods, specifically heterogeneous multi-group transport code DeCART, show that the coupling produces more precise results. A new convergence criterion for the coupled simulation is developed based on the statistical uncertainty in power distribution in the Monte Carlo code, rather than ad-hoc criteria used in previous research. The new convergence criterion is shown to be more rigorous, equally convenient to use but requiring a few more coupling steps to converge. Finally, the influence of Monte Carlo statistical uncertainty on the coupled error of power and thermal–hydraulics parameters is quantified. The results are presented such that they can be used to find the statistical uncertainty to use in Monte Carlo in order to achieve a desired precision in coupled simulation.

1. Introduction

Modern nuclear system simulations emphasize improvements of computational accuracy. One of the directions to achieve this is to use coupled multi-physics approach with high fidelity simulators. The term 'multi-physics' means the requirements of coupling of discrete physics. Coupled systems that integrate relevant phenomena in reactor systems such as neutronics, thermal–hydraulics, chemical and structural mechanics are need to greatly improve design, operation and safety methodologies of modern reactors.

Both deterministic and Monte Carlo neutronics codes have been coupled with system, sub-channel or Computational Fluid Dynamics (CFD) codes for thermal–hydraulics feedback. With the ability to use highly accurate continuous-energy cross-section libraries, as well as simulating detailed geometries without significant spatial approximations, Monte Carlo codes are gaining in popularity over deterministic methods. The coupling of Monte-Carlo (MC) and reactor thermal–hydraulics (TH) significantly improves the MC predictive capability and its applicability to a wider range of reactor problems of practical interest, as right now it is limited to fixed-feedback conditions.

Coupled simulation using MCNP/Fluent (Hu and Uddin, 2008) and MCNP/STAR-CCM+ (Cardoni, 2011) are carried out at University of Illinois to provide a high fidelity multi-physics simulation tools for analysis of the steady-state Pressurized Water Reactor (PWR) core. Many other coupled Monte Carlo neutronics/thermal–hydraulics systems were developed to solve various problems. Seker et al. (2007) used coupled MCNP5/STAR-CD to simulate a 3-D 3 by 3 array of PWR fuel pins. Examples of Monte Carlo coupled with sub-channel codes are MCNP/COBRA-TF (Sanchez and Al-Hamry, 2009) and MCNP5/SUBCHANFLOW (Ivanov et al., 2011, 2013). Both systems are used to predict the pin-power distribution of a PWR fuel assembly. The later was also used for a hexagonal fuel assembly consisting of 271 pins of SCFR (Steam Cooled Fast Reactor) fuel pin clusters. A relaxation method was adopted in the above two coupled systems iteration to speed-up the convergence. Another example of innovative reactors simulated by coupled Monte Carlo and sub-channel codes is the work

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by Vazquez et al. (2012). Coupled MCNPX/COBRA-IV system was successfully applied to a fuel assembly of a SFR (sodium-cooled fast) at sub-channel scale and a full SFR core at channel scale. Monte Carlo based BGCore system is developed at Ben-Gurion University that couples Monte Carlo transport code MCNP and a burnup and decay module SARAF (Kotlyar et al., 2011). A TH module feedback is implemented into this system for a full PWR core analysis.

In general, most of the coupling systems share some common features. Ivanov and Maria (2007) summarized the challenges in coupled thermal–hydraulics and neutronics simulations for LWR safety analysis. If Monte Carlo methods are involved, issues like temperature dependency of nuclear data have to be taken care of. The most obvious differences between different MC/TH coupling systems are (a) the way they deal with the temperature dependency of nuclear data, and (b) convergence criteria for the coupled simulation. Researchers used different convergence criteria, but all of the coupling systems converge fast, usually in less than 10 coupling steps. The results such as temperature and power distribution show good agreement with other codes used for verification purpose. The most obvious drawback of MC/TH coupling is that the computational time is still very long.

The present paper tested the capability of Serpent to be coupled with thermal–hydraulics code RELAP5. In Section 2, a brief overview of the codes used in this paper is presented. Section 3 describes the details of the models used in this paper. The aim of Section 4 is to present the coupling methodology. Moreover, a new convergence criterion based on the statistical uncertainty of power distribution in Monte Carlo code is introduced. The convergence criterion has been tested on both UO_2 and MOX single assemblies. Based on an earlier conference paper (Wu and Kozlowski, 2014), the present paper further compared the convergence criterion with previously proposed convergence criteria based on temperature, eigenvalue or flux (or power). Finally, in Section 5, the results are shown for coupled simulation for UO_2 and MOX single fuel assemblies. The results are compared with reference results from DeCART code. At the end of Section 5 results are presented for the quantification of the correlation between Monte Carlo statistical uncertainty and coupled error of power and thermal–hydraulics parameters such as fuel temperature and coolant mass density.

2. Overview of the codes

A three-dimensional continuous-energy Monte Carlo reactor physics code, Serpent, has been coupled with thermal–hydraulics safety analysis code RELAP5. The coupling results are compared with a deterministic heterogeneous multi-group transport code DeCART. DeCART has an internal thermal–hydraulics feedback solution.

2.1. Monte Carlo code Serpent

Serpent is a three-dimensional continuous-energy Monte Carlo reactor physics burnup calculation code (Leppänen, 2007 and Leppänen, 2012), developed at VTT Technical Research Centre of Finland since 2004. It is specifically designed for reactor physics calculations, particularly at the fuel pin, assembly or core level. The code is best suited for two-dimensional infinite-lattice physics calculations. However, modelling of complicated three-dimensional geometries is also possible.

The Serpent code simulates neutron transport in the geometry based on a combination of conventional surface-to-surface ray-tracing and the Woodcock delta-tracking method (Leppänen, 2010). Woodcock delta-tracking method differs significantly from the ray-tracing methods used by most of the other neutronics codes. The advantages of the delta-tracking method include reduced computing time and relatively simple handling of complex geometrical objects. Neutron interaction data used by Serpent is read from continuous-energy ACE format data libraries. The code version used for coupling is Serpent 1.1.18.

2.2. Thermal–hydraulics code RELAP5

RELAP5 (Reactor Excursion and Leak Analysis Program) is developed by the U.S. Nuclear Regulatory Commission (NRC) (The RELAP5 Development Team, 2010). The code is intended for the best-estimate analysis of operational transients and postulated accidents in water-cooled nuclear power plants and related systems. It solves one-dimension two-phase two-fluid model, with very broad constitutive relation package, applicable to LWR in operating and accident conditions. The code version used for coupling is RELAP5/MODE3.3.

2.3. Whole core transport code DeCART

DeCART (Deterministic Core Analysis based on Ray Tracing) (Joo et al., 2004 and Kochunas et al., 2009) is a three-dimensional whole-core neutron transport code capable of PWR and BWR (Boiling Water Reactor) core simulation. The code can solve steady-state eigenvalue problem, as well as transient fixed source problem. Method of Characteristic (MOC) is used to deal with the heterogeneity at the pin cell level. DeCART obtains multi-group cross-section data from a cross-section library normally used in lattice transport codes.

DeCART incorporates both the neutronics and thermal–hydraulics solution modules, as well as an iterative solution logic controlling the alternate execution of the two modules and the subsequent cross-section update. DeCART takes into account both the Doppler and coolant number density effects in order to incorporate the thermal feedback effect. That is the reason why DeCART is chosen for the validation of the coupled Serpent/RELAP5. The code version used in this paper is DeCART v2.05.

3. Benchmark problem

The UO_2 and MOX single assembly models are based on the OECD/NEA and U.S. NRC PWR MOX/UO_2 Core Transient Benchmark (Kozlowski et al., 2003). This benchmark is a well-defined problem that provides the framework to assess the ability of modern reactor kinetic codes to predict the steady-state and transient response of a core partially loaded with weapons-grade MOX fuel.

3.1. Single assemblies description

The assemblies are based on 17×17 Westinghouse design. Each assembly has 264 fuel pins and 25 guide tubes. Moreover, MOX assembly uses fuel rods with three different Pu enrichment. Two modifications are made to the UO_2 and MOX single assembly models relative to the benchmark specifications. First, the Integral Fuel Burnable Absorber (IFBA) and Wet Annular Burnable Absorbers (WABA) pins are abandoned to simplify the assemblies. Second, gap in the fuel rod is removed and replaced with fuel, so the UO_2 and MOX fuel pellet is surrounded only by clad material. Axial reflector is added at the top and bottom of the single assemblies with thickness of 30 cm. The single assembly configurations are shown in Fig. 1.