



# Advances in the physics and thermohydraulics of nuclear reactors

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## 1 Introduction

The topics covered in this Focus Point collect ideas from many areas in nuclear reactor physics and simulations, ranging from some fundamental questions about the mathematical properties of the solution of the neutron transport equation to the final modelling of energy distribution inside an industrial scale nuclear reactor. They involved the most part of the Italian community working in the field, both on the academic and on the industrial sides, as well as international collaborators.

Historically, the physical description of a nuclear reactor breaks down into the development of a set of models for each of the occurring phenomena—the production of energy by nuclear fission, its transfer from a part of the system to the other, its extraction to be utilized—by means of appropriate different physical and engineering models and corresponding computational tools. This is because very different time (and energy) scales are in action, ranging from  $\sim 10^{-19}$  s for compound nuclear reactions to the order of seconds or more to transfer the energy from one zone of the system to the other, or even to years considering the fuel cycle: this is by far a too much extended range of times because, in practice, the evolution of the neutron population in a reactor happens over times somewhat larger or of the order of  $\sim 10^{-8}$  s, so that all nuclear reactions happening at shorter times are usually considered instantaneous. However, the time range to be considered remains rather wide.

The complete description of a real system has been usually obtained by iterating over the corresponding computational tools. So, to be very schematic, at first one makes use of the neutron linear transport equation—which could be derived from the Boltzmann one—to describe the neutron behaviour in the system on very short time scales, then of the equation of thermal hydraulics to describe how energy is distributed over the system, and finally of the Bateman's equations to describe fuel utilization (and waste production) over the time scale of the reactor industrial utilization. The iteration among these models and computational tools is a very complicated task, not only because of the technical difficulties, but even more because the dependencies among various parts of the problem are not trivial: so, for example, macroscopic cross sections required to transport neutrons over the shorter time scales depend

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both on the temperature distribution in the reactor and on the isotopic composition of fuel and other materials. The latter, on their side, depend on the energy production by fission and on the cumulative irradiation.

This Focus Point originated from a workshop held at the I.N.F.N. Genoa branch, hosted in the Physics Department of the University on 14–15 January 2019 as a conclusion of the project OCAPIE, which was supported by a grant from Compagnia di San Paolo, Turin, Italy. The project aimed at the development and test of innovative advanced computational techniques on high-performance computing (HPC) systems for the full simulation of nuclear systems.

The rapid evolution of computational performances over the last decades, both in terms of computational efficiency and in memory availability, has made it possible to develop a unitary description of the whole process. The OCAPIE project and conclusive workshop were namely motivated by the question on how to put together these different computational schemes into a coherent and unitary simulation effort by using the opportunities of modern high-performance computing systems. We did not consider the broader implications of our studies in terms of practical regulatory and industrial aspects, but there are certainly many.

## 2 Focus Point content

To illustrate the Focus Point, we introduce the papers presented by following a logical, based on topic, approach rather than a purely chronological one, which instead descends from random facts, e.g. the submission times or the time spent for refereeing. Therefore, we begin with a block of more general contributions, or, at least, less directly connected to a specific application context.

### 2.1 Mathematical models

A paper on some new thoughts about the boundary conditions which should be applied to the neutron linear transport equation [1] can then be the logical introduction to the Focus Point, even if this point is clearly not new, since it addresses a very basic point. However, some erroneous formulations of this question are still present in the literature.

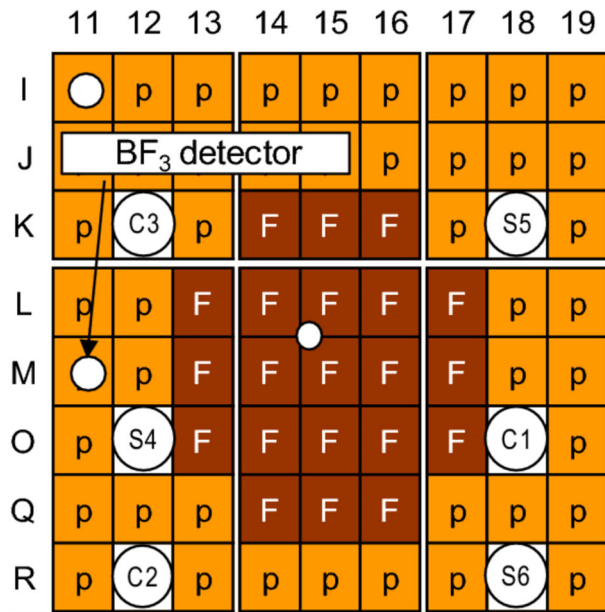
Another paper [2] examining how to qualify a sub-critical system using specific filtering techniques of experimental data is useful to introduce the fundamental distinction between a critical assembly (a reactor), which is in an unstable, but controllable, quasi steady-state, and a sub-critical facility (Fig. 1), which instead is kept stable by an external source of neutrons (some more papers concerning more specifically the design of such facilities are quoted in the last subsection). The second reason to cite here this paper is because it introduces also to the idea of effective models, in particular the widely employed reactor point kinetics.

Then, a re-visitation of neutron space asymptotic theories [3] is presented: such models are based on the idea that some conditions exist such that the space and energy distributions of the neutron population factorize; these methods can provide a deep physical insight into the basics of reactor physics and may still give new ideas for modern computational methods.

A paper follows aiming to enhance diffusion theory by systematic evaluation of correction factors to be used in a multi-group diffusion scheme, where the factors are actually given by the integral transport equation. The corrected solutions are compared against reference results from a discrete ordinate code [4].

A more “fundamental” approach—based on the true stochastic nature of power generation in a reactor core—describes neutron kinetics as a time stochastic process: “reactor noise”—

**Fig. 1** Kyoto University Critical Assembly in a subcritical configuration



Description of subcritical core with 14 MeV neutrons at KUCA

consisting of stochastic fluctuations of the power around the mean field (which is given by the deterministic models)—becomes then the basic topic for nuclear engineering [5]. However, stochastic models have well-known stability problems in that even if the mean field solution is stable, its variance grows linearly in time; this feature is not observed in real measurements and a conjecture is examined assuming that reactivity feedback provides the necessary stabilization mechanism.

## 2.2 Multiphysics simulation tools

The benchmark of a deterministic code (SEnTri/PARTISN) against a Monte Carlo time-dependent simulation (GUARDYAN) has been developed for the Training Reactor of the Budapest University of Technology and Economics: it is a pool-type research reactor giving a maximum thermal power of 100 kW, sufficient to give rise to a (small) thermal feedback [6].

A series of contributions present multiphysics simulation tools and applications. The first concerns molten salt reactors (MSRs): these systems have a unique feature, the presence of nuclear fuel in the form of a molten fluoride or chloride salt containing the fissile and fertile materials. The possible development of inert gas bubbles inside such fluid cores can have an impact on the reactivity. To approach this problem, a model coupling computational fluid dynamics for fluid flow and heat transfer with neutron diffusion equation for neutronics and a balance equation with diffusion and advection terms for taking into account the drift of the delayed neutron precursors has been developed [7].

A computer code for lead fast reactors (LFRs)—a GenIV kind of reactors cooled by liquid lead, characterized by hard (or fast) neutron spectrum—coupled neutron and thermal-hydraulic simulation [8] has been developed at Politecnico di Torino: a consistent comparison between the FRENETIC code results and the reference ones obtained in Serpent/OpenFOAM

is presented for the full core simulation of the ALFRED demonstrator (Fig. 2). This should be the first EU industrial-scale demonstrator of such facilities.

The last contribution pertaining to this subsection is the description of a very ambitious project [9] (and an erratum in [10]). The coupling of neutronic, thermal-hydraulic and fuel cycle analyses within a multiphysics model is again developed in Serpent and OpenFOAM: due to the complexity of the calculation, it is limited to considering a single fuel pin surrounded by water; this simulation cannot be presently carried out for a full-scale system, which will be the topic for the next set of contributions.

### 2.3 Industrial-scale systems

In [11], the simulation of the industrial full-scale European LFR demonstrator ALFRED is addressed within a new multiphysics model developed by coupling Serpent and OpenFOAM, which are well-assessed Monte Carlo simulation and thermal-hydraulic analysis codes. This approach by one side maintains the computational advantages of two computational tools specifically designed for each of the tasks, while, on the other, it fully exploits the possibilities of HPC.

The same topic is addressed also in [12], but with more emphasis on the HPC features of the simulation, in particular analysing the scaling properties of the computation on a farm of Intel XEON-Phi processors. The proposed model focuses on the adoption of spatially non-uniform temperature distributions of materials to compute better on-the-fly estimations of nuclide cross sections and thence a more accurate neutron physics description.

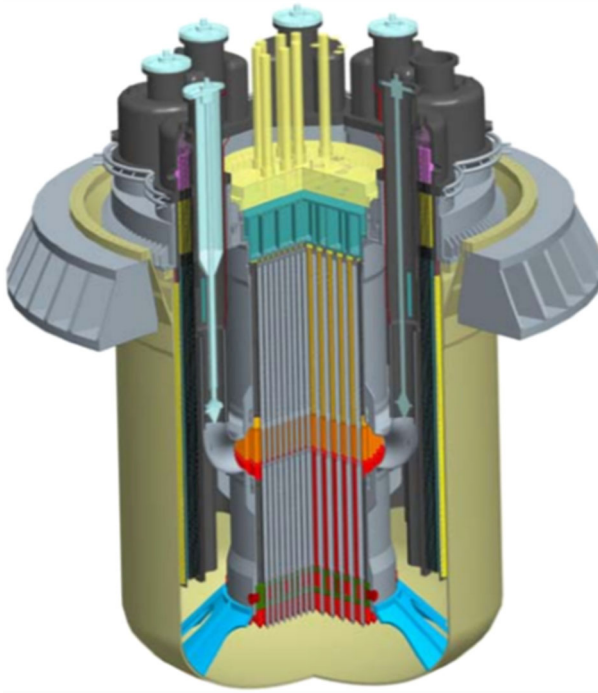
Another paper [13] addresses the coupling of neutronic and thermal-hydraulic simulations, but relying on the well-assessed industrial code Relap5, to describe the time transient following an accidental condition for a 1200 MW<sub>e</sub> pressurized commercial reactor: in this case, the full plant is simulated, within a one-dimensional model, including all the major primary, secondary and safety systems included in advanced PWR designs, upgraded with a three-dimensional thermal-hydraulic representation of the reactor vessel and a three-dimensional neutron kinetic core model (Fig. 3).

The same code Relap5 is used to simulate an innovative passive heat removal system again for the LFR demonstrator ALFRED [14]: the development of passive systems is one of the methodologies envisaged in the framework of GEN-IV to enhance safety levels. Such new designs are based on innovative reactor coolants and imply, as a consequence, a complete change of the technology know-how: simulation is then a fundamental design method.

Ansaldo Nucleare developed a parallel computational tool, MANCINTAP [15], to perform 3D neutron transport, activation and time-resolved dose-rate calculations in 3D complex geometries and transient conditions. This code is based on the automation of the link between MCNP—a code by LANL used to evaluate both the neutron fluxes for activation calculations and the resulting secondary photon dose rates—with Anita2000, a code package for the activation characterisation of materials exposed to neutrons.

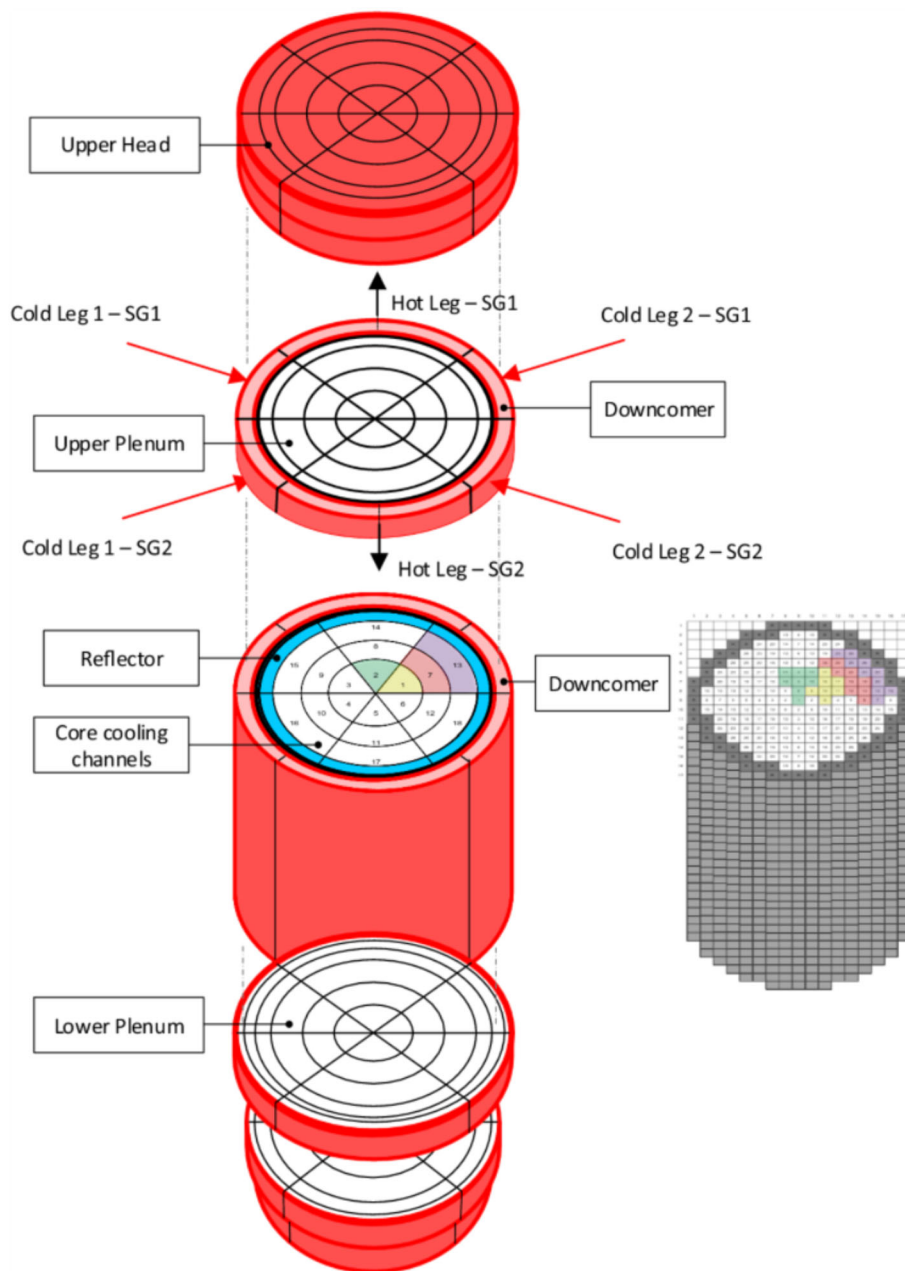
### 2.4 Accelerator-driven systems and fuel cycle considerations

A dual new conceptual design of an accelerator-driven system is described in [16]: the system is dual because the core combines a lead-bismuth-eutectic-cooled fast reactor (LFR) with a MSR, so taking advantages of both reactor core features. A subcritical core allows for loading a high fraction of minor actinides in fuels while preserving safety prescriptions. The possibility of burning 120 kg/year of minor actinides with only the maximum beam power of 13 MW is discussed.



**Fig. 2** 3D sketch of ALFRED LFR Gen IV demonstrator

Logically at last, but not the least, a discussion of the fuel burn-up is addressed in [17] with a specific attention paid to the design of accelerator-driven system: such systems—discussed also elsewhere in other papers of this Focus Point—are naturally more costly than a traditional critical reactor, so that their justification derives from the perspective of serving fuel and waste management strategies, for which a quick and easy way to preview the main features is clearly attractive. Here, an extension to ternary fuels of a previous model is presented.



**Fig. 3** Schematic representation of vessel and core of a PWR

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