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Confronto fra le tecniche di soluzione dell'equazione del trasporto per reattori termici

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CONFRONTO FRA LE TECNICHE DI SOLUZIONE DELL'EQUAZIONE DEL TRASPORTO PER REATTORI TERMICI

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Sommario

The design of nuclear systems through the developments over many years has reached a certain performance level deemed to be satisfactory and subsequently very little innovation has been introduced in the computational procedures employed for the various simulations. The situation has changed recently, when the international scientific and technical community has started developing and upgrading of methods and computational tools for more performing high fidelity codes. Several undertakings are under way all over the world. Some of them are quite ambitious, with the objective to develop a full comprehensive computational tool to accurately describe the full multi-physics behaviour of the nuclear reactor, retaining its full geometrical and material detail. The present report summarizes the main aspects of the current state-of-the-art, with specific attention to the development of methods for neutron transport.

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Assessment of solution techniques for the neutron transport equation applied to thermal reactors

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Assessment of solution techniques for the neutron transport equation applied to thermal reactors

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1. Introduction

The design of nuclear systems through the developments over many years has reached a certain performance level deemed to be satisfactory and subsequently very little innovation has been introduced in the computational procedures employed for the various simulations. The computer codes used for the design of the past generation of reactors have thus remained mainly unchanged in the past twenty years. This is also motivated by the heavy load and procedures usually associated to the validation and qualification of the computational tools with reference to the licensing authorities.

In the latest years the situation has changed quite significantly. At first, the computational power has experienced an enormous increase, thus opening new possibilities in terms of complication and physical detail of problems that can be handled and of accuracy of the evaluations. An advance of the computation capabilities would greatly enhance the design capabilities, leading to better system performances and an improved economy. On the other hand, new nuclear systems (e.g., Generation IV) are under investigation, or, at least new components (e.g., fuels) are being proposed with specific features that may require ad hoc models and computational tools.

The international scientific and technical community is thus oriented to devote resources towards the development and upgrade of methods and computational tools for more performing high fidelity codes. A recent summer school held in Karlsruhe has been fully devoted to examine such issue in the various aspects, concerning neutronics, thermal-hydraulics and material science [1], with the participation of some of the best known specialists in such fields.

Several undertakings are under way all over the world. Some of them are quite ambitious, with the objective to develop a full comprehensive computational tool to accurately describe the full multi-physics behaviour of the nuclear reactor, retaining its full geometrical and material detail.

This report addresses some of the issues related to the neutronic behaviour, with particular regards to the illustration of the state-of-the-art situation as far as computational tools for water reactors is concerned. A critical description of the procedures currently employed is presented, highlighting the shortcomings and evidencing the possible improvements and the requirements in terms of mathematical physics and computational algorithms that are needed to obtain such objectives. The most challenging tasks concern the simulation of reactor transients.

An improved simulation capability in this field can greatly enhance the comprehension of intricate transient phenomena with a better design of the safety features of nuclear reactors.

The basic step in order to obtain the above mentioned multi-physics simulation goals is the assessment of numerical methods to obtain a high fidelity solution of the Boltzmann neutron equation. In the following, some aspects are outlined.

2. The neutronic analysis

The neutronic design of a reactor core requires the solution of the neutron transport equation, in order to determine the neutron density or, better, the neutron flux, from which the various reaction rates can be determined for the following computational steps involving thermal-hydraulic and material evaluations. The approach to the transport problem can be either deterministic or statistic. The statistical approach is implemented in the Monte Carlo codes. While these codes can reach a very detailed description of the geometrical and material complications in a nuclear system, the computational cost for design purposes, for which many parametrical evaluations are required in the engineering optimization process, seems to exclude their application for industrial applications. However, they play an essential role for some specific assessments (e.g., evaluations connected to new systems) and for validation-qualification purposes in conjunction to deterministic methods.

The design of the reactor requires to determine the conditions for a steady-state behaviour in terms of neutron population. This is the main task of the reactor physicist. Therefore, the neutron distribution has to be determined, together with an eigenvalue (criticality) of the transport equation in the case of a source-free problem, as typical for commercial reactors. The time-dependent analysis is required on different scales, for different engineering purposes:

1. Control design
2. Safety assessment
3. Burn-up
4. Transmutation and fuel-cycle

Each item indicated above is characterized by different time scales, which may lead to quite different computational approaches and numerical techniques. The scale needed for the safety analysis may span from the prompt neutron lifetime to the scale of the control and thermal-hydraulic feed-back processes, quite similarly to the scale of the control design. Since delayed neutron emissions and heat transfer phenomena are to be taken into account, the mathematical problem turns out to be stiff. On the other hand, the scale for the burn-up and transmutation analysis is much longer, involving much slower radioactive decay processes.

2.1 *The static simulation*

The classic approach to the static simulation involves a solution through different steps, associated to different spatial scales, namely, the pin level, the assembly level and the full reactor. This decoupling is motivated by the

computational impossibility to retain the full spatial and energy complication and deal with it in one single step. This technique is quite common in many engineering fields and it aims at trying to separate different physical phenomena, appearing at the different spatial scales. This procedure has been standardized in many high-performance computer packages [e.g., 2], which are widely employed by industries and research centres all over the world. The procedure can be synthesized as a homogenization process, aiming at reducing the energy and geometrical complication. Energy point-wise cross sections are available through existing libraries (ENDF, JEF). Cross sections in these libraries are physical quantities, associated to the properties of the nuclides.

The objective of the first step of the procedure is to reduce the energy detail, from many thousands to a much smaller number. Of course, this can be done only through an averaging procedure that takes into account the actual neutron field, typical of the system being considered. Therefore, the averaging process is carried out on the basis of a conservation of reaction rates, using as a weighting function the detailed energy (fine groups) neutron flux obtained by a transport calculation on a cell (spectrum calculation, generation of self-shielded data). A transport solution is needed, because transport effects are very important while considering a very high number of energy groups, while the geometrical configuration can be simplified supposing an infinite periodic lattice, thus highly simplifying the boundary conditions. In Fig. 1 a unit cell for a square-lattice water reactor configuration is presented.

It must be noted that homogenized cross sections turn out to be angle-dependent, as weighted on a direction neutron flux. That means that the homogenized medium has anisotropic properties. Various techniques have been developed to overcome this physical problem, which can however prove to be unsatisfactory. Further development is quite advisable, as recent works have proved [3].

Once the cell are homogenized, a transport calculation is carried out on the fuel bundle (see Fig. 2), with periodic boundary conditions. An homogenization is again performed, further reducing the number of groups (broad groups, typically 2 or 3). It is worth recalling the attention upon the fact that homogenized cross section are specific for the system being considered, they are not basic “physical” data.

The last step of the calculation is the full-core calculation, using the broad group data. This calculation can be performed by either diffusion modules or low-order transport methods in three space dimensions (such as low-order S_N [4] or SP_N [5, 6]). The spatial discretization scheme is adopted on a coarse-mesh scale, of the order of the fuel element, thus requires an appropriate nodal approach. It is worth calling the attention upon the consistency and robustness of such numerical methods [7]. Therefore, the final result includes the neutron distribution over the whole system and the corresponding multiplication (criticality) eigenvalue. Each step of the scheme tries to capture a specific physical feature.

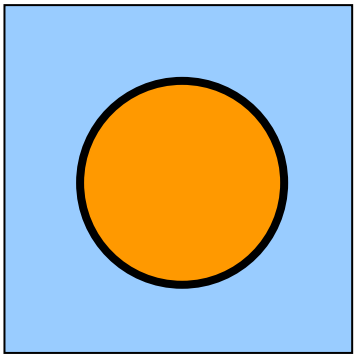

Fig. 1 – Sketch of a unit cell for a square-lattice water reactor.

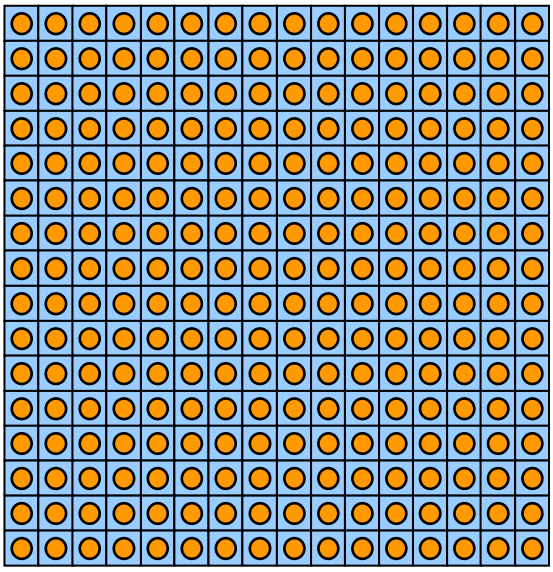

Fig. 2 – Sketch of a fuel bundle scheme for a water reactor.

The procedure described above has proved to be satisfactory for reactor engineering up to now. However, it is worth pointing out at some important shortcomings, which may prevent its applicability in the future and make advisable novel developments. In particular, the procedure is quite unsuitable for accurate multi-physics analyses. The detail of the energy deposition in each fuel pin is completely lost and appropriate schemes have to be set up to be able to reconstruct such information [8, 9, 10]. Moreover, certain important details of neutron asymmetries cannot be retrieved and properly described, specially for advanced thermal-hydraulics, material and fuel-cycle analyses [11].

With special regards to neutronics, new algorithms may be needed to obtain accurate enough results. To attain this goal, completely different simulation techniques may be necessary, such as the method of characteristics [12, 13] or the use of spectral elements [14].

The importance of reliable nuclear data is a very basic and relevant issue, since it would be useless to refine the methods to have highly accurate codes but not to have as accurate and reliable data. This fact should be considered attentively and it may require a great evaluation effort associated to rigorous experimental activities for both differential data (cross sections) and integral data, to be used in

adjustment procedures. In order to focus such work, sensitivity analyses should be carried out.

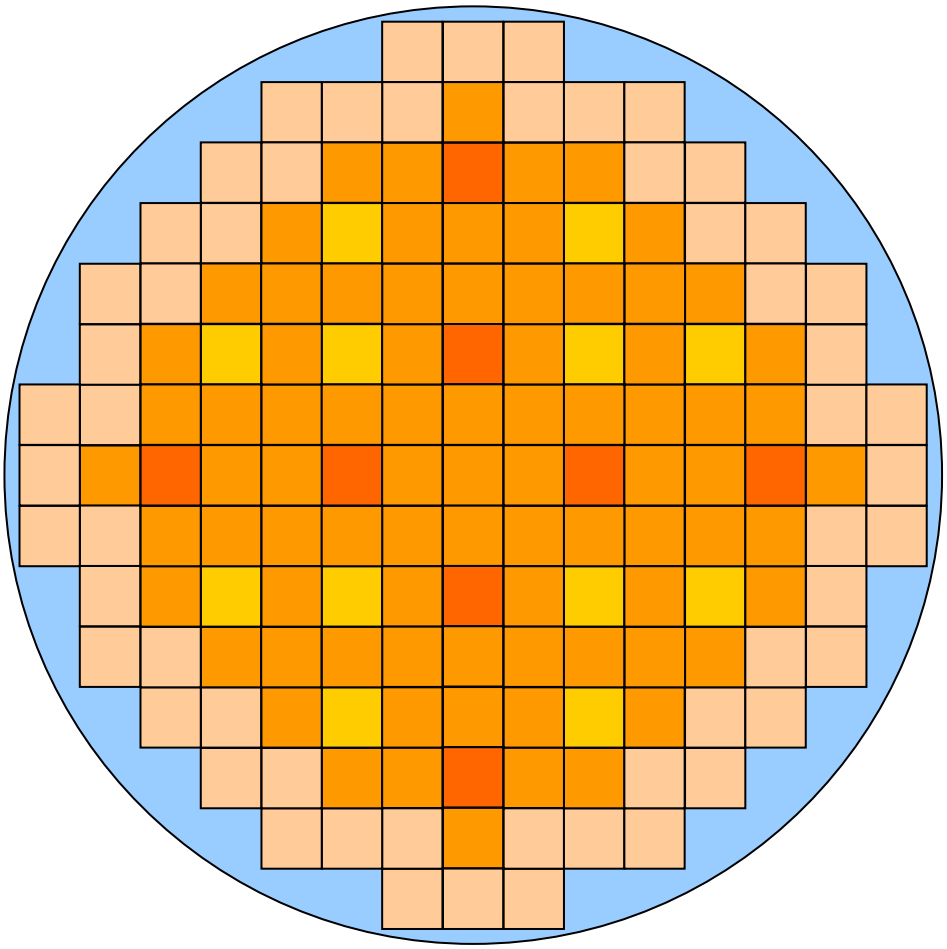

Fig. 3 – Schematics of full core geometry.

2.1 *The dynamic simulation*

The time-dependent simulation requires an efficient, robust and reliable solver for the time-dependent transport equation. Highly simplified, lumped-parameters codes are deemed inadequate for current needs. However, the short scale phenomena involved in the neutronic evolution within a nuclear reactor core demand for a high computational cost when a direct approach is used. However, direct approaches are considered in any case, even in association with multiphysic simulations [15].

As an alternative, the neutronic equations can be efficiently integrated by separation algorithms, which can lead to accurate results with a reasonable computational effort. In recent times, several improvements and enhancements have been proposed and investigated [16, 17]. It appears that these new techniques may be successfully applied for future high-performance dynamic codes, with multi-physics features. Some work is going on in the field of advanced fast reactor simulations [18], with the objective to develop a coupled neutronic-thermal-hydraulic solver for full system transient simulation, to be used for parametric and stability studies.

3. Best-estimate codes

The current status of dynamic, coupled neutronic-thermal-hydraulic full core simulations is based on two different, and somehow complementary, approaches, i.e. best-estimate codes and high-fidelity codes. This and the following sections present some general features of these codes, trying, in particular, to evidence their various aspects together with the need for future developments [19-22].

As already pointed out above, it is believed that spatial neutronics is needed, in conjunction with at least low-order transport approximations, since for many applications diffusion may prove to be inadequate. However, up to now the diffusion approximation in nodal formulation for the neutron balance is usually adopted, with discontinuity factors obtained from assembly calculations. In general, point kinetics is considered not to be reliable, since no spatial and spectral effects can be taken into account. Some improvements, involving the introduction of more degrees of freedom for the neutron distribution in phase space, may demonstrate to be useful in conjunction with quasi-static schemes [23].

As far as the spatial variable is concerned, a nodal coarse mesh approach is needed, to reduce the detail and to keep the computational cost at a reasonable level. Of course, that option requires proper and reliable homogenization techniques for cross sections and other nuclear parameters, starting from the original libraries.

For the energy variable, a small number of groups is to be foreseen, e.g., two groups can be enough for standard safety evaluations of water reactors in less-than-severe accident conditions. However, that may introduce some important physical shortcomings that should be attentively considered. In fact, a two group model for a thermal system does not allow to satisfactorily account for the different importance of delayed neutrons with respect to prompt neutrons. This fact may introduce unacceptable inaccuracies in the results [24]. It is recommended that this problem is taken into consideration and given an adequate solution.

All evaluations are given with a statistical evaluation of reliability of the results obtained, to have a reliable definition of the safety margin and possibly, to improve them. Examples of such codes are the TRACE/PARCS system [25].

There are pros and cons for these codes. A favourable aspect is the ability to predict asymmetrical modification, a feature that is not accessible for point kinetics based codes. Moreover, these are well-assessed codes, with well-established, embedded uncertainty analyses and have proven to provide good results in comparison to international benchmarks (OECD/NRC PWR Main Steam Line Break, OECD/NRC BWR Turbine Trip, OECD/NRC Oskarshamm 2 BWR Stability, …) [26]. On the contrary, the spatial resolution at the fuel assembly level may be not enough to obtain useful data for fuel performance evaluations and to detect important localized phenomena. Also, large distortions may be introduced by the spatial and energy collapsing that is needed to produce the input data. At last, if a detailed CFD resolution is required, this has to be coupled to a more refined neutronic evaluation, reaching a finer detail than the fuel assembly.

4. High-fidelity codes

It has been stressed in the previous section that there is a real necessity to move to simulation capabilities up to the pin level. This requires a big effort for a consistent refinement of the neutronic and thermal-hydraulic modelling. This leads to a class of high-fidelity multiphysics computational tools that are under development in this respect with a large effort in research. It is worth recalling the following programs:

- The EU supported projects NURESIM and NURISP in Europe [27];

- The establishments of the Consortium for Advanced Simulation of LWR's (CASL) in the USA [28].

Within the CASL undertaking, it is foreseen to develop computer models that simulate nuclear power plant operations, forming a "virtual reactor" for the predictive description of light water reactors, accelerating the deployment of the next-generation reactor system designs.

The characteristics (and "desiderata") for the neutronics of high-fidelity codes are the following:

- The spatial resolution should reach the pin level, or even be extended at sub-pin level, for the evaluations of interest in burn-up assessments, to estimate the spatial distribution of the production of Pu and higher actinides;

- A very large number of energy groups should be adopted, to reduce the inherent error associated to self-shielding and group collapsing procedures;

- All efforts should be made to replace the diffusion model with a higher-order transport approximation.

The possibility to use higher-order transport models for the neutron transport modelling is an important issue that may require a large interdisciplinary effort, involving numerics, reactor physicists and code developers. The P_n and S_n approximations are standard techniques which are well-assessed and little is hidden as far as their advantages and shortcomings are concerned. In particular, discrete ordinates are affected by ray-effects in multi-dimensional problems and it may be quite difficult to treat scattering with large anisotropy effects. Works carried out on angular finite element method may be able to overcome this problem [29]. On the other hand, the spherical harmonics P_n model is ray-effect free, while it may become rather complicated when used to high angular orders. The SP_n may be an adequate solution, although there are some important questions about its convergence to the effective transport solution.

In general, these codes require large CPU times for realistic configurations and, in any case, they still need a rather wide energy group discretization.

Monte Carlo can be used as reference solution for benchmarking purposes (but not as a standard tool for time-dependent problems). The validation-qualification process is mandatory and a very essential issue [30].

Various alternatives are being investigated. Different methods can be composed, such as a two-dimensional characteristics approach coupled with a one-dimensional diffusion or SP_n model. Also hybrid deterministic-stochastic methods are considered, in both space and energy domains. Deterministic methods can be envisaged in order to accelerate stochastic simulations, e.g. to obtain a converged fission source distribution for a Monte Carlo k_{eff} estimate or to determine information on the importance function in the framework of the contributon theory. An interesting and challenging topic that may turn out to be very important for such application is the domain decomposition technique [31, 32].

5. Conclusions and recommendations

As a conclusion of the review collection of information reported above, it is worth to gather some recommendations as itemized in the following, which, in the opinion of the authors, are deemed important in order to direct future research and development activities in the field of reactor physics and multi-physics simulation of nuclear systems:

- development of innovative high-performance transport solvers for core analysis with enhanced physical capabilities;
- development of dynamic simulators with multi-physics capabilities for advanced reactor description;
- participation to qualified benchmark activities, analytical, numerical and experimental;
- participation to international undertakings for the generation of updated and more reliable nuclear data libraries;
- development of experimental facilities for the validation of thermal-hydraulic models and multi-physics simulation tools;
- validation and qualification of numerical schemes and computational tools for reactor physics evaluations;
- participation to international experimental activities in the field of reactor physics and fuel studies.

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