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The Numerical Multi-Physics project (NUMPS) at VTT Technical Research Centre of Finland

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ABSTRACT

The four-year Numerical Multi-Physics (NUMPS) project funded by the Academy of Finland was initiated at VTT Technical Research Centre of Finland in September 2012, for the purpose of studying and developing high-fidelity computational methods for nuclear reactor analysis. The project is built around calculation codes developed at VTT, and it aims at the coupled three-dimensional modeling of neutronics, thermal hydraulics and fuel behavior of nuclear reactors. The work involves the continuous-energy Monte Carlo code Serpent and CFD code PORFLO, together with two light-weight solvers, COSY and FINIX, coupled to Serpent at source code level. This paper is a review on the current status and development activities, reflecting the status of the NUMPS project at the beginning of its second complete year.

1. Introduction

Development of calculation codes has been an important part of the nuclear safety related work carried out at VTT Technical Research Centre of Finland since the construction of the first Finnish nuclear power plants in Loviisa in the 1970s. The value of in-house code development is recognized and supported within the organization, and still considered one of the best means to maintain a high level of national competence in the nuclear field. The advances in calculation methods and computer capacity necessitates that, in order to keep up with the latest developments, the codes and methods developed at VTT need to be periodically revised. In addition to legacy codes, the work often involves initiating entirely new projects, which provides good opportunities for educating a new generation of experts, with not only a comprehensive knowledge on theory and methods, but also source-code level understanding of the calculation tools.

In recent years, there has been an increasing interest in the use of high-fidelity numerical methods in reactor analysis and the simulation of coupled problems encountered when modeling an operating nuclear reactor. The need for a capability to simulate neutronics, fuel behavior and fluid dynamics using state-of-the-art calculation tools has also been recognized at VTT, which lead to the initiation of the Numerical Multi-Physics (NUMPS) project in 2012. The project is funded for four years by the Academy of Finland, and in addition to the development of new modeling capabilities, the project has important educational goals as well. Of the six active members of the project staff, four are currently working on their doctoral theses on topics related to neutronics, fluid dynamics and fuel performance coupling.

The work carried out within the NUMPS project is mainly built around two calculation codes developed at VTT already before the initiation of the project: the Serpent Monte Carlo reactor physics code and the PORFLO CFD code. The coupling of the two codes is carried out by adapting the transport methods used in Serpent to be specifically suited for multi-physics applications, in practice, for the exchange of data via an interface based on an unstructured CFD mesh. In addition to the externally-coupled high-fidelity CFD solver, the NUMPS project also involves the development of an internal light-weight solver COSY, which is to be coupled to Serpent at the source code level. The applications often necessitate including fuel behavior in the coupled simulation, which is taken into account in the development of the multi-physics interface. This coupling also forms an important connection to another code development project at VTT, involving the FINIX fuel behavior model.

This paper is a review on the recent activities and current status of the VTT's NUMPS project in early 2014, at the beginning of its second complete year. The work carried out so far has been focused on each calculation code separately, and the codes and methods involved in the project are introduced in the following section.

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Even though the coupling between Serpent and PORFLO is yet to be accomplished, some significant work has already been carried out for the development of the multi-physics interface, with preliminary test calculations involving fuel performance codes and CFD calculations with OpenFOAM (OpenFOAM, 2014). The coupling scheme is described in Section 3, and some example results introduced in Section 4. The future directions of the project are discussed in Section 5. The FINIX code is covered more comprehensively in a paper by Ikonen et al. (2014), published in this multi-physics issue of Annals of Nuclear Energy.

2. Description of codes and methods

The multi-physics calculation scheme in the NUMPS project involves the external coupling of continuous-energy Monte Carlo code Serpent and the PORFLO CFD code, together with two light-weight solvers, COSY and FINIX, internally coupled to Serpent at source code level. The codes and solvers are introduced in the following.

2.1. Serpent

Serpent is a continuous-energy Monte Carlo code developed at VTT since 2004 for reactor physics applications, such as fuel depletion and spatial homogenization (Leppänen, 2007). The development of a new code version, Serpent 2, started in 2010, and a major part of the work is currently devoted to multi-physics applications. In the NUMPS project, Serpent 2 is used as the neutronics solver for the coupling scheme described in Section 3. The methods relevant for this coupling are briefly introduced below, and a more complete and up-to-date description of the code is found in Leppänen et al. (2013) and the Serpent website.[1]

The main challenge in the coupling of neutronics to thermal hydraulics and fuel performance calculations lies in the passing of state-point information into the transport simulation as local variation of temperature and density. For the Monte Carlo tracking routine this means that the macroscopic cross section changes along the sampled flight path, even though the material composition remains homogeneous. The changes in density caused by heat expansion or boiling are directly reflected in the macroscopic total cross section, while the temperature-induced changes in the relative motion between the neutron and the nuclides in the medium are seen in the effective (Doppler-broadened) microscopic cross sections. The result is that the corresponding interaction probabilities cannot be treated as constants, which affects the sampling of the neutron path length.

The traditional solution is to handle the distributions as part of the geometry model, and divide the material into a number of homogeneous sub-regions with different temperature and density. Instead of taking this conventional approach, the solution applied in Serpent 2 relies on a rejection sampling scheme, which has three major advantages:

(1) Since the material zones are not divided into separate sub-regions, the state-point information can be easily separated from the actual geometry model.
(2) Reaction cross sections are needed only at discrete collision sites for rejection sampling, which makes it possible to handle temperature and density distributions as continuous functions of the spatial coordinates.
(3) The rejection sampling based tracking algorithm moves the neutron directly to the next tentative collision site. For piece-wise homogeneous (mesh-based) distributions this means that computational performance is not strongly dependent on spatial resolution, as there is no need stop the track at each boundary surface.

The fact that the interaction probability can be allowed to change, even continuously, over the sampled path length results from the rejection algorithm, which replaces the space-dependent macroscopic total cross sections with a constant majorant. The procedure is described in Leppänen (2013b), where the method is applied for modeling continuously-varying coolant density distributions.

The rejection algorithm is very similar when applied to temperatures, but the effects of thermal motion on microscopic interaction probabilities makes the implementation more complicated in practice. For this purpose Serpent uses the Target Motion Sampling (TMS) temperature treatment technique, which handles the thermal motion of target nuclides explicitly for each collision.[2] The velocity of the target is sampled from a Maxwellian based distribution, followed by a coordinate transformation into the target-at-rest frame, in which the reaction probabilities are characterized by cross sections at zero Kelvin temperature. The fact that the interaction probabilities become distributed quantities is handled using the rejection sampling routine: the neutron path length is sampled using a majorant cross section, which takes into account the variation in relative energy within the range of thermal motion, and each collision is accepted or rejected according to the probability given by the ratio of the sampled target-at-rest cross section to the majorant. The method is currently limited to unbound nuclei outside the region of unresolved resonances.

The TMS method was first introduced in Viitanen and Leppänen (2012b) and the very first results reported at the PHYSOR 2012 conference (Viitanen and Leppänen, 2012a). The computational overhead of this preliminary implementation was more than a factor of two relative to a comparable reference calculation with Serpent 2. Considerable effort has since then been devoted to optimizing the routines (Viitanen and Leppänen, 2013b). Increasing the temperature of the basis cross sections above zero Kelvin (Viitanen and Leppänen, 2014a) and optimizing the generation of the majorant cross sections (Viitanen and Leppänen, 2014b) has lead to improved performance, and the computational overhead is no longer considered a major limitation for the TMS method.

Since it was anticipated that the added stochasticity due to the explicit sampling of thermal motion would increase the standard deviation of reaction rate tallies, the performance of the TMS method was also assessed using true performance indicators (Viitanen and Leppänen, 2013a). According to test calculations, the use of TMS has no significant impact on figures-of-merit when the reaction rate tallies are integrated over a wide energy range, which is typical for coupled multi-physics calculations.

Since the simulation of reactivity transients is an important part of reactor safety analyses, the multi-physics coupling scheme should be capable of modeling time-dependent neutronics. In Serpent 2 this capability is covered by a dynamic simulation mode (Leppänen, 2013a), which extends the conventional time-dependent external source simulation to super-critical reactivity excursions. The exponentially growing neutron population is managed by sequential population control, which makes it possible to handle simulations in which the initial source is multiplied by several orders of magnitude. The method is internally coupled to the

[1] http://montecarlo.vtt.fi.

[2] Functionally this technique serves the purpose of on-the-fly Doppler-broadening, but since no cross sections are actually Doppler-broadened during the transport simulation, the term temperature treatment technique is preferred in this context. It has been later learned that a method very similar to TMS in Serpent has been used for many years in Russian Monte Carlo transport code PRIZMA (Ogibin and Orlov, 1984).

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