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Ph.D. Thesis: Methods for safety and stability analysis of nuclear systems

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The content of the thesis has led to the publication of 7 journal articles and 6 conference proceedings, provided in a separate file.

Introduction

The risk perception of nuclear power and, consequently, its public acceptability are probably the aspects that limited the most, during the last 40 years, the worldwide diffusion of nuclear power plants as an effective, reliable, and carbon-free electricity source. This aspect and some economic considerations motivated the development of innovative, safe-by-design reactor concepts, like Gen-III+ reactors and Gen-IV reactors.

With respect to Gen-III+ reactors, which can benefit from the design and operational experience coming from the LWRs fleet, Gen-IV reactors are mostly first-of-a-kind systems, with very limited design and operational experience. Their unique features and working principles introduced the need for more sophisticated modelling and computational techniques for both the design and the licensing phases. For example, the inherent multiphysics features of these reactors put a larger emphasis on the multiphysics simulations, and the presence of uncommon isotopes requires the quantification of the nuclear data uncertainties on the reactor macroscopic parameters. Hence, the successful deployment of these revolutionary concepts requires the development of new experiments, methods, tools, safety and construction standards.

It is clear that both the operation of Gen-III+ reactors and the design, licensing and construction of Gen-IV reactors entail a keen effort towards the adoption of state-of-the-art methodologies to perform thorough safety assessments. One possibility to accomplish this goal could lie in the integration of practices pertaining to safety analysis into the different aspects of the reactor design and operation, like neutronics, thermo-hydraulics, and fuel performance. Due to the vastness of these disciplines, this Ph.D. thesis focuses on the neutronic aspects and their role in safety studies.

Objectives

The considerations made previously highlight two current needs of reactor physics, namely:

- the necessity of new methods for the fast and accurate analysis of innovative Gen-IV systems, for incorporating safety aspects from the early stages of the design;
- the need for more efficient computational frameworks to support the core monitoring and, consequently, the safe and reliable operation of Gen-III/III+ systems.

Effectively addressing the above issues is extremely challenging from a practical point of view. Only a few among the several codes available for reactor analysis are accepted by the licensing authority, after having passed a complex set of qualification steps, which aims at ensuring the quality and reliability of the calculation tools. Modifying existing codes with state-of-the-art methods would be unpractical for operating reactors, while could be feasible for Gen-IV reactors. The time scale for the deployment of the Gen-IV reactors would probably be compatible with the qualification procedure needed for the extended codes, but the peculiarities of these systems may require too invasive modifications that could make this solution unworthy: new reactor concepts may also require new safety regulations, which may require new codes. Therefore, the development of new methods and codes is often the only possible approach for the deployment of these systems.

Hence, this thesis has the double objective of proposing new methods, mainly concerning the safety and stability analyses of nuclear reactors, and, at the same time, of extending available techniques to make them compliant with the industrial requirements and constraints discussed previously.

Discussion

The first part of the thesis, composed of chapters 2 through 5, is devoted to investigating and developing reactor physics methods for the criticality eigenvalue arising in the Neutron Transport Equation (NTE).

In chapter 2, the numerical framework based on the P_N and S_N multi-group models is presented, with the goal of solving the eigenvalue problem formulations arising in neutron transport, i.e. the multiplication eigenvalue k , the time eigenvalue α , the collision eigenvalue γ and the density/streaming eigenvalue δ . After the implementation and verification of the [TEST](#) (Transport Equation Solver In Turin) in-house Python package for the numerical solution of neutron transport eigenvalue problems with some benchmarks in the literature, some old-fashioned but still relevant questions are addressed. First, the equivalence between the odd P_N equation and the succeeding even order P_{N+1} is formally established. Then, the impact of the boundary conditions and the parity order on the angular convergence is assessed for the fundamental eigenvalues of the various formulations. These interesting features are then exploited to study the numerical acceleration of the eigenvalue sequences to the asymptotic values with the Wynn- ϵ scheme. The cases analysed in this work prove that the acceleration is very effective, yielding the same level of accuracy of discretisation-free Monte Carlo calculations. Moreover, this scheme seems a useful tool to estimate the various numerical errors affecting the non-accelerated values.

In chapter 3, the different eigenvalue formulations to the neutron transport equation available in the literature (k , α , γ and δ) are presented, discussing thoroughly their physical and mathematical peculiarities. Moreover, a novel eigenvalue, associated with the capture reaction, is introduced in this work for the first time (the θ eigenvalue). The chapter focuses mainly on the behaviour of the different eigenvalue spectra (i.e., the distribution of the eigenvalues on the complex plane) according to the spatial, angular, and energetic models employed for the numerical discretisation and to the degree of spatial heterogeneity. This analysis, led with the TEST code, highlighted the tight connection between the spectra and the approximation used to solve the NTE, and allowed drawing some practical conclusions for driving the eigenvalue solvers toward the fundamental eigenpair (i.e., the solution of practical interest) according to the spectral formulation employed. Finally, a possible application of the spectrum as a concise figure of merit for the optimal selection of the group boundaries for the group constant collapsing is suggested.

In chapter 4, the generation of multi-group neutron constants for time-dependent calculations, which is one of the current open issues in reactor physics, is addressed focusing on the flux energy spectrum used for the group collapsing. The use of the fundamental eigenfunctions associated with the eigenvalue formulations studied in chapter 3 is investigated as an alternative to the usual choice of the k -eigenvalue spectrum. Due to the problem complexity and the large number of parameters involved, the analysis is carried out by performing some numerical experiments for a simplified system, i.e. a homogeneous slab, for which the calculation of the various eigenfunctions is possible using the TEST code. The collapsed group data are then employed to solve some reference time-dependent problems. The analysis shows that the performances of each weighting eigenfunction strongly depends on the type of the reactivity insertion, the few-group grid, and the energy spectrum of the reactor. Nevertheless, in most cases, the k -eigenfunction, i.e. the one traditionally employed, is the one yielding the worst results, especially for strong off-critical systems. The best option for the energy collapsing seems to be the γ -energy spectrum, which causes a lower distortion of energy spectrum of the system compared to the other formulations.

In chapter 5, it is shown that any eigenvalue formulation to the NTE can be traced back to a generalised eigenvalue formulation, called ζ . This eigenvalue can be introduced for filtering specific regions of the phase

space. After discussing the main physical and mathematical aspects of this formulation, relevant engineering problems are evaluated using this new approach, by considering the main types of components encountered in the design of a reactor core, e.g., the fuel, the coolant, the moderator and the localised absorbers. These applications provide remarkable results, showing the efficiency and capability of this approach in the determination of all the possible critical configurations for a given off-critical system. Compared to the iterative calculation of k_{eff} carried out in the core-design process, ζ yields equivalent results but with a strong reduction of the computational effort. More importantly, the existence of one or more design solutions is related to one or more real and positive ζ eigenfunctions. This feature should facilitate rigorously assessing whether criticality can be attained or not acting on the selected nuclides, even in case of complex systems. The knowledge of all the possible criticality arrangements featuring a system is fundamental for safety studies involving the re-criticality phenomena. The ζ eigenvalue spectrum suggests that, in the absence of competing phenomena, only one positive solution may exist, associated with an eigenvalue separation that is large enough to ensure an efficient numerical convergence on the dominant one.

The second part of the thesis focuses on problems of industrial interest, concerning Gen-III+ and Gen-IV reactor concepts.

Chapter 6 proposes computationally efficient methods for the analysis of safety-critical, complex systems. Bearing in mind the constraints related to the industrial code qualification, this objective can be accomplished with Non-Intrusive Reduced-Order Models (NIROM). Such methods allow reducing the computational burden of the long-running calculations (i.e., those needed for the safety assessment) without any intervention on the reference codes, at the price of acceptable approximations. After an initially expensive training phase, carried out with the reference codes, the NIROMs require a fraction of the time needed by the high-fidelity codes. In this work a NIROM based on a Proper Orthogonal Decomposition (POD) and Radial Basis Function (RBF) techniques is presented and applied to different industrial applications to prove its effectiveness. The first case study focuses on Gen-III+ LWR cores. These large thermal reactors are endowed with heavy reflectors, which make them very sensitive to localised operational perturbations, e.g., density variations in the moderator. The adequate characterisation of the flux and power spatial effects induced by these disturbances would be computationally cumbersome with legacy codes, demanding a more efficient computational framework. The NIROM model developed for this application is featured by two steps. First, the perturbed group constants are approximated via a polynomial chaos expansion regression model, with an acceptable accuracy. Then, the POD-RBF model is trained to replace the expensive full-core diffusion calculations. Due to the spatial dependence of the input perturbations, some ad hoc strategies are proposed in the thesis and successfully applied in the reduced order model training phase. Finally, the bootstrap technique is employed to assess the quality of the meta-model approximations and to provide an estimation of the modelling error distribution.

Another application of the POD-RBF approach regarded the simulation of accidental neutronic scenarios featuring the Gen-IV ALFRED core design, triggered by the accidental insertion of a control rod in the initially critical core. Exploiting a set of training simulations computed with the FRENETIC nodal diffusion code, the POD-RBF NIROM can reproduce the responses of the reference FRENETIC calculations with a good accuracy on both the local and global spatial scales and for the whole-time interval of the simulation. Except for the off-line, expensive training phase, the POD-RBF model outperforms FRENETIC, computing the power density snapshots with a fraction of the time requested by the original code.

The last chapter is devoted to propagating the uncertainty from the raw nuclear data to the energy collapsed and spatially homogenised cross sections featuring the ALFRED core design. The epistemic uncertainty characterising the heavy isotopes of the MOX fuel used in ALFRED is propagated to the response of interest (i.e., the homogenised and condensed capture and fission cross sections) using the first-order sandwich rule, which combines the nuclear data covariances and the first-order sensitivities, evaluated in this case with the Generalised Perturbation Theory implemented in the Serpent 2 Monte Carlo code.

This study shows that the two most abundant isotopes, i.e. Pu-239 and U-238, are also the most relevant one from the point of view of the epistemic uncertainty. This work also suggests that an adequate number of low-energy groups is mandatory also if the system under analysis is featured by a fast spectrum. Finally, an assessment between the GPT and XGPT (eXtended GPT) methods is carried out, focusing on the impact of the energy grid resolution used for scoring the covariances and the sensitivities on the accuracy of the propagated uncertainty.