ADVANCED NUMERICAL SIMULATION AND MODELLING FOR REACTOR SAFETY – CONTRIBUTIONS FROM THE CORTEX, HPMC, MCSAFE AND NURESAFE PROJECTS

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ABSTRACT

Predictive modelling capabilities have long represented one of the pillars of reactor safety. In this paper, an account of some projects funded by the European Commission within the seventh Framework Program (HPMC and NURESAFE projects) and Horizon2020 Program (CORTEX and McSAFE) is given. Such projects aim at, among others, developing improved solution strategies for the modelling of neutronics, thermal-hydraulics, and/or thermo-mechanics during normal operation, reactor transients and/or situations involving stationary perturbations. Although the different projects have different focus areas, they all capitalize on the most recent advancements in deterministic and probabilistic neutron transport, as well as in DNS, LES, CFD and macroscopic thermal-hydraulics modelling. The goal of the simulation strategies is to model complex multi-physics and multi-scale phenomena specific to nuclear reactors. The use of machine learning combined with such advanced simulation tools is also demonstrated to be capable of providing useful information for the detection of anomalies during operation.

1. Introduction

The safe and reliable operation of nuclear power plants relies on many intertwined aspects involving technological and human factors, as well as the relation between those. On the technological side, the pillars of reactor safety are based on the demonstration that a reactor can withstand the effect of disturbances or anomalies. This includes the prevention of incidents and should an accident occur, its mitigation.

Predictive simulations have always been one of the backbones of nuclear reactor safety. Due to the extensive efforts the Verification and Validation (V&V) of the corresponding modelling software these represent, most of the tools used by the industry are based on coarse mesh in space and low order in time approaches developed when computing resources and capabilities were limited. Because of the progress recently made in computer architectures, high performance computing techniques can be used for modelling nuclear reactor systems, thus replacing the legacy approaches by truly high-fidelity methods.

In parallel with the more faithful modelling of such systems, the monitoring of their instantaneous state is becoming increasingly important, so that possible anomalies can be detected early on and proper actions can be promptly taken. On the one hand, over 60% of the current fleet of nuclear reactors is composed of units more than 30 years old, therefore operational problems are expected to be more frequent. On the other hand, the conservatism in design previously applied to the evaluation of safety parameters has been greatly reduced, thanks to the increased level of fidelity achieved by the current modelling tools. As a result, nuclear reactors are now operating more closely to their safety limits. Operational problems may be also accentuated by other factors (e.g. use of advanced high-burnup fuel designs and heterogeneous core loadings).

In this paper, a brief account of four projects previously or currently funded by the European Commission in the area of the simulation and the monitoring of nuclear reactor systems is given. Despite the differences in nature between those projects, the key objectives and achievements with respect to advanced numerical simulation and modelling for reactor safety will be given particular emphasis. The paper will conclude with some recommendations for the future.

2. Short description of the respective projects

2.1 CORTEX

The CORTEX project (with CORTEX standing for CORe monitoring Techniques and EXperimental validation and demonstration) is a Research and Innovation Action financed by the European Commission. The project formally started on September 1st, 2017 for a duration of four years. The overall objective of CORTEX is to develop a core monitoring technique allowing the early detection, localization and characterization of anomalies in nuclear reactors while operating.

Being able to monitor the state of reactors while they are running at nominal conditions is extremely advantageous. The early detection of anomalies gives the possibility for the utilities to take proper actions before such problems lead to safety concerns or impact plant availability. The analysis of measured fluctuations of process parameters (primarily the neutron flux) around their mean values has the potential to provide non-intrusive on-line core monitoring capabilities. These fluctuations, often referred to as *noise*, primarily arise either from the turbulent character of the flow in the core, from coolant boiling (in the case of two-phase systems), or from mechanical vibrations of reactor internals. Because such fluctuations carry valuable information concerning the dynamics of the reactor core, one can infer some information about the system state under certain conditions.

A promising but challenging application of core diagnostics thus consists in using the readings of the (usually very few) detectors (out-of-core neutron counters, in-core power/flux monitors, thermocouples, pressure transducers, etc.), located inside the core and/or at its periphery, to backtrack the nature and spatial distribution of the anomaly that gives rise to the recorded fluctuations.

Although intelligent signal processing techniques could also be of help for such a purpose, they would generally not be sufficient by themselves. Therefore, a more comprehensive solution strategy is adopted in CORTEX and relies on the determination of the *reactor transfer function* or *Green's function*, and on its subsequent inversion.

The Green's function establishes a relationship between any local perturbation to the corresponding space-dependent response of the neutron flux throughout the core. In CORTEX, state-of-the-art modelling techniques relying on both deterministic and probabilistic methods are being developed for estimating the reactor transfer function. Such techniques are also being validated in specifically-designed experiments carried out in two research reactors.

Once the reactor transfer is known, artificial intelligence methods relying on machine learning techniques are used to recover from the measured detector signals the driving anomaly, its characteristics features and location.

More information about the CORTEX project can be found in [1].

2.2 HPMC and McSAFE

The projects HPMC (High Performance Monte Carlo Methods for Core Analysis) and McSAFE (High Performance Monte Carlo Methods for SAFEty Analysis) are two collaborative research projects funded by the European Commission in the seventh Framework Program (2011 to 2013) and Horizon 2020 Program (2017 to 2020) with the main goal of developing high fidelity multi-physics simulation tools for the improved design and safety evaluation of reactor cores. The peculiarity of HPMC and McSAFE is the focus on Monte Carlo neutronics solvers instead of deterministic ones, in order to take profit of the huge and cheap available computer power currently available.

The scientific goal of the HPMC was the “proof of concept“ of newly developed multi-physics codes for depletion analysis taking into account thermal hydraulic feedbacks, static pin-by-pin full LWR core analysis considering local feedbacks, and the development of time-dependent Monte Carlo codes including the behaviour of prompt and delayed neutrons for accident analysis.

Based on the success and promising results of the HPMC-project, the goal of the McSAFE-project that started in September 2017 is to become a powerful numerical tool for realistic core design, safety analysis and industry-like applications of LWRs of generation II and III [4], [5]. For this purpose, the envisaged developments will permit to predict important core safety parameters with less conservatism than current state-of-the-art methods and it will make possible to increase the performance and operational flexibility of nuclear reactors. Moreover, the multi-physics coupling developments are carried out within the European Simulation platform NURESIM developed during different FP7-projects such as NURESIM, NURISP and NURESAFE [6], heavily relying on the open-source SALOME-software platform. In this context, the European Monte Carlo solvers MONK, SERPENT, and TRIPOLI are coupled with the subchannel thermal-hydraulic code SUBCHANFLOW and with the thermo-mechanic solvers TRANSURANUS using the ICoCo-methodology [7]. At the present, the application and demonstration are done for LWR and SMR reactors. However, the peculiarity of the codes and methods make possible their application to the Gen- III and Gen-IV reactors as well as to research reactors, for which the complicated geometry and physics of the core can only be adequately simulated by Monte Carlo codes.

Finally, all developed methods and codes are validated against plant data of European VVER- and PWR-plants as well as using test data of the SPERT Series IV E REA.

2.3 NURESAFE

NURESAFE (NUclear REactor SAFEty simulation platform) is a collaborative research project funded by the European Commission in the seventh Framework Program [7], [8]. The project started early 2013 for a duration of three years. The main objective of NURESAFE was to develop a European reference tool for higher fidelity simulation of LWR cores for design and safety assessment.

The simulation tool developed by the NURESAFE project includes deterministic core physics codes, thermal-hydraulics and fuel thermo-mechanics codes, all integrated in a software platform whose name is *NURESIM*. This platform provides a capability for code coupling, capability of paramount importance as main phenomena occurring in reactors involve an interaction between the above-mentioned physics. The NURESIM platform also offers an uncertainty quantification, which is necessary for validation and safety evaluation.

The scope of the NURESIM platform includes the simulation of steady states of LWRs and design basis accidents of LWRs. This platform was initially created in the framework of former FP6 and FP7 collaborative projects (NURESIM and NURISP), during which core physics and thermal-hydraulics codes were first integrated. In NURESAFE, the platform was extended to more codes, particularly fuel thermo-mechanics codes. An important part of the NURESAFE work was also dedicated to:

- The demonstration of the multi-physics capability of the platform.
- Advanced CFD modelling.
- Uncertainty quantification and validation.

3. Key objectives with respect to advanced numerical simulation and modelling for reactor safety

3.1 Introduction

As earlier mentioned, most of the modelling tools used by the nuclear industry were developed when computing resources and capabilities were limited. Although nuclear reactors are by essence multi-physics and multi-scale systems, the techniques that were then favoured relied on modelling the different fields of physics and sometimes the different scales by different codes that were only thereafter coupled between each other. In the current best-estimate approaches, the modelling of neutron transport, fluid dynamics and heat transfer is thus based on a multi-stage computational procedure involving many approximations.

On the neutronic side, deterministic approaches have been used primarily, due to their lower computational cost compared to probabilistic methods (i.e. Monte Carlo). Deterministic tools nevertheless rely on many approximations, with the neutron transport equation solved explicitly after reducing the complexity of the task at hand (typically using space-homogenization, energy-condensation, and angular approximation techniques) [2]. The problem is first solved over a small region of the computational domain using approximate boundary conditions, and the “fine-grid” solution then computed is used for producing equivalent average properties locally. In a second step, a global “coarse-grid” solution is found for the full computational domain, in which only average local properties are considered, i.e., in which the true complexity of the system is not represented explicitly. Typically, three to four of such “bottom-up” simplifications are used to model a full reactor core. Although used on a routine basis for reactor calculations, the approximations used in each of the computational steps are almost never corrected by the results of the calculations performed in the following steps when a “better” (i.e. taking a larger computational domain into account) solution has been computed.

In the probabilistic approach on the other hand, no equation as such is solved. Rather, the probability of occurrence of a nuclear reaction/process of a given type on a given nuclide at a given energy for a given incoming particle (which can still exist after the nuclear interaction) is used to sample neutron life histories throughout the system [3]. Using a very large number of such histories, actual neutron transport in the system can be simulated without requiring any simplification, and statistically meaningful results can be derived by appropriately averaging neutron tallies. However, due to the size and complexity of the systems usually modelled, Monte Carlo techniques are extremely expensive computing techniques, which limited their use for routine applications in the past.

With the advent of cheap computing resources, both the deterministic approach and the probabilistic approach are now being used on massively parallel clusters to circumvent the limitations mentioned above. In the deterministic case, the process of averaging (“bottom-up”) is now being complemented by a de-averaging process (“top-down”) in an iterative manner, so that a better modelling of the boundary conditions can be achieved using the information available from the coarser mesh. The modelling of full cores in a single computational step is also being contemplated. In the probabilistic case, the use of large clusters allows modelling full reactor cores, and efforts are being pursued to include the feedback effects induced by changes in the composition and/or density of the materials [9], [10] [8]. Due to the complexity and level of details in the deterministic approach based on the averaging/de-averaging process, there are situations where the deterministic route can become quite expensive, being almost on par with the probabilistic route for high-fidelity simulations.

On the thermal-hydraulic side, the strategy is to average in time and in space the local conservation equations expressing the conservation of mass, momentum and energy. The double averaging results in a set of macroscopic conservation equations that are tractable for a large system as a nuclear reactor, unfortunately at the expense of filtering the high-frequency and small-scale phenomena [2]. In addition, the averaging process introduces new unknown quantities (expressing for instance the wall transfer and possible interfacial transfer between the phases) that are usually determined using empirical or semi-empirical correlations. These correlations are heavily dependent on the flow regimes. Such a modelling strategy is often referred to as a system code approach. With the advent of cheap computing power, current efforts focus on modelling much finer scale using Computational Fluid Dynamics (CFD) tools instead.

3.2 CORTEX

For the CORTEX project, since a majority of the diagnostic tasks are based on the inversion of the Green's function, the key objectives in the area of advanced numerical simulation and modelling can be summarized as follows: (a) the development of modelling capabilities for estimating the transfer function, (b) the validation of such tools against experiments specifically designed for that purpose, and (c) the inversion of the reactor transfer function using machine learning.

Concerning (a), one of the strategic objectives of the project is to determine the area of applicability of existing tools for noise analysis and to develop new simulation tools that are specifically dedicated to the modelling of the effect of stationary fluctuations in power reactors with a high level of fidelity. The ultimate goal is to develop modelling capabilities allowing the determination, for any reactor core, of the fluctuations in neutron flux resulting from known perturbations applied to the system. Two tracks are followed. Existing low-order computational capabilities are consolidated and extended. Simultaneously, advanced methods based on deterministic neutron transport and on probabilistic (i.e. Monte Carlo) methods are developed so that the transfer function of a reactor core can be estimated with a high resolution in space, angle and energy. Since the modelling of the response of the system to a perturbation expressed in terms of macroscopic cross-sections is equally important as the modelling of the actual perturbation, large efforts are spent on converting actual noise sources into perturbations of cross-sections. For that purpose, emphasis is put on developing models for reproducing vibrations of reactor vessel internals due to Fluid-Structures Interactions (FSIs). Finally, the evaluation of the uncertainties associated to the estimation of the reactor transfer function is given particular attention, together with the sensitivity of the simulations to input parameters and models.

Concerning (b), although the tools allowing estimating the reactor transfer function can be verified against analytical or semi-analytical solutions for simple systems and configurations, the validation using reactor experiments specifically designed for noise analysis applications is essential. Two types of neutron noise measurements are considered: a so-called absorber of variable strength and a so-called vibrating absorber.

Finally, concerning (c), the backtracking of the driving perturbation (not measurable) from the induced neutron noise (measurable at some discrete locations throughout the core) is performed using machine learning. With the tools referred to above, the induced neutron noise for many possible scenarios of considered perturbations is estimated. The results of such simulations are then provided as training data sets to machine learning techniques. Based on such training sets, the machine learning algorithms have for primary objective to retrieve the actual perturbation (and its location) existing in a nuclear core from the neutron noise recorded by the in- and ex-core neutron detectors.

3.3 HPMC and McSAFE

The major objectives of the HPMC-project were the following:

a) Optimal Monte Carlo-thermal-hydraulics coupling: the objective was to realise efficient coupling of the Monte Carlo codes SERPENT and MCNP with the thermal-hydraulic subchannel codes SUBCHANFLOW and FLICA4, suitable for full-core application.
b) Optimal Monte Carlo burn-up integration: the objective was to realise an efficient integration of burnup calculations in the Monte Carlo codes SERPENT and MCNP, suitable for full-core application.
c) Time-dependence capabilities in Monte Carlo methods: the objective was to develop an efficient algorithm for modelling time-dependence in the Monte Carlo codes SERPENT and MCNP, applicable to safety analysis and full-core calculations.

Based on the promising results of the HPMC-project, the McSAFE-projected started in September 2017 with the goal to move the Monte Carlo-based multiphysics codes towards industrial applications, e.g. simulation of depletion of commercial LWR cores taking thermal-hydraulic feedback into account, analysis of transients such as REA. For this purpose, a generic and optimal coupling approach based on ICoCo and the open-source NURESIM platform is followed for the coupling of European Monte Carlo solvers such as MONK, SERPENT and TRIPOLI with subchannel codes e.g. SUBCHANFLOW and fuel thermo-mechanics solvers e.g. TRANSURANUS. Moreover, dynamic versions of TRIPOLI, SERPENT and MCNP6 coupled with SUBCHANFLOW are developed for analysing transients. Especially, SERPENT/SUBCHANFLOW is being coupled with TRANSURANUS for the depletion analysis of commercial western PWR and VVER cores while considering thermal-hydraulic feedback. Emphasis is put on the extensive validation of the tools being developed within McSAFE. For the validation of the depletion capability, plant data are used for, whereas for the validation of the dynamic capability of the coupled Monte Carlo – thermal-hydraulics codes under development, experimental data of unique tests e.g. the SPERT REA IV E are used. Finally, high fidelity tools based on Monte Carlo requires a massive use of HPC in order to solve full cores at the pin level. Methods for optimal parallelization strategy, scalability of Monte Carlo-based simulations of depletion problems and time-dependent simulations, are also scrutinized in the McSAFE project. Since memory requirements for such problems may represent a limiting factor, methods for the optimal use of memory during depletion simulations of large problems needs to be further developed.

3.4 NURESAFE

The main objectives of NURESAFE were:

- To enhance the prediction capability of the computations used for safety demonstration of the current LWR nuclear power plants through the dynamic 3D coupling of the codes simulating the different physics of the problem into a common multi-physics simulation scheme.
- To advance the fundamental knowledge in two-phase thermo-hydraulics and develop new multi-scale thermo-hydraulics models.
- To develop multi-scale and multi-physics simulation capabilities for LOCA, Pressurized Thermal Shock (PTS) and BWR thermo-hydraulics, thus allowing more accurate and more reliable safety analyses.
- To develop generic software tools within the NURESIM software platform and to provide a support to developers for integration of the codes into this platform.

4. Key achievements with respect to advanced numerical simulation and modelling for reactor safety

4.1 CORTEX

Since the start of the project, the key achievements in the area of advanced numerical simulation and modelling along the three objectives identified in Section 3.2 can be summarized as follows.

Development of modelling capabilities for estimating the transfer function

The work carried out so far is performed along several lines, as schematically represented in Fig. 1.

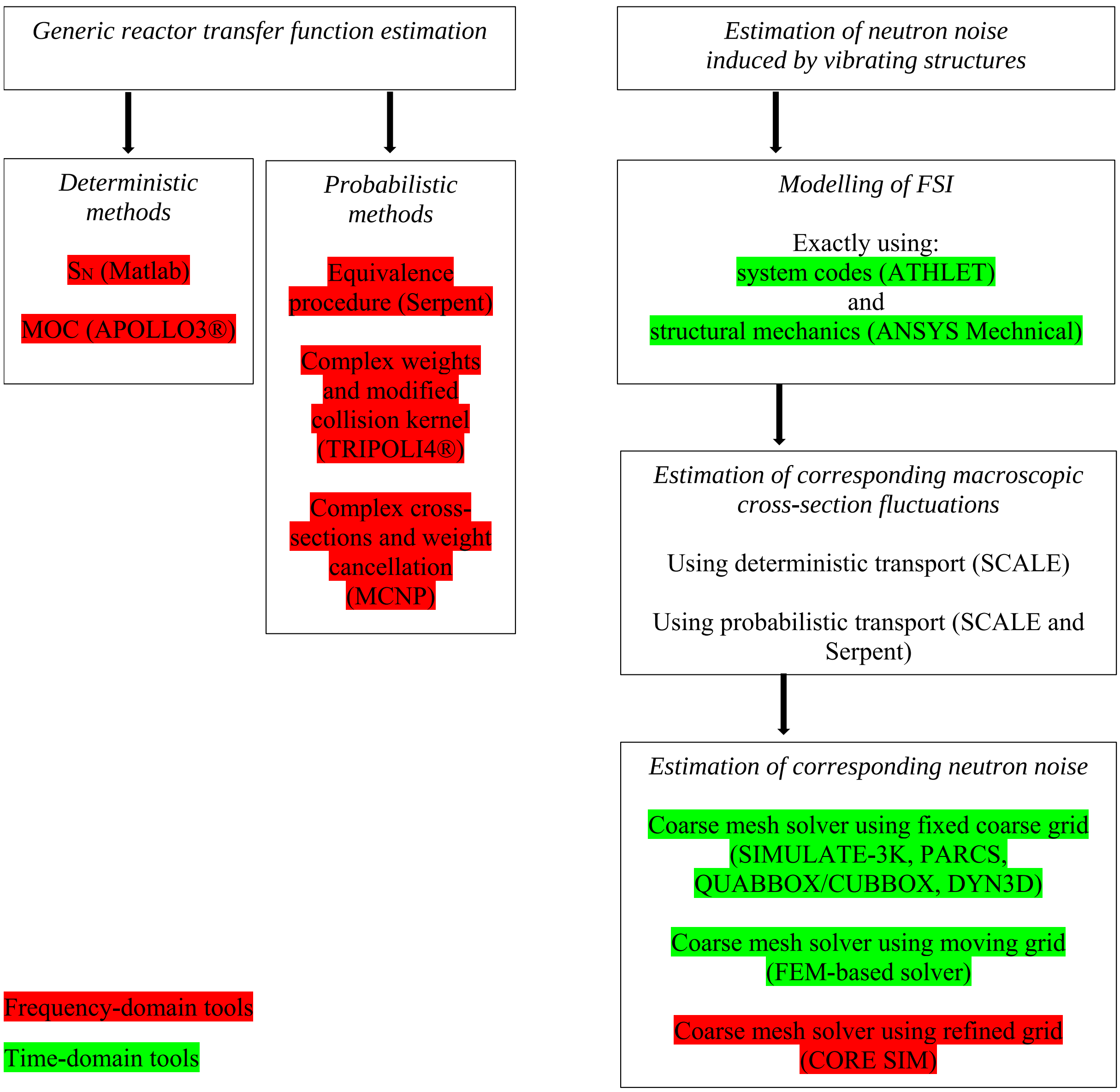


Fig. 1 Overview of the simulation alternatives targeted at estimating the neutron noise and the reactor transfer function.

In the area of mechanical vibrations, an extensive review of the past work on vibration of reactor internals was carried out. The focus was on both obtaining a coverage of all possible sources of neutron noise, a phenomenological description of each corresponding scenario, and of the observed neutron noise patterns when actual plant measurements were available. First simulations using thermal-hydraulic perturbations generated by the ATHLET system code were later fed into the Finite Element Method (FEM) code ANSYS Mechanical.

In parallel to those activities, neutronic capabilities are being developed. For *coarse mesh* approaches, three parallel tracks are pursued. Nodal codes used for the simulation of other core transients in the time-domain are used. Such codes are SIMULATE-3K, PARCS, QUABBOX/CUBBOX and DYN3D. To use some of these codes, the first step is to generate a set of time-dependent macroscopic cross-sections that simulate the movement of the fuel assemblies on a fixed computational coarse grid, based on the results of the FSI simulations. Procedure are being implemented using either the SCALE simulation suite or the Monte Carlo code Serpent to generate the whole set of cross-sections. In addition to the use of existing time-dependent tools with a set of time-dependent cross-sections, another approach is pursued based on the development of an ad-hoc software relying on FEM. The FEM method has a large versatility for solving balance equation using different spatial meshes. A code, called FEMFFUSSION, is being developed. It will offer the possibility in the future to have a moving mesh following the vibration characteristics determined from the FSI calculations. The main advantage of the FEM route lies with the fact that only static macroscopic cross sections for the initial configuration of the core are necessary. Finally, a third and complementary approach based on a mesh refinement technique in the frequency domain is being developed. The modelling of vibrating reactor internals requires the definition of perturbations on very small spatial domains compared to the size of the node size used in coarse mesh modelling tools. This makes it necessary to development mesh refinement techniques around the region where the perturbation exists. This mesh refinement technique is currently implemented in the frequency-domain core simulator CORE SIM, and the code being developed is referred to as CORE SIM+. For *fine mesh* approaches, deterministic methods relying on the method of discrete ordinates (Sn) are being developed. Moreover, a neutron noise solver relying on the method of characteristics is being implemented within the transport code APOLLO3®. In probabilistic methods, an equivalence procedure between neutron noise problems in the frequency-domain and static subcritical systems is being developed. A method using complex statistical weights and a modified collision kernel for the neutron transport equations in the frequency domain have been implemented in TRIPOLI-4®. Likewise, another method using complex-valued weights in the frequency domain has been implemented in MCNP.

As can be seen above, several complementary approaches are being developed. They either rely on existing codes or codes specifically developed for noise analysis. Moreover, these codes work either in the time- or in the frequency-domain. These tools use either a coarse-mesh approach (possibly with a moving mesh) or a fine-mesh approach regarding the spatial discretization. Finally, both deterministic and probabilistic methods are considered.

Validation of the modelling capabilities against experiments

Concerning the validation of such tools against experiments specifically designed for neutron noise, two research facilities are used: the AKR-2 facility at the Technical University of Dresden (TUD), Dresden, Germany, and the CROCUS facility at the Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland. Pictures of those two facilities are given in Fig. 2.

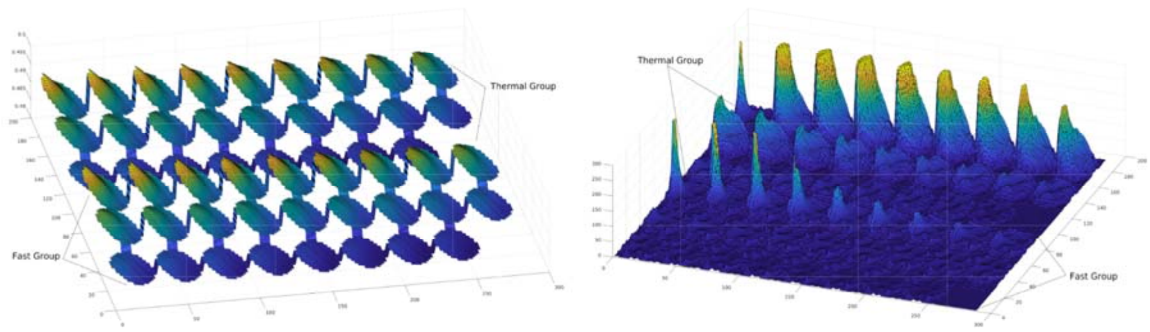
(a) CROCUS (courtesy of EPFL) (b) AKR-2 (courtesy of TUD)

Fig. 2 Overview of the CROCUS and AKR-2 facilities.

At both facilities, the data acquisition systems allow the simultaneous recording of seven and 11 neutron detectors, for AKR-2 and CROCUS, respectively, located throughout the respective cores, together with the recording of the actual perturbation introduced. The data acquisition systems were successfully benchmarked against an industry-grade data acquisition system from TUV Rheinland ISTec GmbH. In terms of perturbations, AKR-2 has the ability to perturb the system in two ways: either by rotating a neutron absorbing foil (thickness of 0.02 cm x length of 25 cm x width of 2 cm) along a horizontal axis or by moving a neutron absorbing disc (thickness of 1.0 mm x diameter of 12.7 mm) along a horizontal axis. In the former case, the foil rotates at a distance of 2.98 cm from its axis at a frequency of up to 2.0 Hz, whereas in the latter case, the disc is moving horizontally with a maximum displacement amplitude of 20 cm at a frequency up to 2.0 Hz. At CROCUS, up to 18 fuel rods located at the periphery of the core can be displaced laterally with a maximum displacement up to ±3 mm from their equilibrium positions at a frequency up to 5 Hz. The first noise measurements for the three types of noise sources (rotating absorber and vibrating absorber at AKR-2; vibrating fuel rods at CROCUS) have been performed as part of the validation of the data acquisition systems.

Since both the perturbations and the corresponding induced neutron noise are recorded in the experiments described above, such experiments can be used to validate the neutronic tools aimed at estimating the Green's function of the reactor and being developed within CORTEX. Such noise measurements, where both the perturbations and the corresponding neutron noise are recorded, represent a world premiere.

Inversion of the reactor transfer function using machine learning
Preliminary tests were performed using simulated signals, either in the time-domain or in the frequency-domain. Several scenarios corresponding to different types of noise sources were considered: localized absorbers of variable strength in the frequency-domain, travelling perturbations along fuel channels in the frequency domain, fuel assembly vibrations in the time-domain, and inlet coolant perturbations in the time-domain. The frequency-domain simulations were performed using CORE SIM at frequencies of 0.1, 1.0 and 10.0 Hz. The time-domain simulations were performed using SIMULATE-3K for either white noise sources or monochromatic noise sources at a frequency of 1.5 Hz. First successful machine learning tests on the absorbers of variable strength were based on "unrolling" the three-dimensional induced neutron noise into the juxtaposition of two-dimensional images, each corresponding to the plane-wise response of the reactor core to the perturbation. Fig. 3 represents such two-dimensional information that was then fed to a Deep Convolutional Neural Network (CNN) to retrieve the actual location of the perturbation. The recovery of the exact spatial location of the noise source was thereafter improved by using instead a three-dimensional CNN, so that the axial coupling information could be fully exploited in the unfolding. In addition, both the absorber of variable strength data and the travelling perturbation data were used. The network could both recognize the type of perturbation applied and recover the actual location of the perturbation being applied. For the time-domain data, the different scenarios could be successfully identified using a Long Short-Term Memory (LSTM) network.



(a) Phase information (b) Amplitude information

Fig. 3 Example of the reactor response to a localized absorber of variable strength unrolled as two-dimensional images (courtesy of University of Lincoln, UK).

4.2 HPMC and McSAFE

Optimal Monte Carlo-thermal-hydraulics coupling
The HPMC project demonstrated the potentials and capabilities of Monte Carlo based multi-physics coupled codes for improved static core analysis taking local interdependencies between neutronics and thermal hydraulics into account. At the completion of the project, two coupled codes, SERPENT/SUBCHANFLOW and MCNP/SUBCHANFLOW, had been

developed for static full core simulations at the pin level. Those codes were successfully applied to the analysis of a PWR core with UOX and MOX fuel assemblies, while taking local thermal hydraulic feedbacks into account and using HPC clusters [9], [10]. As an illustrative example, the capability of the coupled code SERPENT/SUBCHANFLOW to perform a pin-level analysis of a full PWR core with local thermal hydraulic feedback is shown in Fig. 4. The problem consists of 55777 neutronic nodes (pins and guide tubes), 2.2 million fluid cells, as well as 23.4 million solid cells (thermal-hydraulic solver). A total of 4×10^6 neutrons per cycle and 650 inactive and 2500 active cycles were used in the SERPENT calculations. The simulation was performed at the KIT IC2 HPC cluster using 2048 cores. A converged solution was achieved after 5.8 CPU-year (1.03 days).

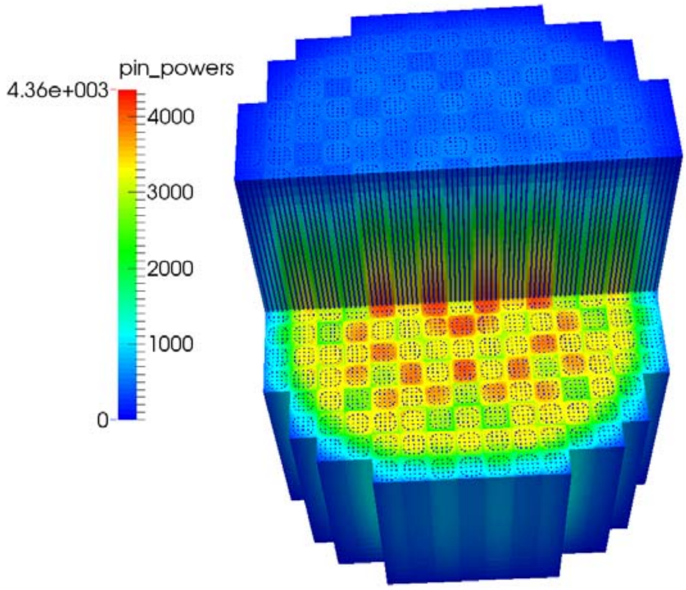


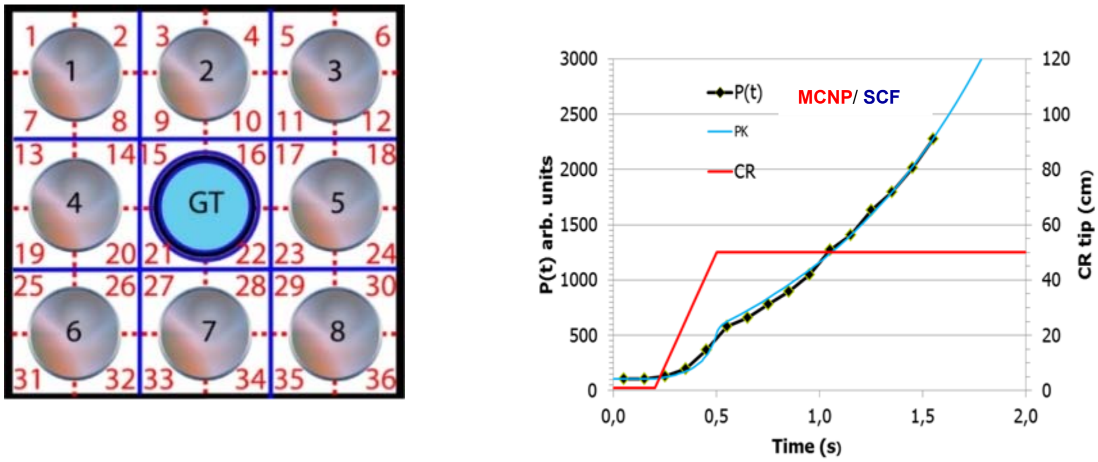
Fig. 4 3D Pin power predicted by SERPENT/SUBCHANFLOW for the PWR UOX/MOX core [10].

Optimum Monte Carlo burn-up integration

Another important outcome was the exploration and development of various schemes for stable depletion calculation using Monte Carlo codes such as the Stochastic Implicit Euler (SIE) method [11] for stable steady state coupled Monte Carlo-thermal-hydraulics calculations.

Time-dependence capabilities in Monte Carlo methods

A highlight of the project was the implementation of a time-dependence option in MCNP5 (dynMCNP) that required source code modifications [12]. This option includes the generation and decay of delayed neutron precursors, possible control rods movement, etc. To reduce the statistical error in the generated reactor power in successive time intervals, a method of forced decay of precursors in each time interval was implemented. Moreover, variance reduction methods (like the branchless collision method) were introduced. Thermal-hydraulic feedback was also implemented. To let the time-dependent thermal-hydraulics calculations take the heating history into account, further extensions of the codes were necessary. The new capabilities were demonstrated with the simulation of a mini fuel assembly consisting of 3x3 PWR fuel rods, where the central rod is a control rod. This rod is moved from its critical position upwards to initiate a relatively large reactivity effect. The time-dependent results for the assembly power are in good agreement with those calculated for a point-kinetics (PK) approximation, as illustrated in Fig. 5. Those results show the new capabilities of dynMCNP and demonstrate the potentials of MC-code to solve transient problems without any approximation to the physical modelling.



a) 3x3 fuel rod cluster

b) Power excursion after control rod withdrawal

Fig. 5 Comparison of the power excursion caused by the control rod ejection as predicted by MCNP5/SUBCHANFLOW and Point Kinetics (PK) [12].

Finally, various ways for parallel execution of a Monte Carlo calculation using the MPI and OpenMP application programming interfaces were investigated and their efficiency measured in terms of the speedup factor. For application on large computer clusters with different computer nodes and multiple processors per node, the optimum combination of MPI and OpenMP was determined. Application of OpenMP was introduced in the SERPENT2 code. The MCNP code was modified to use all available processor cores for neutron history simulation [13].

The main achievements close to the midterm of the McSAFE-project are described hereafter.

Full core multiphysics depletion
Methods for depletion of full core using Monte Carlo codes are being developed. First of all, the efficiency and stability of Monte Carlo burnup simulations were studied by optimal combination of free parameters that allow to solve full core problems [14]. In addition, a collision-based domain decomposition scheme for SERPENT2 is being developed to solve large-scale high-fidelity problems with large memory demands (e.g. full core pin-by-pin depletion). For this purpose, memory-intensive materials are split among MPI tasks, enabling the memory demand to be divided among nodes in a high-performance computer [15]. Investigations were also performed to identify the computational requirements for depletion calculations taking thermal hydraulic feedbacks into account for of 3D problems (e.g. 5x5 fuel assemblies mini-core) [16]. Potential bottlenecks and limitations, e.g. huge RAM-requirements which increase linearly with the number of fuel assemblies – 40 GB for eight fuel assemblies, could be identified. Alternatives were also proposed to overcome the challenges, such as a collision-based domain decomposition. In Fig. 6, the memory requirement for SERPENT2 is plotted against the number of fuel assemblies. Keeping in mind that available memory of e.g. the KIT ForHL-2 cluster is around 50 GB, merely few fully-resolved fuel assemblies can be considered for depletion calculations.

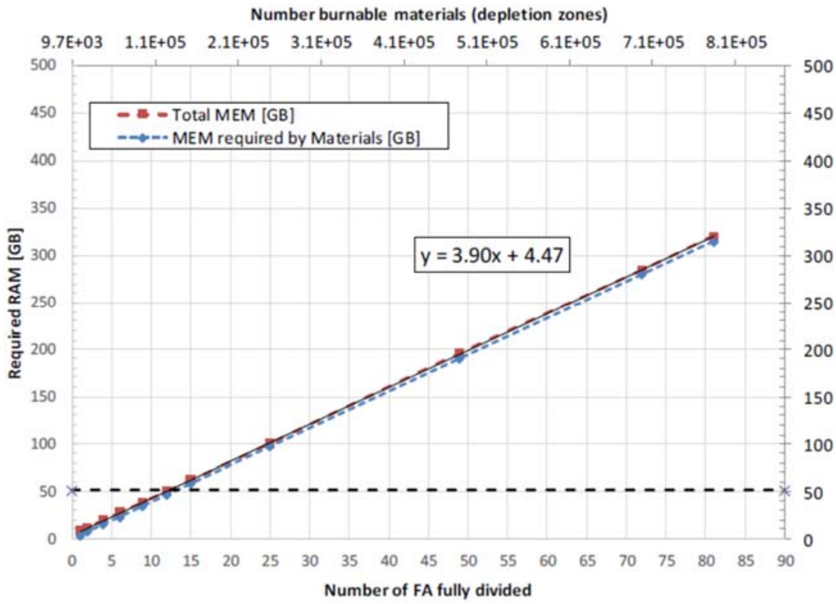
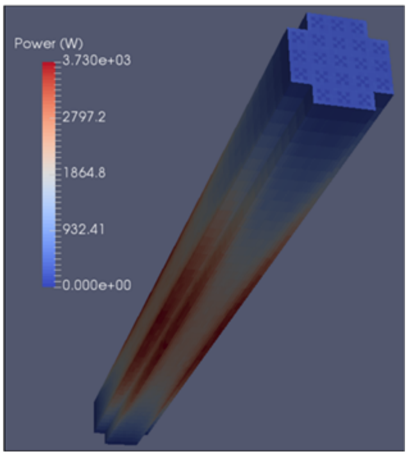
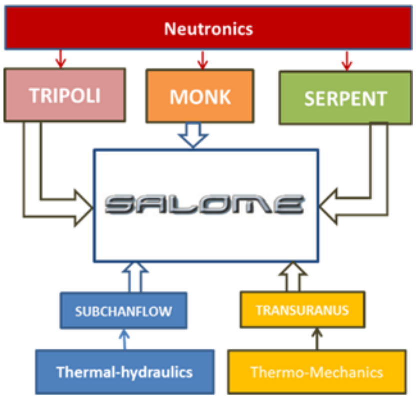


Fig. 6 SERPENT2 RAM-requirements as function of the number of fuel assemblies [16].

Code integration

The European Monte Carlo codes TRIPOLI, SERPENT, and MONK as well as the fuel thermo-mechanics code TRANSURANUS were fully integrated into the European NURESIM simulation platform (SUBCHANFLOW – SCF was already part of the platform), as Fig. 7 illustrates. Each solver owns a specific meshing. New flexible and object-oriented coupling schemes based on the ICoCo-methodology are being developed for each of the codes integrated into the NURESIM platform. The following coupled code versions are available: MONK/SCF, SERPENT/SCF, TRIPOLI/SCF.





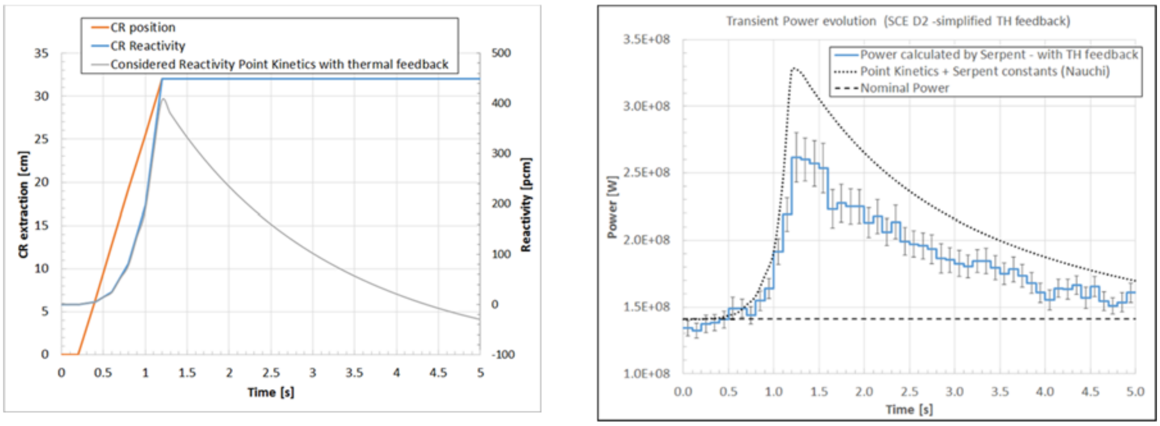
a) Meshing of the TH-solver (SCF)

b) NURESIM Platform: Implemented codes for ICoCo-based coupling

Fig. 7 McSAFE tools implemented in the NURESIM-platform and meshing capability.

Dynamical multiphysics calculations

Another important task in the McSAFE project is to extend general-purpose Monte Carlo codes (SERPENT2, TRIPOLI-4 and MCNP6) to dynamic version that can accurately calculate transient behaviour in nuclear reactors considering local thermal-hydraulic feedback. New versions of Monte Carlo codes with time-dependent capabilities (called dynamicMC) are at the end of the development phase for the analysis of transients. These Monte Carlo codes are coupled with the SCF thermal-hydraulic solver, thus leading to the coupled codes: dynMCNP/SCF, dynTRIPOLI/SCF, dynSERPENT/SCF. The code extensions and modifications are described in more detail in [12], [17] and [18]. The coupling schemes must be appropriate for massive HPC-simulations. The peculiarity of time-dependent Monte Carlo is to describe the behaviour of delayed neutrons, which have a significant influence on the statistical uncertainty (standard deviation) of the power prediction. An additional challenge is the short lifetime of prompt neutrons (roughly 100 µs in a LWR) compared to the large decay time of precursors of delayed neutrons for the method development. To test the dynamic capability of the Monte Carlo codes, different REA scenarios are being developed within McSAFE. One of these scenarios consists of a control rod withdrawal with constant velocity within one second. A SERPENT2 simulation considering thermal-hydraulic feedback was performed [19]. The obtained results are presented in Fig. 8 and demonstrate that the global trends are similar with the ones obtained using point-kinetics. The different scenarios will be calculated with the dynamic versions of the MC-codes under development in McSAFE.



a) REA transient scenario indicating the control rod movement and the introduced reactivity

b) Comparison of the power predicted by SERPENT2 and a point-kinetics model

Fig. 8 REA scenario and power increase predicted by SERPENT2 and Point Kinetics [19].

4.3 NURESAFE

Simulation platform

One of the main outcomes of the NURESIM and NURISP projects was the release of the NURESIM platform that is heavily used in NURESAFE. The NURESIM platform is based upon the software simulation platform SALOME. SALOME is an open-source project, (http://salome-platform.org), which implements the interoperability between a CAD modeller, meshing algorithms, visualisation modules and computing codes and solvers, as represented in Fig. 9. It mutualises a pool of generic tools for pre-processing, post-processing and code coupling. Its supervision module provides functionalities for code integration, dynamic loading and execution of components on remote distributed computing systems, and supervision of the calculation. Support is provided to developers for integration of the codes into the SALOME software and for producing and managing the successive versions of the NURESIM platform on a dedicated repository. Innovative deterministic and statistical methods and tools for quantification of the uncertainties developed within NURESAFE give a better knowledge of conservatisms and margins.

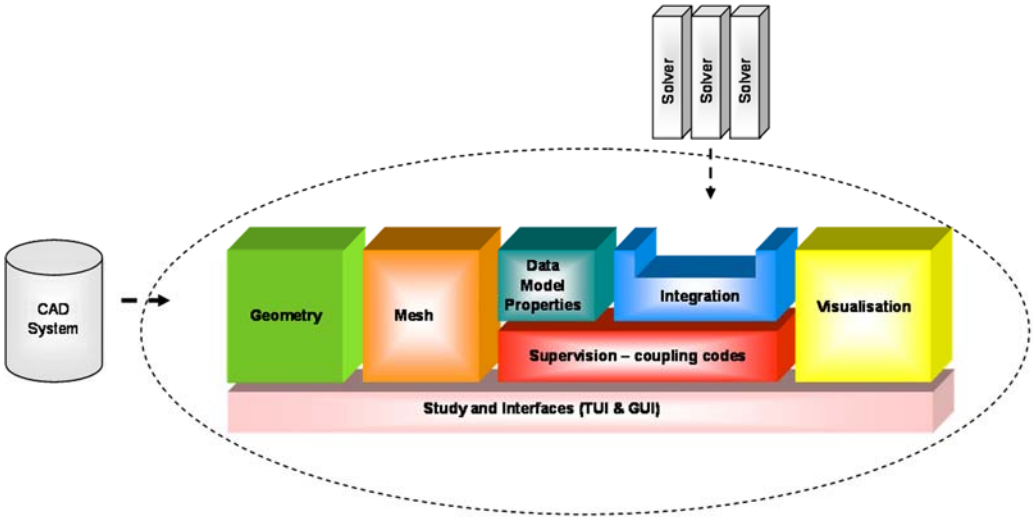


Fig. 9 SALOME global view.

The NURESIM platform provides a set of state-of-the-art software devoted to the simulation of normal operation and design basis accidents of LWR (i.e. BWR, PWR, and VVER). The platform includes 14 codes covering different physics: neutronics, thermal-hydraulics, fuel thermo-mechanics at different scales, 2 thermal-hydraulics system codes, 2 single-phase CFD codes, 2 two-phase CFD codes, 3 sub-channel thermal-hydraulic analysis codes, 2 advanced fuel thermo-mechanics codes, 2 DNS codes, 3 neutron-kinetics codes. All these codes were extensively benchmarked and validated against experiments during the course of the NURESAFE project.

SALOME is connected to URANIE, an open-source platform aimed at providing methods and algorithms about Uncertainty and Sensitivity (US) and Verification and Validation (VV) analyses in the same framework (https://sourceforge.net/projects/uranie/). The URANIE and SALOME platforms work nicely together. Any calculation scheme developed in SALOME can be used within URANIE.

Through the link with URANIE, users of the NURESIM platform successfully performed in the NURESAFE project sensitivity analyses and model calibration studies. For instance, the NURESAFE partners performed a sensitivity analysis within the context of the OECD/NEA Oskarshamn-2 stability event benchmark, with the event induced by a feedwater transient [20]. This benchmark provides qualitatively very good data for validating coupled thermal-hydraulics with neutron kinetics tools. A benchmarking of several methods to determine input uncertainties of system codes in a LOCA situation was also conducted.

3D dynamic coupling of codes

Individual models, solvers, codes and coupled applications, were run and validated through modelling “situation targets” corresponding to given nuclear reactor situations and including reference calculations, experiments, and plant data. As safety analysis was the main issue within the project, all these situation targets consisted in some accidental scenarios. The challenging “situation targets” were selected according to the required coupling between two different disciplines. Industry-like applications were released at the end of the project for the following “situation targets”:

- Square lattice PWR Main Steam Line Break (MSLB).
- One selected BWR Anticipated Transient Without Scram (ATWS).
- VVER MSLB.

The analysis also included uncertainty quantification using the URANIE open-source software. The BWR ATWS analysis framework featuring coupled simulations combining system thermo-hydraulics, 3D neutronics, thermo-mechanical evaluation of fuel safety parameters, and uncertainty evaluation. The MSLB transient analysis provided more accurate assessment of margins between predicted key parameters and safety criteria. The outcome of the transient simulation was evaluated with respect to local re-criticality and maximum reactor power level. As an illustrative example, the results of the PWR MSLB are presented hereafter.

A two-step modelling approach was applied. In the first step, reference results were produced using the platform codes with higher resolutions of coupling between core nodal and sub-channel scale. In the second step, CFD evaluations were included into the solution. In that way, an improvement in the prediction of the target safety parameters could be achieved. In order to increase the confidence of the CFD results, a validation was also performed by comparing the calculation results with experimental data from the HZDR test facility on coolant mixing ROCOM. The cross-section libraries were created using new methods of grid point selection [21]. Various combinations of system codes, core thermal-hydraulic codes and neutronic codes were used. Fig. 8 highlights the 3D distributions at time t=86s after the initiation of the MSLB. The quantitative comparison of the results revealed that the discrepancies were dominated by differences created on the secondary side during the depressurisation. The source of these differences comes mainly from the application of different models for the two-phase leak flow available in the different system codes. The use of different thermal-hydraulic system codes had thus a much bigger impact than expected.

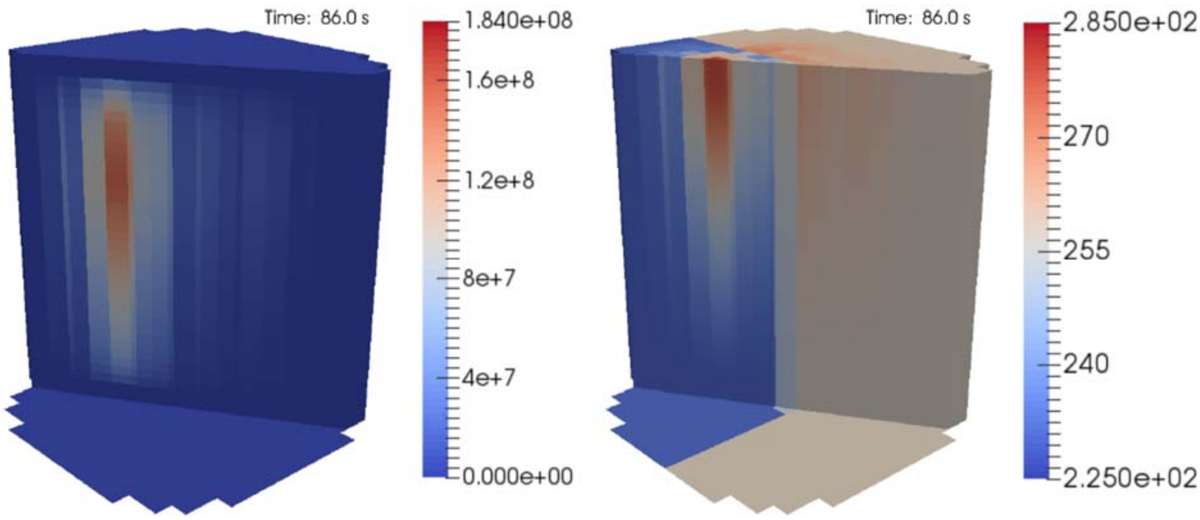


Fig. 10 Distribution of power density (MW/m^3, left) and coolant temperature (°C, right) at 86 s after the initiation of the MSLB event.

The obtained results confirmed that the NURESIM platform is applicable for challenging coupled transients in PWR. Furthermore, by accomplishing the coupling of reactor dynamics codes and CFD codes, the superiority of the NURESIM platform was demonstrated. The conducted advanced calculations demonstrated the excellent status and the readiness for industrial applications of the NURESIM platform and the integrated codes.

Advanced CFD modelling

advancement in the fundamental knowledge of CFD modelling was pursued and new models based on detailed Direct Numerical Simulation (DNS) for momentum exchange and boiling heat transfer issues typical of LWR thermal-hydraulics were developed. New benchmark data bases for fundamental and applied problems were developed. The existing computational multiphase flow strategies were first extended in order to cope with a wider range of practical applications. Novel methods for pool and convective boiling in a channel were also developed. Advanced strategies for modelling turbulent bubbly flow in a channel and in a rod bundle were analysed. Finally, the novel models and simulation techniques were implemented in codes, validated and applied in this context. New versions of the CFD platform codes NEPTUNE_CFD, TransAT and TRIO_U were delivered to end-users, including the most advanced numerical simulation features and the associated modelling approaches for the physics pertinent to both PWR and BWR.

Three specific issues were addressed within NURESAFE:

- All-topology flow modeling by coupling interface tracking models with phase-average models.
- DNS and LES of pool and convective boiling [22].
- DNS and LES of bubbly flows [23], [24].

As an illustrative example, the first issue is addressed below.

Multiphase flows involve a hierarchy of length scales intricately combined into interfaces and dispersed entities interacting with turbulence. The issue here is that there is no unified approach capable to treat the various topologies at once on the same grid and using one single strategy everywhere necessarily reduces the predictive performance of the model. The aim in NURESAFE was to develop a unified approach while treating each sub-portion of the flow individually using massively resolved grids (DNS). Correspondingly, the models could be fed with the pertinent physics (phase transition/inversion criteria) that cannot be quantified using today's experimental technology. Two new All Flow regime Models were developed. One was implemented in the TransAT computer code and the second model was implemented and used within the NEPTUNE_CFD code.

Both models use Interface Tracking Models (ITM) within the mixture phase-averaged models. In other words, they combine the two computational approaches most suitable for topologies of flows that exhibit large interfaces as well as dispersed flow features (small bubbles or droplets). The ITM is suitable for simulating flows with interfaces and mixture phase-averaged strategies are more suitable for simulating dispersed flows.

New models developed within NURESAFE were tested on some numerical and physical test cases: 1D advancing front, breaking droplet, impinging water jet, and rising bubble. The results obtained in these test cases were assessed as adequate to continue development and to apply the models to three experimental set-ups:

- Impinging jet experiment, where water is injected down into a stagnant pool along the vertical axis, from various heights and with various jet velocities.
- Szalinski's experiment, in which large air bubbles are injected into a tall vertical pipe filled with liquid water from the bottom.
- Castillejos' experiment, in which air is injected into the liquid at the bottom of a large pool. This experiment presents a range of bubble sizes from about 6 cm to smaller than 1 mm. Using classical two-phase two-field models such as the Euler-Euler dispersed two-phase approach is thus difficult, because of the difficulty to set up correlation for the closure laws when the range of bubble size and shapes are so wide. The experiment was simulated in NEPTUNE_CFD code with the two-field and two-phase and with the three-field and two-phase approaches. The mesh contained about 5.8 million of cells. The filtering scale at the centre of the domain was 5 mm for the located gas structure in the flow. The dispersed field of the three-field and two-phase approach was modelled through a simplified mono-dispersed approach with a constant bubble diameter set to 1 mm. Comparison of the calculated averaged void fraction of the gas phase with the experimental data is shown in Fig. 11. It can be seen that the three-field and two-phase model provides a larger plume near the free surface. The higher averaged void fraction at the centre of the plume suggests that additional efforts should be made on the transfer terms between the two gas fields that have numerically been set here. The approach has proved to be numerically robust, even used on a non-conforming mesh.

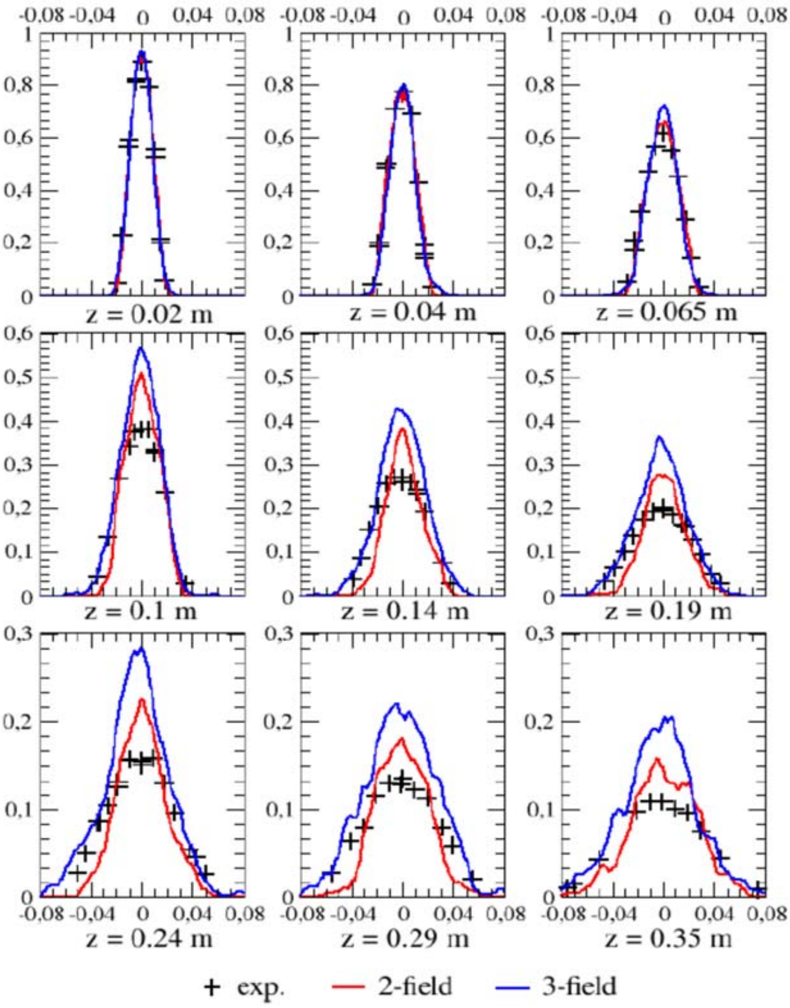


Fig. 11 Profiles of the averaged void fraction of the gas phase. The experimental data are represented with the black crosses, the results of the two-field and two-phase simulations correspond to the red line, and the results of the three-field and two-phase simulations are given by the blue line.

Multi-scale and multiphysics simulations

In the area of multi-scale and multiphysics simulations of LOCA, PTS and BWR thermal-hydraulics, multi-scale and multiphysics simulation capabilities for more accurate and more reliable safety analyses were developed.

LOCA is usually simulated with industrial versions of thermal-hydraulics system codes such as CATHARE and ATHLET. Although system codes are able to answer most safety needs, the status and limits of current methods and tools for plant analysis were reviewed during the NURISP project and areas for improvements were pointed out. Advanced tools and methods for multi-scale and multi-physics analyses and simulations of LOCA, including situations with deformed or ballooned rods and possible fuel relocation, were developed. The addition to system thermal-hydraulic codes of two-phase CFD tools and of advanced fuel models allowed revisiting these transients for more accurate and reliable predictions. This required improving and coupling CFD to system codes or improving system codes and system codes coupled with fuel thermo-mechanics codes. Furthermore, methods for uncertainty and sensitivity analysis applied to system codes were improved. In this framework, a special focus was put on the issue of the quantification of the uncertainties of the closure laws. This work was based on a benchmarking of the possible methods using reflooding experimental data (FEBA and PERICLES).

Concerning PTS, better simulation capabilities were achieved by improving the CFD modelling thanks to the analysis of new experimental data (including TOPFLOW steam-water tests and KAERI CCSF test). In addition, sensitivity and uncertainty methods were applied to CFD codes and state-of-the-art methods on validation uncertainty and uncertainty of CFD applications to reactor issues were reviewed.

In the field of BWR thermal-hydraulics, progress in the simulation of two-phase thermal-hydraulics phenomena specific to BWR was achieved. This includes dry-out prediction, transient core thermal-hydraulics and steam injection in pressure suppression pool. CFD codes, and sub-channel codes were used, improved and validated during the project.

5. Future recommendations

Using the NURESIM platform, challenging DNS & LES simulations were performed within NURESAFE to analyse bubbly flow with and without phase change in order to understand intricate phenomena that are beyond measurements capabilities. New modelling routes were proposed based on these results and were documented and implemented in the platform available to all stakeholders. Novel ideas were explored, and some others were further refined, such as combining large-scale and small-scale prediction techniques. Such techniques should in the medium term replace state-of-the-art methods that are limited to one flow regime. These novel techniques are applicable to more complex core-level thermal-hydraulics situations involving boiling. Solution procedures taking advantage of the coupling between various codes tackling different physics and scales were successfully developed.

In the area of Monte Carlo methods, the methods for depletion and dynamic calculations are close to their culmination. The developed coupled codes based on the ICoCo-methodology are now implemented in the European simulation platform NURESIM and the testing and validation phase will start soon. For this purpose, different benchmark problems of different size are being developed so that all partners will apply the developed tools for the analysis of those problems. Moreover, the validation of the codes under development using plant /experimental data is of paramount importance for McSAFE. Therefore, plant data of two European reactors (PWR-KONVOI, VVER-1000) are being prepared and documented for the validation of the advanced depletion capability of the tools. On the other hand, selected SPERT III REA E test data will be used for the validation of the dynamic versions of the Monte Carlo codes. Finally, application to LWR and SMR are foreseen to demonstrate the extended capabilities of the multi-physics codes. Generally, it can be stated that considerable efforts are still needed for high fidelity simulations based on Monte Carlo codes in an HPC-environment in order to perform core analysis with acceptable statistics for the key parameters of interest.

Beyond the major developments in computing capabilities for normal operation and design basis accidents, the monitoring of reactors and the early detection of anomalies will become increasingly important, due to the ageing fleet of reactors in Europe. By extending the current simulation platforms to the modelling of stationary fluctuations and their effect, such simulation tools csn be used for creating large data sets that can thereafter be used to detect from given measured reactor parameters possible anomalies. For such a purpose, machine learning was demonstrated in CORTEX, using simulated test data, to be potentially capable of retrieving anomalies. Tests on actual plant data remain nevertheless to prove the viability of this technique. In addition, although the phenomena considered so far in CORTEX do not require taking the thermal-hydraulic feedback into account, other scenarios might require the estimation of the coupled neutronics/thermal-hydraulics reactor transfer function.

In essence, the different situations needing accurate modelling require the inclusion of more and more physics. Beyond neutronics, thermal-hydraulics, and thermo-mechanics, other as important physics might need to be included: fuel physics, structural mechanics, coolant and radiation chemistry, radionuclide transport, etc. Truly multiphysics and multi-scale modelling approaches still need to be developed at a more mature level for tackling such situations. This include the development of new models, their coupling, as well as the use of the latest advancements in numerical analysis optimized for HPC. In this respect, the development of hybrid methods, such as deterministic and probabilistic methods in neutron transport, or DNS, LES, CFD, and macroscopic approaches in fluid dynamics and heat transfer, should be favoured and optimized. This requires having different scientific communities collaborating and capitalizing on each other's strengths and expertise. With so challenging modelling targets, the use of machine learning for predictive modelling should also be considered, where machine learning could be used in place of or in addition to more traditional modelling approaches. The enormous amount of measured data at commercial reactors, research reactors, and experimental facilities represent a definite asset, in a machine learning-based modelling strategy, that should be utilized as much as possible.

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