ENS High Scientific Council – PhD Award 2024 – Extended Summary of the PhD Thesis Application of Boglárka Babcsány

Development of a finite-element-based reactor physics code system for the solution of the SP_3 approximation of the neutron transport equation

For the safe, reliable and economic operation of power reactors, the accurate determination of the core power distribution at all times is of paramount importance. To determine the core power distribution, reactor physics codes are used in the core monitoring system. These reactor physics codes are most often based on the diffusion transport approximation, since, in addition to their accuracy, high computational speed is desired for core monitoring purposes. However, the modelling of highly inhomogeneous core regions with significantly varying material composition or with high absorption cross section, i.e. those regions where the spatial gradient of the neutron flux is high, is a challenge for the diffusion approximation, which is a low-order transport approximation. However, the increasing material and geometric complexity of the new Generation III, III+ and IV reactor designs increasingly requires the use of reactor physics codes based on higher-order transport approximations for core design and monitoring purposes.

The SP_N, or simplified P_L method, which is based on the Legendre polynomial expansion of the angular neutron flux, allows higher order angular anisotropy of the neutron flux to be considered than in diffusion theory [1]. Furthermore, the mathematical form of the SP_N approximation as a second-order partial differential equation is analogue to that of the multi-group diffusion equations; hence, multi-group diffusion solvers can be easily further developed for their solution. Accordingly, the SP_3 transport approximation can describe up to third-order angular anisotropy of the neutron flux, and the corresponding equations can be solved using numerical solution algorithms optimised for multi-group diffusion calculations.

During my PhD studies, I started working on the development of SP_3-based reactor physics codes with potential use for core monitoring purposes. I carried out this research in close cooperation with the Reactor Physics Department of the Paks Nuclear Power Plant. The main objective of the multi-year collaboration was to enable their in-house reactor physics code C-PORCA to perform SP_3-based core computations in addition to its multi-group diffusion capabilities. As the C-PORCA code uses a hybrid finite element method to solve the multi-group diffusion equations, it was a straightforward choice to develop finite element methods to solve the multi-group SP_3 equations.

During my PhD research, I first developed and implemented a continuous Galerkin finite element method for solving the multi-group SP_3 equations [2]. One can model arbitrary core geometry and composition by applying the continuous Galerkin finite element method. However, it requires pre-generated finite element meshes for the solution process. I used the free open-source three-dimensional modelling software Gmsh to generate the finite element meshes. I verified the developed SP_3 solution method using analytical reference problems and one- to three-dimensional mathematical problems, including VVER reactor benchmark problems. I also participated in a comprehensive measurement and computational benchmark performed for the BME Training Reactor. As part of this analysis, I demonstrated that the developed continuous Galerkin finite-element-based SP_3 solution method can accurately model small, high-leakage, highly heterogeneous systems, such as the BME Training Reactor, by comparing SP_3 computational results with reference measurements and Monte Carlo transport solutions [3]. Using the continuous Galerkin finite-element-based SP_3 solution method, I have been able to provide reference SP_3 solutions for well-known VVER reactor benchmarks using high-resolution finite element meshes that were not previously solved using

the SP_3 method. Such calculation results can be effectively used to verify nodal numerical SP_3 solvers.

Besides, I further developed the hybrid finite element, multi-group diffusion solver of the C-PORCA code, applied by the Reactor Physics Department of the Paks Nuclear Power Plant, to solve the SP_3 equations [4-5]. The hybrid finite element method, being a nodal solution technique, leverages the fact that the space dependence of the neutron flux is less steep in the axial than in the radial direction. Accordingly, finite element mesh is only applied in the radial direction, while axially higher nodes (volumetric elements) can be allowed. Although such a solution algorithm is computationally more efficient, it limits the analysis of arbitrary core geometries compared to the continuous Galerkin finite element method. However, this is not a drawback in repeated core calculations performed for the same system, as typically needed in the frame of core monitoring. In such cases, minimizing computation speed is also essential, in addition to accuracy. I implemented the further developed hybrid finite element SP_3 solution algorithm as a supplementary module besides the continuous Galerkin finite-element-based solver in my code, SPNDYN and in the C-PORCA code applied by the Reactor Physics Department of the Paks Nuclear Power Plant. Similarly to the continuous Galerkin finite-element-based SP_3 solution method, I verified the solver using analytical and mathematical benchmark problems, considering also the high-resolution SP_3 reference solutions obtained with the continuous Galerkin finite-element-based SP_3 module of SPNDYN.

Core calculations performed with diffusion or SP_3 transport approximation necessitate a pre-generated group constant database that covers the potential core parameter space. This so-called parametrized group constant database is generated with the HELIOS lattice physics code based on the collision probabilities method for the C-PORCA calculations in the case of the Reactor Physics Department of the Paks Nuclear Power Plant by governing the core states that well-describe the potential operational states of the VVER-440 reactors. The HELIOS calculations do not need to be performed before each core calculation; group constants characterizing the actual operational state of the reactor are derived by substituting into previously fitted functions using the pre-generated and parametrized group constant database. However, HELIOS is a commercial code; hence, during my PhD research, I applied a free software, the Serpent 2 Monte Carlo code for group constant generation. Serpent 2 is also commonly used for group constant generation for diffusion codes. I modeled two-dimensional VVER-440 and VVER-1000 reactor problems using the Serpent 2 code based on detailed geometric and material composition data. For these problems, I performed Monte Carlo transport simulations to provide reference transport solutions and generate group constants for SP_3 calculations. In this research phase, I started to focus on examining the considerations that may apply to Serpent-generated group constants in higher-order transport approximations. I examined the accuracy of diffusion and SP_3 calculation results in the frame of the mentioned VVER reactor problems by comparing the obtained results to reference Serpent 2 solutions and by considering the limitations of the Serpent-generated group constants. I derived how to apply the so-called discontinuity factors, introduced initially to increase the accuracy of diffusion calculations, in the hybrid finite element SP_3 solution scheme, and showed that they are also necessary in the case of SP_3 core calculations if one would like to obtain more accurate SP_3 solutions compared to discontinuity-factor-enhanced diffusion calculations.

I showed that the approximate method of scalar flux weighting of higher-order anisotropic scattering matrices needed for higher-order transport calculations, which is also implemented in Serpent 2 instead of flux moment weighting, can result in significantly decreased accuracy of higher-order transport calculations [6]. Reliable codes for parametrized group constant generation – as the HELIOS code applied at the Paks Nuclear Power Plant – is a prerequisite

for using SP_3-based reactor physics codes for core monitoring purposes and also for the verified and validated application of the SP_3 module of the C-PORCA code for core design, verification and core monitoring purposes by the Reactor Physics Department of the Paks Nuclear Power Plant. My current research focuses on developing reliable SP_3 group constant generation methods, vital for future SP_3 core calculations.

I would like to emphasise that during my PhD studies and after obtaining the PhD degree, I have used the knowledge gained on reactor physics applications of finite element methods in education and talent management at the Budapest University of Technology and Economics. I have introduced the teaching of finite element methods as potential alternatives to finite difference and finite volume methods for solving the heat, diffusion and SP_3 equations in the courses Thermal Hydraulics of Nuclear Power Plants and Reactor Physics Calculations. Several of my students have participated in university- and national-level Scientific Student Associations' Conferences with excellent results and have been employed as reactor physicists at the Reactor Physics Department of the Paks Nuclear Power Plant. The SPNDYN code developed by me is currently being used to design a Supercritical Water Cooled Small Modular Reactor (SCW-SMR) concept in the framework of a Horizon 2020 project funded by the European Union (ECC-SMART). In the framework of the ECC-SMART project, the code was also coupled with the Apros thermal hydraulics system code. In addition, we also started investigating the accuracy of pin-level SP_3 core calculations with SPNDYN, besides the assembly-level calculations that have been performed so far. Regarding further developments of the SPNDYN code, I also plan to develop a burn-up module, as well as a quasi-static numerical scheme as an efficient alternative to the currently available finite difference time discretisation, which would be more suitable for long-term transient core calculations.

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