Multi-physics Coupling Scheme in the Serpent 2 Monte Carlo Code

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INTRODUCTION

The computational modeling of an operating nuclear reactor is a challenging task, which requires detailed solutions for fundamental physical problems at several levels: 1) neutron transport process and fission heat production and deposition in the fuel, 2) heat transfer from fuel to coolant and 3) coolant flow and final heat removal from the system. The fact that each partial solution produces source terms for the next stage, together with the strong feedbacks between fission power, fuel temperature and coolant density, imply that the different parts cannot be separated from each other. Instead, the problem requires a coupled, iterative solution, and applications dealing with coupled neutronics / thermal hydraulics calculations are often categorized under term "multi-physics".

The advances in computer capacity and parallel computing have made it possible to use computing-intensive state-of-the-art methods for large scale problems and realistic reactor geometries. By looking at the number of recent scientific publications related to nuclear multi-physics applications, it is easy to see that the coupling of Monte Carlo neutronics to CFD and thermal hydraulics codes is becoming an increasingly important research topic in the field. This topic is also included in the near-term development plan for the Serpent Monte Carlo code[a] at VTT Technical Research Centre of Finland, and the project was recently granted a major research fund specifically for this purpose.

This paper brings together the methodologies developed and planned for the multi-physics coupling of the Serpent 2 code. The work is still in progress, and so far mainly focused on the built-in methods needed for passing the thermal hydraulics solution into the Monte Carlo neutron transport simulation.

COUPLING SCHEME IN SERPENT 2

Serpent 1 continuous-energy Monte Carlo reactor physics code is currently used in 73 organizations and 27 countries around the world. Serpent 2 is the development version of the code, and the main platform for developing new features. One of the main features under development is multi-physics coupling to thermal hydraulics and fuel performance codes, which is handled at two levels:

1. Internal temperature feedback module that solves heat transfer inside fuel pins.

2. External coupling to a thermal hydraulics solver via a universal multi-physics interface.

The coupling and the internal temperature feedback module take advantage of built-in capabilities for handling continuous temperature and density distributions inside material regions. These methods are briefly introduced below, before going into the actual coupling scheme. The flow chart for the coupling scheme is presented in Fig. 1.

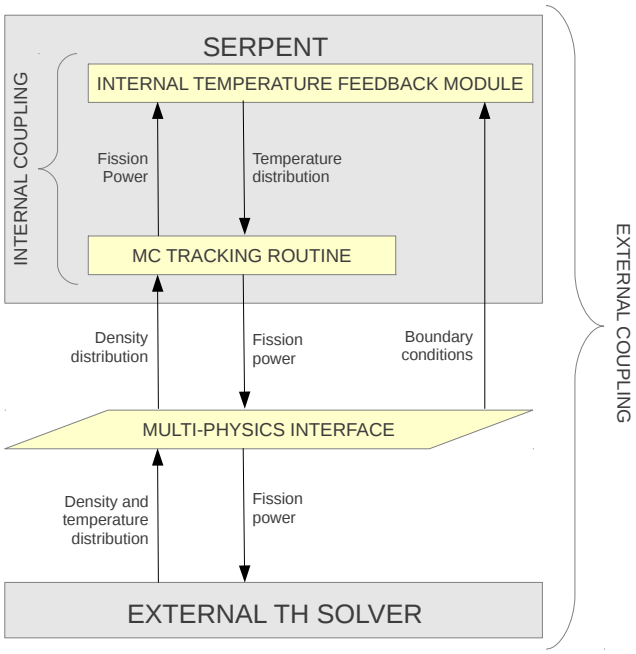

Fig. 1. Multi-physics coupling scheme in Serpent 2.

Continuous Temperature and Density Distributions

Geometry models in Monte Carlo particle transport codes are constructed of homogeneous cells, defined using elementary and derived surface types. In order to account for spatial distributions for material temperature or density – the solutions of a thermal hydraulics calculation – these cells must be divided into a number of sub-regions, each assigned with a different homogeneous material composition. This type of approach requires a somewhat rigid coupling between the two codes, in which the thermal hydraulics solution is essentially written in the form of Monte Carlo geometry input.

One of the main motivations for implementing temperature and density distributions in Serpent 2 is to decouple the thermal hydraulics solution from the actual geometry model. The distributions can be provided in a separate file, without any modifications in the main input, which considerably simplifies the interface between the two codes. The second reason is the possibility of representing temperatures and densities as actual continuous distributions, which brings them much closer to the thermal hydraulics solution.

The capability to treat these distributions as continuous functions of the spatial coordinates is based on rejection sampling performed on the particle path lengths. The procedure is very similar to the Woodcock delta-tracking method [1], which is a geometry tracking routine used for extending particle path lengths over one or several material boundaries, without calculating the distances to the boundary surfaces. In this case, however, the tracking is not performed between cells, but inside bounded material regions, and rejection sampling is needed to account for the fact that the total interaction probability changes along the particle path.

The temperature treatment routine is based on the use of zero-Kelvin cross sections and explicit treatment of target motion. When a collision occurs, the velocity of the target nucleus is sampled from a Maxwellian distribution, and coordinate transformation is made in the target-at-rest frame. Interaction physics is handled using the 0K data, and in the case of scattering, the emitted neutrons are transfered back to the original frame of reference. The fact that total interaction probability becomes a distributed quantity is handled by rejection sampling, as described above.

The method allows the on-the-fly modeling of non-uniform temperature distributions, which is essential for the internal temperature feedback module described below. There is no need to store cross sections at several temperatures, which significantly reduces the memory requirements compared to methods based on tabular interpolation. Currently the method works for isotopic continuous-energy cross sections, and work is on the way for extending the procedure to unresolved resonance probability table sampling and $S(\alpha,\beta)$ thermal scattering data. Theoretical background and the details of the method, including its limitations, are discussed in Refs. [2] and [3].

The capability to model continuous density distributions relies on a very similar rejection sampling based approach, but instead of acting on microscopic cross sections via thermal motion, the total interaction probability is affected by heat expansion or boiling, which reduces the macroscopic cross sections of the materials. The main application for the method is the modeling of density and void distributions inside the coolant channels of fuel assemblies [4], which is essential for coupling the external thermal hydraulics solution to the Monte Carlo calculation.

These two recently implemented capabilities form the basis of the two-stage multi-physics coupling scheme, as described in the following.

Stage 1: Internal Temperature Feedback Module

The solution of temperature distributions inside fuel pins can effectively be separated from the solution of coolant flow by the use of appropriate boundary conditions at the cladding-coolant interface. What is needed for the solution is the source term, which is given by the Monte Carlo transport simulation, and the models and parameters for the heat transfer correlations. Currently the work is focused on 2D fuel pins, consisting of nested annular material regions [5].

The temperature distribution in the fuel pins is solved separately in each region of the pin, starting from the outermost region, by demanding that the surface heat flux in the pellet is continuous and assuming a steady state of heat conduction. The heat conductivities for each material zone are obtained either from state-of-the-art correlations or as user input. Heat transfer in the gas gap is handled using a model similar to that proposed by Ross and Stoute [6], which has been modified to make use of Serpent's internal thermodynamical model. The thermomechanical changes in the fuel rod geometry are taken in account by correlations for fuel and cladding thermal expansion.

The solution of the heat transfer calculation – the temperature profile inside each fuel pin – is passed on to the built-in on-the-fly temperature treatment routine, which is used in the Monte Carlo neutron transport simulation. The procedure is carried out separately for each criticality source cycle, and the power distribution from the previous cycle is used as the source term for the next temperature calculation. The result is an iteration between the two solutions, which essentially describes the Doppler-feedback between fuel temperature and fission power. Everything is done within a single transport simulation without outer iterations.

Stage 2: Multi-physics Interface

Unlike heat transfer in fuel, the modeling of coolant flow is considered too complicated to be handled by an internal module. The solution is instead based on external coupling to a thermal hydraulics code via a multi-physics interface that takes on the following main functions:

1. Passing coolant density distributions from the thermal hydraulics solver to the Monte Carlo simulation.

2. Passing fuel temperature distributions or boundary conditions from the thermal hydraulics solver to the Monte Carlo simulation or the internal temperature feedback module.

3. Passing fission power distribution from the Monte Carlo simulation back to the thermal hydraulics solver.

The density distribution is applied directly in the Monte Carlo transport simulation, using the method described above. Temperature data can be applied either directly, or used as boundary conditions for the built-in solver. The interface is designed to be as versatile as possible, without considering any particular code-to-code coupling. Some of the data format options are introduced in Ref. [4].

CURRENT STATUS AND EXAMPLE RESULTS

The work for developing the multi-physics coupling capability in Serpent 2 is still in progress, and the scheme is missing some features that are crucial for performing calculations that are coupled in both directions, most importantly the output format for passing power distributions back to the thermal hydraulics solver. For this reason, all test calculations performed so far have focused on the newly implemented features: the on-the-fly temperature treatment routine [3], the capability to model continuous density distributions [4], and the internal temperature feedback module [5].

Figure 2. shows, as an example, results produced by the internal temperature feedback module. The calculation case is a two-dimensional 10×10 BWR fuel assembly with 10 burnable absorber pins. Average linear power is set to 300 W/cm, and coolant void fraction to 40%. The figure shows the pin-wise volume averaged temperatures in the assembly, when the boundary condition (cladding outer temperature) is fixed to 500 K. The difference between the hottest and the coldest pin is almost 400 K, and the differences in reactivity and local reaction rates become significant when compared to a calculation in which all fuel pins are assumed to be at a constant average temperature.

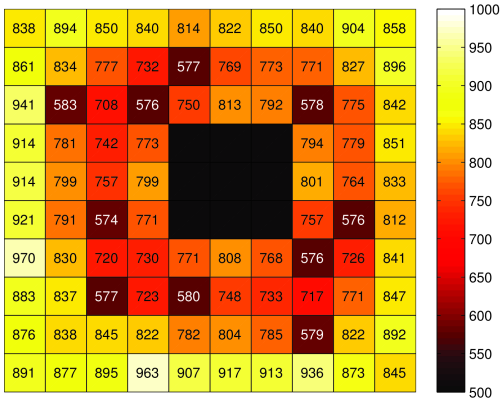

Fig. 2. Pin-wise temperature distribution (in K) in a BWR fuel assembly, produced by the internal temperature feedback module in Serpent 2. Burnable absorber pins, shown in dark red, are 300 - 400 K colder than the assembly average.

In addition to completing the multi-physics interface by coupling the power distributions to the thermal hydraulics calculation, other topics for future studies include implementing an unstructured mesh type interface for coupling with CFD codes. Photon and coupled neutron/photon transport simulation, which is another new feature currently under development for Serpent 2, will enable the modeling of direct heat deposition in the coolant channel. The code is currently in a beta-testing phase and public distribution is scheduled for 2013-2014.

ACKNOWLEDGMENTS

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ENDNOTES

[a]For a complete and up-to-date description of the Serpent code, see website: http://montecarlo.vtt.fi

REFERENCES

1. E. R. WOODCOCK et al., “Techniques Used in the GEM Code for Monte Carlo Neutronics Calculations in Reactors and Other Systems of Complex Geometry,” ANL-7050, Argonne National Laboratory (1965).

2. T. VIITANEN and J. LEPPÄNEN, “Explicit Treatment of Thermal Motion in Continuous-energy Monte Carlo Tracking Routines,” *Nucl. Sci. Eng.*, **171**, 165-173 (2012).

3. T. VIITANEN and J. LEPPÄNEN, “Explicit Temperature Treatment in Monte Carlo Neutron Tracking Routines – First Results,” *Proc. PHYSOR 2012*, Knoxville, TN, April 15-20, 2012.

4. J. LEPPÄNEN, “Modeling of Non-uniform Density Distributions in the Serpent 2 Monte Carlo Code,” article submitted to *Nucl. Sci. Eng.*

5. V. VALTAVIRTA, “Designing and Implementing a Temperature Solver Routine for Serpent,” M.Sc. Thesis, Aalto University (2012).

6. A. M. ROSS and R. L. STOUTE, “Heat Transfer Coefficient Between UO2 and Zircaloy-2,” AECL-1552, Atomic Energy of Canada, Ltd. (1962).