EPJ Nuclear Sci. Technol. **8**, 29 (2022)

https://doi.org/10.1051/epjn/2022026

EPJ Nuclear Sciences & Technologies

Euratom Research and Training in 2022: challenges, achievements and future perspectives, Roger Garbil, Seif Ben Hadj Hassine, Patrick Blaise and Cécile Ferry (Guest editors)

Available online at:
https://www.epj-n.org

Review Article

Open Access

Advanced numerical simulation and modeling for reactor safety – contributions from the CORTEX, McSAFER, and METIS projects

Christophe Demazière[1*] and Victor Hugo Sanchez-Espinoza[2] and Irmela Zentner[3]

[1] Chalmers University of Technology, Department of Physics, Division of Subatomic, High Energy and Plasma Physics, SE-412 96 Gothenburg, Sweden
[2] Karlsruhe Institute of Technology (KIT), Institute for Neutron Physics and Reactor Technology (INR), Hermann-vom-Helmholtz-Platz-1, 76344 Eggenstein-Leopoldshafen, Germany
[3] EDF R&D, Lab Paris – Saclay, ERMES – Earthquake Engineering, 7, Boulevard Gaspard Monge, 91120 Palaiseau, France

Received: 16 March 2022 / Received in final form: 7 September 2022 / Accepted: 16 September 2022

Abstract. This paper gives an account of three projects funded by the European Union that heavily rely on numerical modeling and simulations of nuclear reactors: the CORTEX project (CORe monitoring Techniques and EXperimental validation and demonstration), the McSAFER project (High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors), and the METIS project (MEthods and Tools Innovations for Seismic risk assessment). The CORTEX project focuses on neutronic simulations, the McSAFER project considers neutronic, thermal-hydraulic, and thermo-mechanic simulations, whereas the METIS project investigates simulations for seismic assessments. Although the projects have different objectives, they present some common features in terms of the complementary modeling approaches used in each project and in terms of verification and validation programs. The main achievements of the projects are presented in the paper covering the technical aspects of the respective projects, training, education, and dissemination activities, as well as utilization and cross-fertilization. All three projects lead to the advancement in nuclear reactor modeling in the above areas, with the development of new simulation capabilities beyond the state-of-the-art.

1 Introduction

Numerical simulations have always represented one of the pillars of nuclear reactor safety, with safety analyses carried out either in a deterministic or a probabilistic sense. Although well-established methods have been used for the current fleet of reactors for decades, recent developments in modeling capabilities make it possible to address new situations and conditions. This paper overviews the latest advancements in simulation and modeling in the Euratom-funded projects CORTEX, McSAFER, and METIS.

In CORTEX, deterministic and Monte Carlo neutron transport simulations of postulated anomalies are combined with machine learning architectures to detect existing perturbations in operating nuclear reactors, classify them and, when relevant, identify the location of the perturbation. In McSAFER, the existing simulation platforms based on the multi-physics and multi-scale approach are adapted to Small Modular Reactors, focusing on neutron transport, thermal-hydraulic and fuel thermo-mechanic simulations, and their interdependencies. An experimental program in three European facilities (MOTEL, COSMOS-H, and HWAT) to investigate safety-relevant thermal-hydraulic phenomena in the core, reactor pressure vessel, and heat exchanger of integrated SMR concepts complements the numerical investigations. In METIS, a multidisciplinary approach is proposed for the seismic safety assessment of reactors, based on numerical simulations, the use of observations for model updating, and the uncertainty propagation through the three steps of the analysis, from hazard via structural and equipment fragility analyses to risk quantification.

Although the three projects have different objectives, they also present common features. First, various complementary modeling tools with different levels of sophistication are used depending on the target conditions and situations. This also allows for assessing the area of validity of low order fast running models versus high-fidelity computationally intensive tools. Second, all modeling approaches require extensive verification of the tools and validation against experiments. Finally, the assessment of the reliability of the simulations requires complementing the

* e-mail: demaz@chalmers.se

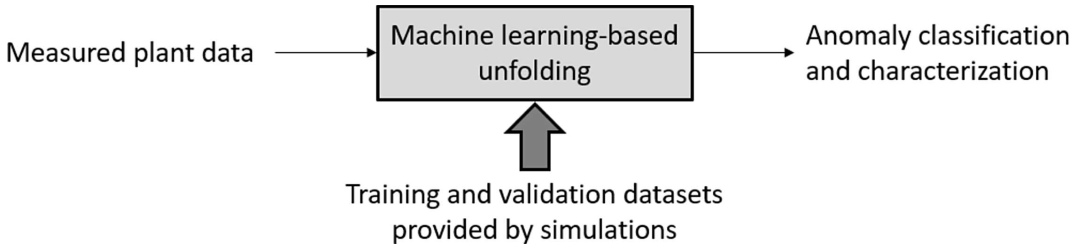

Fig. 1. Overview of the overall core monitoring methodology applied in the CORTEX project.

simulations with uncertainty and sensitivity estimates. The paper details the development of the modeling capabilities within the three projects, the lessons learned, and the required future developments.

2 Short description of the respective projects

2.1 CORTEX

Maintaining the high availability of nuclear reactors has always been a top priority for the industry. With the aging fleet worldwide, operational problems become more frequent and may impact plant availability. Being able to detect anomalies early before they have any inadvertent effect on plant operation, availability and safety is thus of paramount importance. As nuclear power plants are very large and complex systems, detecting anomalies is particularly challenging, despite the multitude of sensors monitoring the health of the system and the recent progress in surveillance, diagnostic and prognostic techniques [1]. The part of the system where this is most difficult is the nuclear reactor core, i.e., the part of the system containing the nuclear fuel assemblies. The system contains very few detectors, especially in-core. The existence of neutrons originating from the core nevertheless offers a unique opportunity for monitoring: due to the transport of neutrons via fission and scattering reactions, a neutron detector can "sense" any perturbation, even when this perturbation is far away from the considered neutron detector.

In this respect, the spatial dependence of the inherent time fluctuations in the neutron flux – the so-called *neutron noise* – may also be used for core monitoring [2]. Neutron noise is formally defined as the instantaneous neutron flux at a given spatial point from which its mean value in time has been subtracted. The main advantage of using neutron noise is that such fluctuations are always present. They are the results of mostly turbulence (in the case of a Pressurised Water Reactor – PWR) and possibly coolant boiling (in the case of a Boiling Water Reactor). The evolution, during the fuel cycle, of the spatial signature of the neutron noise and its spectral content is thus of high diagnostic value, as the monitoring of the neutron noise may help in the early identification of conditions possibly leading to a reactor transient or malfunction. In general, core diagnostics using noise analysis can be seen as a set of hierarchical tasks. The first task is to detect the anomalies. The second task is to classify them, i.e., to determine the type of anomaly. Subsequently, and depending on the type of anomaly, further characterization is possible, such as locating the perturbation, determining the vibration pattern, if relevant, etc.

In the Horizon 2020 CORTEX project (which ran from September 1st, 2017, to August 31st, 2021 – https://cortex-h2020.eu/), advanced reactor modeling tools were combined with Artificial Intelligence/machine learning techniques for detecting, characterizing, and potentially localizing anomalies [3]. As annotated measurement data, i.e., measurement data for which the anomaly is known, do not exist, another approach was followed in CORTEX, as presented in Figure 1. The training and validation data sets were provided by simulations. By postulating a neutron noise source, the induced neutron noise can be calculated accordingly, assuming that the necessary modeling tools are available. The training and validation data sets can thus be built by varying the type of noise sources and their characteristics.

The method was demonstrated to be efficient for identifying anomalies in commercial nuclear reactors – see, e.g., [4–6]. Machine learning-based unfolding can thus correctly identify and classify different types of perturbations and, when relevant, successfully localize such fluctuations.

Although the entire core monitoring methodology highlighted above is based on simulations, measurement plant data, and processing, all combined in dedicated machine learning architectures specifically developed for neutron noise-based core monitoring, emphasis is put in the following of this paper on the simulation tools only.

2.2 McSAFER

The High-performance advanced methods and experimental investigations for the safety evaluation of generic Small Modular Reactors (McSAFER) project is a research and innovation project funded by the Horizon 2020 research program of the European Commission (www.mcsafer-h2020.eu). McSAFER started in September 2020 and will last until August 2023. Thirteen partners from nine countries form the consortium. The main objective of McSAFER is, first of all, to provide new experimental data gained in three different facilities (at KIT, KTH, and LUT) under conditions relevant to light water-cooled Small Modular Reactor (SMR)-concepts. Moreover, the purpose of the project is to compare different safety analysis methodologies (industry-like standard methods, advanced and high-fidelity numerical tools) to analyze the behavior of the core, the Reactor Pressure Vessel (RPV), and the integral plant under selected transient conditions [7]. The safety evaluations focus on four SMR concepts: the French F-SMR, the Argentinian CAREM design, the US NuScale design, and the Korean SMART reactor. The advanced numerical tools selected for the safety investigations are based on multi-scale (RPV and plant) and multi-physics (core) methods. Beyond the involvement of industry (PEL, JACOBS, TRACTEBEL) and research centers (VTT, CEA, HZDR, UJV, CNEA), universities (KIT, KTH, LUT, UPM) are also engaged.

The McSAFER project is structured around six Work Packages (WP) – WP2 (Experimental investigations and validation), WP3 (Multi-physics core analysis), WP4 (Multiscale RPV-analysis), and WP5 (Multi-scale and physics plant analysis). WP6 is devoted to dissemination, exploitation, and communication, and the last one is devoted to project management (WP1).

2.3 METIS

Methods and Tools Innovation for Seismic Safety Assessments (METIS https://metis-h2020.eu/) started in September 2020 under the EURATOM Horizon 2020 program and is running until 2024. It addresses the three ingredients of seismic safety assessment in an overall approach: seismic hazard, structural and equipment fragility analyses, and integration in the full Probabilistic Safety Assessment (PSA) framework to determine plant failure probabilities. In nuclear and non-nuclear engineering, the general concepts of seismic risk assessment are due to the pioneering work of Cornell and co-workers [9]. The overall framework for probabilistic safety assessment is well established, but the partitioning into disciplines prevents the integration of common approaches, for example, uncertainty propagation. It is proposed to work in a multidisciplinary framework based on advanced methodologies that will be jointly applied to different parts of safety assessment. Moreover, in the last decades, there have been notable advancements in the development of the Performance-Based Earthquake Engineering (PBEE) approach [8,10]. The PBEE is now entering international civil engineering design codes such as FEMA 2012, ASCE/SEI in the USA but has not yet fully impacted nuclear engineering practice and codes. On the other hand, there have been significant advances in nuclear engineering regarding modeling and tools for dynamic structural and mechanical analyses. METIS follows these paths and further develops methods to improve the predictability of (non-linear, best-estimate) beyond design analyses required to consider Design extension earthquakes. The project further develops the use of databases, numerical simulations, and machine learning to improve the fidelity and accuracy of the engineering models and to comfort, confront and update expert judgment by Bayesian approaches. The developed methodologies will allow for a more objective assessment of safety margins and failure probabilities, thus improving the plant safety analyses.

3 Key objectives in modeling needs

3.1 Introduction

As highlighted above, CORTEX, McSAFER, and METIS heavily rely on simulations. Despite the complexity of the systems being considered, it is important to develop simulation tools adapted to the target situations being investigated. Although state-of-the-art high-fidelity simulations capable of handling all types of scenarios might be desirable, the associated computing time is, in some cases, unnecessarily prohibitive.

In addition to developing such “high-order” solvers, “low-order” solvers, i.e., solvers resolving the dominating physics in simplified terms while giving meaningful results, might represent in some situations a reasonable alternative. Low-order solvers also have the advantage of much cheaper computing costs compared to their high-order counterparts.

3.2 CORTEX

Various modeling approaches were followed in CORTEX. At the frequencies of interest, the effect of the thermal-hydraulic feedback is negligible, and thus the modeling of neutron transport solely is sufficient. In this respect, existing low-order computational capabilities were consolidated and extended. Simultaneously, new and advanced solution methods were developed. In essence, the different approaches are the result of simulation choices and paradigms that can be summarized as follows:

- the calculations can be performed in the time or frequency domain. The time domain requires a sufficiently small time discretization to be able to capture phenomena at typical frequencies of 0.1–20 Hz. The frequency domain, on the other hand, directly considers the frequency of interest. Whereas time-domain codes can easily handle non-linear terms and possible thermal-hydraulic feedback, the modeling in the frequency domain is often limited to linear terms only.
- The calculations can be performed using deterministic or probabilistic methods (i.e., Monte Carlo). Whereas deterministic approaches have a much lower computing cost as compared to Monte Carlo, Monte Carlo approaches do not need to rely on a discretization of the multi-dimensional phase space.
- For deterministic methods, as they rely on discretization, several levels of refinement are possible:
  - for the angular variable, from coarse (i.e., diffusion) to fine (i.e., transport) discretization.
  - For the spatial variable, from coarse (i.e., fuel assembly) to fine (i.e., fuel pin) discretization.
  - For the energy variable, from coarse (i.e., two energy groups) to fine (i.e., several tens of energy groups).

Different tools were used and/or developed in CORTEX depending on a combination of the various alternatives listed above. As those tools use macroscopic cross-sections as input data, a model representing the noise source in terms of perturbations of macroscopic cross-sections needed to be developed for each noise source type, irrespective of whether the solver used for estimating the induced neutron noise is deterministic or probabilistic. The modeling of the noise source is equally important as the modeling of the corresponding induced neutron noise. While expert opinion was, in most cases, used for expressing the effect of physical perturbations in terms of nuclear macroscopic cross-sections, the application of structural mechanics models was demonstrated to be of great help – see, e.g., [11].

3.3 McSAFER

The overall goal of the McSAFER project is to validate and apply advanced numerical tools for safety analysis of water-cooled SMRs taking into account the national regulatory guidelines for the deployment of SMRs in Europe, as well as to generate unique thermal-hydraulic data for the validation of thermal-hydraulic codes to be used for the safety demonstration. Specific goals of the McSAFER project are:

- the development and improvement of multi-physics and multi-scale numerical simulation tools.
- The generation of key experimental data at three facilities, e.g., COSMOS-H, MOTEL, and HWAT, relevant for water-cooled SMRs.
- The demonstration of the advantages of the use of high-fidelity codes for safety demonstration and the complementarity of low-order and high-order solvers.
- The reduction of the degree of conservatism in safety margins.

3.3.1 Multi-physics core analysis tools

Improved reactor physics, thermal-hydraulics, and thermo-mechanics coupled tools are used in addition to industry codes for analyzing four different SMR-cores under nominal and accidental conditions (Rod Ejection Accident – REA, cold water injection). The goal is to demonstrate the complementarity of multi-physic high-fidelity methods with traditional ones. Hence, the following methods are considered:

- the development of advanced deterministic solvers (SP3-pin-by-pin/subchannel) to improve core analysis, achieving higher prediction accuracy, i.e., at the pin level compared to the traditional lower-fidelity codes.
- The demonstration of the need for high-fidelity novel multi-physics and multi-scale codes to improve the traditional low-fidelity codes and methods in use by the industry and regulators for routine simulations.
- The verification of the appropriateness of the high-fidelity multi-physics solutions based on Monte Carlo methods as the reference solution for reduced-order solutions, especially in cases where no experimental data are available.
- The extension of core analysis tools for simulating an SMR core loaded with Accident Tolerant Fuel (ATF).

3.3.2 Multi-scale Reactor Pressure Vessel (RPV) analysis method

Improvement of the simulation of three-dimensional thermal-hydraulic phenomena inside the RPV of integrated SMR designs is achieved by applying multi-scale thermal-hydraulic tools (CFD, sub-channel TH, and system TH) in addition to the traditional ones. Therefore, the spatial resolution of the computational domains is increased to achieve a higher prediction accuracy than traditional one-dimensional coarse mesh codes. The Design Basis Accident (DBA) sequence selected for NuScale is a boron dilution event, and for SMART, an Anticipated Transient Without Scram (ATWS).

3.3.3 Multi-scale/multi-physics plant analysis method

The multi-scale/multi-physics plant analysis is oriented towards the application of the improved and validated numerical tools to the analysis of selected accidents in SMR plants, e.g., SMART and NuScale, and comparing the results with the ones of the traditional methods. The selected accident scenario for NuScale and SMART is a Main Steam Line Break (MSLB). A comparison of the different safety analysis approaches will be performed and discussed.

The thermal-hydraulic models developed in WP4 are extended to include the relevant safety systems of the SMART and NuScale SMRs that are necessary for the simulation of the Steam Line Break (SLB) scenarios. For this purpose, plant data, including the one for the involved control and safety systems and reactor control and protection system of each design (setpoints), were collected in the databases.

3.4 METIS

One major technical objective of the METIS project is to develop, improve, and disseminate open-source tools for seismic hazard, fragility, and risk assessment.

Open-source tools for Probabilistic Seismic Hazard Assessment (PSHA) and structural analyses are getting more and more commonly used both by the scientific and engineering communities and allow for numerous collaborations. None of the PSA tools currently used in the industry are open-source though this would help to improve quality and simplify the exchange of methods and data. One of the high-level objectives of METIS is the development and dissemination of an open-source tool for PSA computations.

The open-source tools identified for METIS are summarized in Figure 2. Openquake [12], code_aster [13] and OpenSees are already largely used for engineering and research. New studies cases will be created, and the codes will be further developed to fully support METIS methodologies. Moreover, METIS will create a new PSA tool based on the existing SCRAM open-source code.

The project then relies on numerical “best-estimate” simulations accompanied by uncertainty quantification and propagation to improve the fidelity and accuracy of seismic response and reliability analysis.

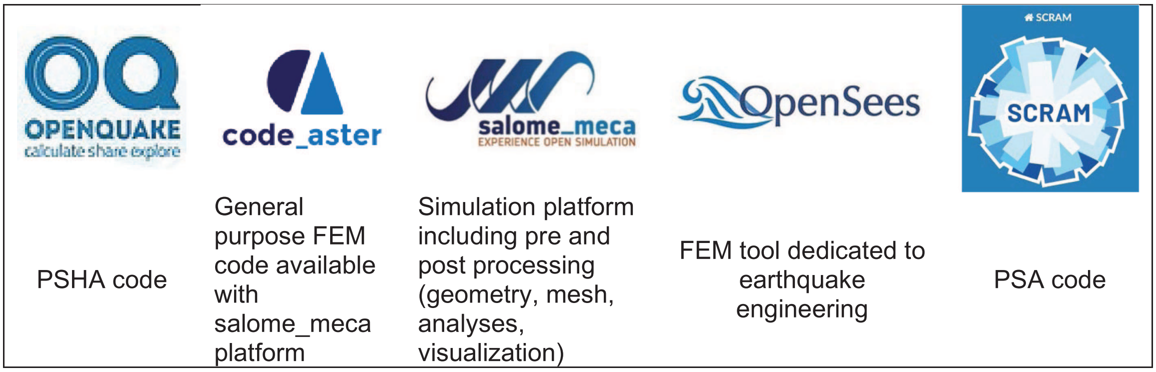

Fig. 2. Existing open-source codes used and developed by METIS.

In addition to simulation, METIS also takes advantage of growing databases and experience feedback for validation and to detect and eliminate bias or misfits in models. The developed methodologies will allow for a more objective assessment of safety margins and failure probabilities and, thus, an improvement in the plant safety analyses.

4 Key achievements

4.1 Introduction

In the area of simulations, the verification and validation of the modeling tools are essential [14–16].

Verification targets the demonstration of the proper numerical implementation of the governing equations corresponding to a chosen model. Typically, verification consists in comparing the results of the modeling software to reference analytical or semi-analytical solutions. To derive such reference solutions, the system to be modeled needs to be drastically simplified. Validation, however, relies on comparing the results of the modeling tool and experimental data. Validation also includes the comparison against any other verified and validated software, which may use other assumptions compared to the tool being validated. The corresponding modeling exercises are thus referred to as benchmarks.

Furthermore, estimating the effect of uncertainties on the modeling results has become increasingly important in recent years, as demonstrated in some international efforts, such as [17]. Uncertainty analysis aims at assessing the variability of the output of a modeling software due to the variability of the input parameters. Sensitivity analysis aims to estimate how sensitive the code output is to the variability of the input parameters. This allows identifying the input parameters having the largest effects on the code results. From this knowledge, efforts can be targeted at reducing the uncertainties of those input parameters so that the uncertainty of the code output can be significantly reduced.

4.2 CORTEX

In CORTEX, all newly developed algorithms were verified by comparing the results of code simulations to analytical or semi-analytical solutions – see, e.g., an illustrative example of a verification exercise in [18]. Moreover, an extensive program of validation of the tools was undertaken, based either on benchmarking exercises between codes or comparisons between simulations and experiments. Representative cases in each of the two categories are given below. A methodology to evaluate the uncertainties associated with the code inputs and the corresponding sensitivities was also developed.

4.2.1 Benchmarking activities

In terms of benchmarking, different exercises were developed. An example is reported in Figure 3 [19]. In this exercise, a fuel assembly in an infinite lattice was considered, and the properties of a fuel pin were assumed to oscillate around a mean nominal value at a frequency of 1 Hz. The figure represents the amplitude and phase of the Fourier transform of the neutron noise calculated by the various codes along the main diagonal of the fuel assembly crossing the perturbed fuel pin. As Figure 3 demonstrates, all codes provide similar answers.

4.2.2 Comparisons between simulations and experiments

Beyond the successful comparisons of the various codes, a great effort in CORTEX was dedicated to validating the codes against neutron noise measurements carried out at the AKR-2 reactor at TUD, Dresden, Germany, and the CROCUS reactor at EPFL, Lausanne, Switzerland. Three experimental campaigns were undertaken at each facility [20]. The first experimental campaigns aimed to give a first fingerprinting of the neutron noise and resolve the issues for the following campaigns. The second experimental campaign targeted general improvements, better estimates, uncertainty reduction, and better coverage of the spatial distribution of the noise for CROCUS. The third experimental campaign had objective repeatability and enhanced spatial dependence of the induced neutron noise.

As illustrative examples, the summary of some of the comparisons between measurements and calculations is given in Figure 4 for AKR-2 and CROCUS, for a representative experiment of the second campaigns at each facility. As seen in those figures, the code predictions typically fall within the uncertainty band of the measured

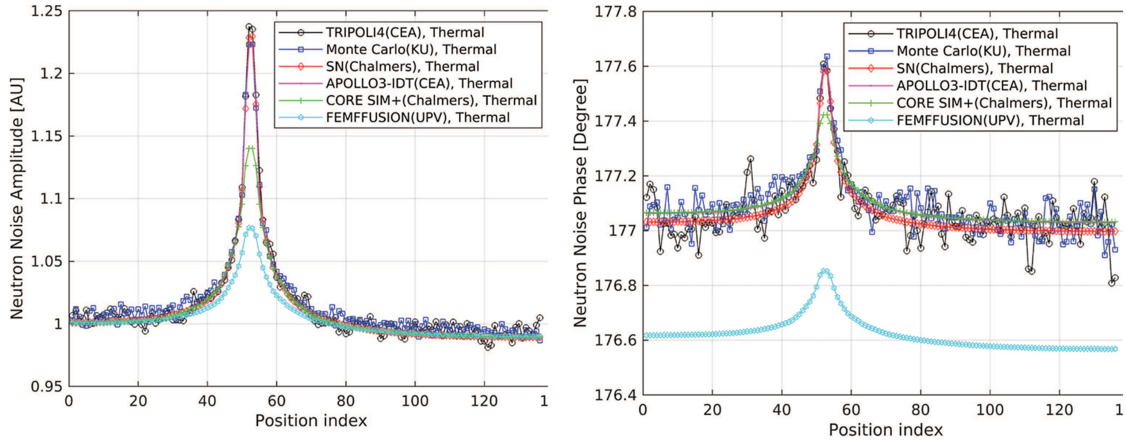

Fig. 3. Spatial variation of the amplitude (left) and phase (right) of the Fourier-transform of the thermal neutron noise induced by a vibrating fuel pin in an infinite fuel assembly lattice in one of the benchmark exercises. Figure derived from [19].

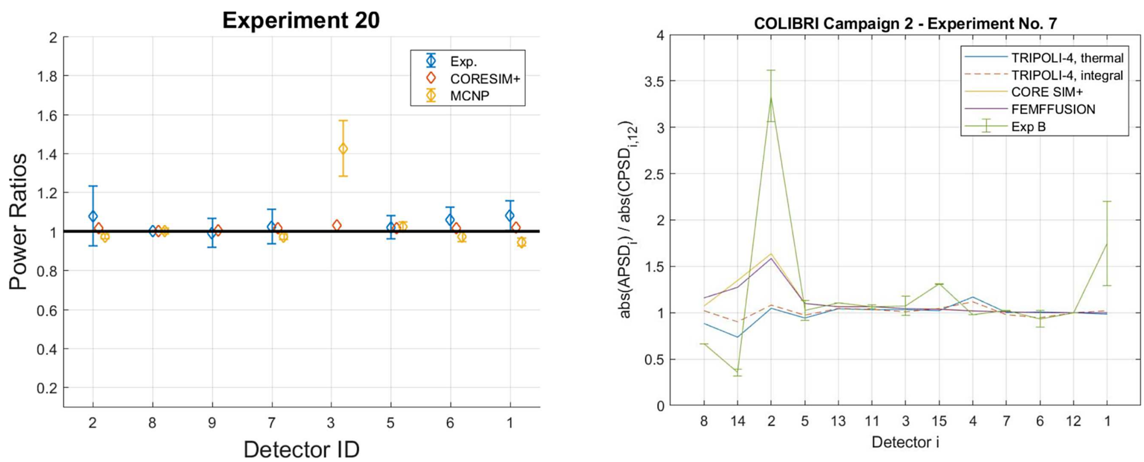

Fig. 4. Comparisons between the calculated and measured neutron noise (given with uncertainties) of the 2nd campaign at AKR-2, experiment #20 (left) and of the 2nd campaign at CROCUS, experiment #7 (right). The figures give the amplitude of the auto-power spectral density of the relative neutron noise (estimated in relation to a reference detector). Figure derived from [21].

values. The comparisons are given at the location of the detectors, ordered at increasing distances from the noise source. It can nevertheless be noticed that in the extreme vicinity of the noise sources, some larger discrepancies can be observed. At those locations, the diffusion-based and transport-based codes also give slightly different predictions, resulting from the difficulty for diffusion theory to properly reproduce steep flux gradients.

4.2.3 Assessment of uncertainties and sensitivity analysis

In CORTEX, a methodology for estimating the uncertainties associated with neutron noise calculations was also developed based on the GRS methodology [22]. In this approach, the input data are perturbed as random variables following their respective uncertainty distributions. By constructing samples of input parameters using Simple Random Sampling, the corresponding samples of output parameters can be computed by the code, from which the uncertainty of the code estimates can be assessed. This method is often referred to as a sampling-based approach.

The sensitivity of the code output to the input parameters can also be evaluated. In the present case, a variance-based approach was considered [23]. It was found that the sensitivity of the neutron noise on the input parameters greatly depends on the spatial distance between the computed neutron noise and the noise source. The closer one is to the noise source, the bigger the effect of the uncertainties on the noise source parameters is. Further away from the noise source, the sensitivity of the computed neutron noise to the uncertainties in the nuclear data becomes more significant [24].

4.3 McSAFER

4.3.1 Experimental investigations

The experimental program is progressing as expected at the MOTEL facility and with some delays at the other facilities (COSMOS-H and HWAT) due to technical and/or delivery issues in the supply chain. In general, the status of the tests can be summarized as follows:

- the commissioning, calibration, and instrumentation checking tests were successfully performed at the three facilities [25].
- The preparation of the first test series at HWAT and COSMOS-H is ongoing, with the following tests being planned:
  - at the HWAT facility: heat transfer for subcooled boiling and CHF, the study of the appropriateness of two critical components (heated riser and pool type condenser) for future transient tests [26].
  - At COSMOS-H: the first test plan consists of a single heated tube made of Zircalloy-4 arranged in an annular gap with an outer glass tube [27]. The heat transfer between the cladding and the coolant is measured for an increasing heat flux. It ranges from subcooled boiling up to critical heat flux conditions.
- The first test series at MOTEL was successfully performed and focused on the helical coil steam generator behavior, including primary/secondary heat transfer at different steady states with different core power levels [28].

Figure 5 shows the axial temperature distribution of the primary side steam generator measured at four different power levels during the MS SG02 test. The averaged axial temperature profiles of the four helical tube groups of the steam generators measured for different power levels are given in Figure 6.

The first results have shown that the MOTEL facility behaves as expected. These data are made available by LUT to the partners involved in code validation. As soon the data of COSMOS-H and HWAT are measured, they will be used to validate the codes by partners. The following MOTEL tests focus on the investigations of the core behavior, including cross-flow under non-symmetrical core conditions considering different axial power profiles.

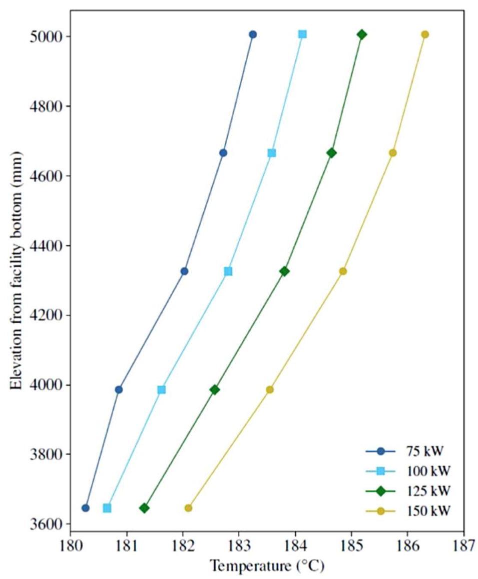

Fig. 5. Primary side steam generator axial temperature profiles with different core power levels during the MS-SG02 experiment.

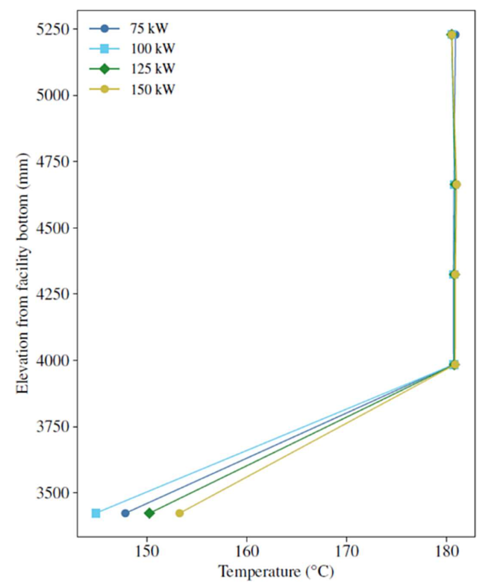

Fig. 6. Averaged axial temperature profiles of all steam generator tubes with different core power levels during the MS-SG02 experiment.

4.3.2 Code validation program

Another important part of the work program is the validation of the thermal-hydraulic codes (Computational Fluid Dynamics – CFD, subchannel, and system thermal-hydraulic codes) with the experimental data generated within the consortium to increase the confidence in the numerical tools used for a safety demonstration. More precisely, the following activities are considered:

- the validation of CFD codes, e.g., CFX, FLUENT, OpenFOAM, TrioCFD, using the experimental data of COSMOS-H, MOTEL, and HWAT.
- The validation of subchannel thermal-hydraulic codes, e.g., CTF, Subchanflow, VIPRE, with the experimental data obtained from the proposed tests.
- The validation of system thermal-hydraulic codes, e.g., TRACE, RELAP-3D, APROS, using the generated test data.

4.3.3 Multi-physics core analysis

Different numerical simulation tools are applied to analyze the core behavior under rod ejection (NuScale, SMART) and cold water injection (CAREM, F-SMOR) transients. Nuclear data libraries for the different simulations are generated with lattice physics codes (deterministic and Monte Carlo), considering the geometrical and material data and operational conditions of the different SMR-cores. The analysis with coupled nodal diffusion codes of the mentioned transients is in an advanced stage, while the high-fidelity simulations are under preparation (SP3 transport and Monte Carlo). Details about the geometry/material of the cores can be found in [29] while the cross-section generation methods for the different solvers (diffusion:

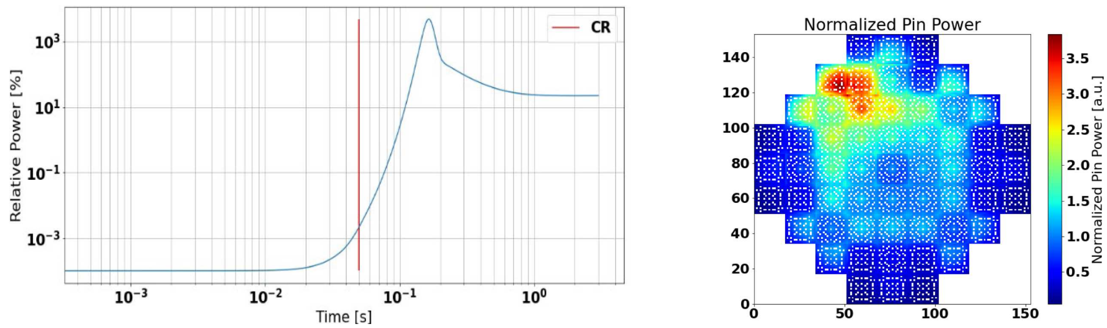

Fig. 7. PARCS/Subchanflow Relative power evolution (left) and radial power distribution (right) in the SMART-core during a REA.

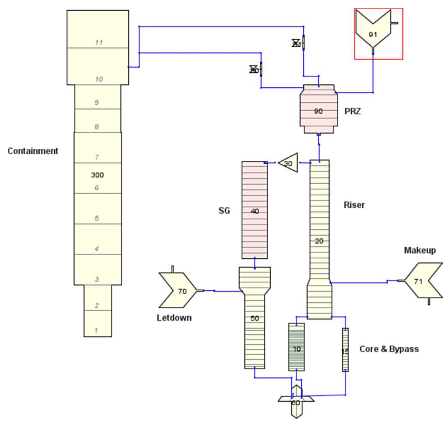

Fig. 8. SMART RPV one-dimensional model for TRACE developed by TRACTEBEL [34].

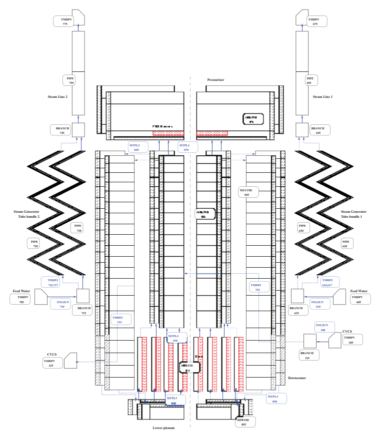

Fig. 9. NuScale RPV three-dimensional model for RELAP-3D developed by UJV [35].

DYN3D, PARCS, APOLLO3, SIMULATE S3K, ANTS, PUMA, PANTHER, transport: PARCS-SP3, APOLLO3, DYN3D-SP3) are described in [30].

In Figure 7, the relative power increase and the 3D radial power distribution predicted with PARCS/Subchanflow for the SMART core in the case of an REA scenario are shown [31]. There, the localized power release at each pin of the fuel assemblies around the position of the ejected control rod is clearly seen.

The methods for the generation of cross sections at pin level for the different low-order transport solvers are developed [31] and the respective REA analysis is at an advanced stage.

4.3.4 Multi-scale RPV and multi-physic/-scale plant analysis

Different coupled versions of thermal-hydraulic codes will be applied to evaluate the three-dimensional thermal-hydraulic phenomena inside the RPV and core of the NuScale and SMART reactors. In Figures 8 and 9, one-dimensional and three-dimensional models of the RPV of SMART and NuScale are shown, developed for TRACE and RELAP5, respectively [32,33].

In Figures 10 and 11, the different CFD models being developed for the SMART and NuScale SMRs and the analysis of the SLB with multi-scale/physic coupled codes are shown. An important step for multi-scale analysis of SMRs is the development of the thermal-hydraulic models of the whole plant and parts of it with different codes, which later on will be combined based on domain decomposition to analyze the plant behavior under accidental conditions.

4.4 METIS

4.4.1 Numerical simulation to allow for site-specific analyses

Seismic risk assessments require the analysis of structural response in order to evaluate the reliability of structures, systems, and components (SSCs). This includes accounting for the impact of local site conditions and soil-structure interaction analysis. This can be achieved simply through generic empirical models, however, these cannot accurately account for the particular conditions of a particular site.

The accurate evaluation of site effects requires the simulation of seismic wave propagation from the source to the site under study. Detailed site response analyses require costly numerical computations. The first task aims to develop simplified (1-D) models that can be used for conducting Soil–Structure Interaction (SSI) analyses. EDF has started working on a strategy to identify 1-D

Fig. 10. TrioCFD model of the downcomer and lower plenum of NuSCALE developed in [36].

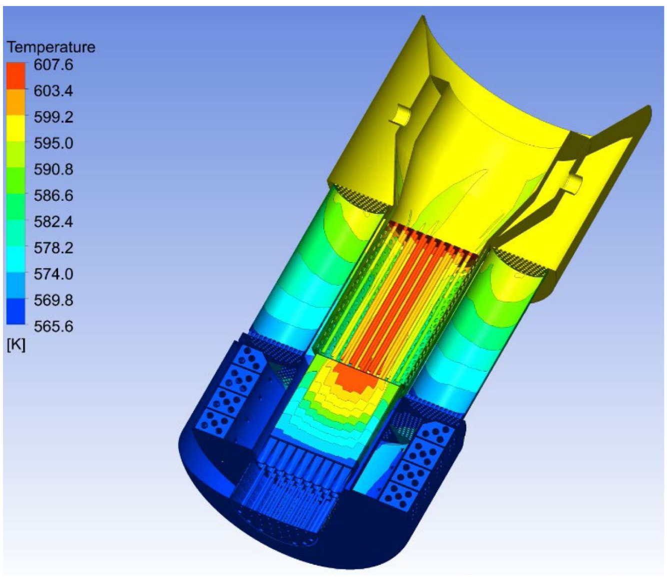

Fig. 11. CFD model of the integral SMART plant developed by KIT [37].

soil columns reflecting observed variability and realistic attenuation due to damping and wave scattering. However, because more complex configurations exist, such as the presence of a sedimentary basin, folded non-horizontal layering, or significant topography, it might be necessary to develop 2-D or 3-D numerical models. For this purpose, we are developing a probabilistic classification scheme to identify sites more likely to be affected by 2-D/3-D side effects, indicating that more complex ground-motion modeling is required. Realistic physics-based 3-D earthquake simulation for source-to-structure wave propagation consists of a powerful numerical tool for seismic response prediction of critical structures submitted to high safety standards [38]. Structural response considering SSI is usually estimated by the Finite Element Method (FEM) approach, as it is considered the most flexible numerical approach for non-linear structural dynamics. The Domain Reduction Method (DRM), which allows for considering a 3-D complex incident wave field as an input to the SSI model, is used here in a Spectral Element Method (SEM) – FEM weak coupling approach with code_aster (see [38] for more details). Moreover, a strategy to represent soil variability at a local scale has been developed. The soil variability is modeled by random fields; the approach is made feasible in a 3D context by HPC capabilities and by optimizing the random field generator by means of the selection of predominant eigenmodes in the Karhunen-Loève representation of the 2-D and 3-D random fields.

The resulting seismic load time histories are then used for the numerical computation of structural and component fragility curves, that is, the failure probability as a function of seismic load intensity.

4.4.2 Uncertainties

One of the main issues in seismic safety assessments is the problem of double counting uncertainties and the accumulation of conservative assumptions arising from the partitioning in disciplines when conducting the analysis from the source to the equipment – see, e.g., [39]. Collective brainstorming has allowed for the development of an integrated approach to account for uncertainty in site response and soil-structure interaction analysis.

4.4.3 Testing model performance by comparison to data and model updating

The work related to verifying and validating Probabilistic Seismic Hazard Assessment (PSHA) models and tools used to define seismic load has started. For this purpose, PSHA models from France and Germany have been implemented into the OpenQuake Engine format, which in conjunction with the 2020 European Seismic Hazard Model, will provide an important suite of complex PSHA models with large numbers of seismic sources and logic tree branches to account for epistemic model uncertainty from which to make comparisons against observations. For the test data, a database of strong and weak motion records has been compiled from the European Integrated Data Archive, and work is ongoing to assess the station quality, database completeness, and the feasibility of using weak motion data to complement the observed strong motions in Europe and to expand the number of sites that can be used for potential testing purposes. Work is underway to begin implementing the "testing, verification and updating toolkit" developed by the partner GFZ Potsdam, Germany.

5 Utilization and cross-fertilization

The CORTEX project had clear ambitions to develop an innovative core monitoring technique for industrial applications. The project required scientists from different disciplines to collaborate and understand each other's paradigms. Those disciplines were: reactor physics, reactor dynamics, reactor modeling, experimental reactor physics, measurement techniques, signal analysis, and artificial intelligence. The project resulted in the demonstration of the usefulness and application of the proposed technique to the industry. In addition to the technical achievements, the project established tight collaborations between the project partners, which extended beyond the project itself. Two project partners were from outside the European Union: an American partner and a Japanese partner. Those collaborations made the partners well equipped for tackling complex problems requiring a cross-disciplinary approach in the future. In order to remain aligned with the needs of the industry, the project made extensive use of its Advisory End-User Group, made of five utilities, two fuel/reactor manufacturers, one technical support organization, and one additional research organization. In the consortium, two consultancy companies servicing the industry were also present. Contacts were also initiated with other US projects using machine learning applied to nuclear engineering.

McSAFER ambitions are twofold: (a) to provide key-experimental data for safety-relevant phenomena of water-cooled SMR for the validation of CFD, subchannel, and system thermal-hydraulic codes and (b) to demonstrate the potentials of advanced and high-fidelity numerical simulation tools for the safety demonstration compared to the traditional codes used in current licensing processes. The wider application of multi-scale/multi-physics numerical tools will contribute to improving the prediction accuracy and reducing the conservatism embedded in current methods. The new generation of tools has large potential to be used not only in safety evaluations (by regulators, TSOs, etc.) but also in the nuclear industry to optimize the design of reactor systems towards higher operational flexibility and enhanced economics while keeping high-safety levels. Many stakeholders may profit from those "new generation" tools if sufficient validation is provided. Finally, yet importantly, the Monte Carlo-based multi-physics tools can provide reference solutions to any low-order simulation, especially for situations where experimental data is not easily available. In view of the powerful HPC cluster nowadays available to the research community at low cost or free of cost, the role of simulation-driven design and optimization, as well as safety evaluations, will greatly increase in the next years.

The open-source strategy adopted by METIS facilitates innovation, international collaborations, and knowledge transfer, and by this means, contributes to increasing the innovation capacity of the nuclear industry and consulting companies. By developing and validating modern state-of-the-art seismic risk assessment methods and open-source simulation tools, it is expected that METIS will contribute to developing new knowledge related to seismic PSA and facilitate innovation in European practice. METIS will influence several technical and scientific sectors, including seismology, seismic hazard analysis, and seismic risk assessment, with opportunities for cross-fertilization among different scientific sectors. The proposed open-source tools help advance the state-of-the-art while at the same time lowering the barrier of entry for aspiring researchers.

6 Conclusions and future recommendations

In CORTEX, it was demonstrated that, for large PWRs, machine learning-based unfolding of the measured neutron noise could correctly identify different types of perturbations and, when relevant, successfully localize such fluctuations. In terms of localization of the noise source, the method can predict the actual location of the perturbation with a mean absolute error below the radial size of one single fuel assembly [40]. Considering the complexity of a nuclear reactor core, its large size (about 4 m in height and radial diameter), and the limited core instrumentation, these results are truly remarkable. To develop an industrial demonstrator, the core monitoring methodology needs to be further refined, improved and tested so that its robustness in industrial setups can be guaranteed. Moreover, following the European Commission Coordinated Plan on Artificial Intelligence 2021 Review [41], the machine/deep learning methods should be transparent, trustworthy, and accountable so that the analysts and users of the methods can better understand the estimates provided by such techniques. Finally, the core monitoring technique should be user-friendly and easy to use so that it can be utilized by analysts and nuclear engineers without any intervention from machine learning or nuclear reactor modeling experts.

At the current stage of advancement of McSAFER, it can be stated that the project is developing as scheduled in the work program. Despite minor delays in delivering some devices for one experimental facility, the test program has started. The development of the models of the core for the four SMR designs is done, and a large part of the analysis is close to being finalized. For the multi-scale analysis of the RPV behavior during the ATWS (SMART) and boron dilution (NuScale) transients, work has been started with the different simulation roots. Finally, the optimization and development of the multi-scale coupling of different thermal-hydraulic codes are near their end. The coupling approaches are being tested with the combination of different TH-modelling approaches for the SMR plants (SMART, NuScale). First, results are produced and evaluated. At the end of the project, a systematic comparison of the different simulation methodologies applied to various SMR designs will be performed, and important conclusions and recommendations to the end-users will be proposed and given.

The METIS project is developing as scheduled with a short delay due to difficulties in the selection and obtaining of data for the METIS case study. The upcoming milestones related to the above-discussed topics are:

- methodology and tools to compute fragility curves (report and code developments + documentation).

- Improved and new tools to compute PSHA with aftershocks and vector-valued seismic intensity measures in Openquake (code and documentation available on github and Openquake website).
- New seismic ground motion simulation tools (codes & documentation).
- METIS Andromeda-SCRAM PSA tool available (report and PSA tool developments with documentation).

All three projects have/had activities dedicated to training, education, and dissemination. Those typically included courses/workshops, publications in open-access journals or conference proceedings, many public deliverables, presentations at conferences/workshops/meetings, the involvement of young scientists in the project, and networking activities with other international projects/initiatives. In addition, various communications channels were developed (websites, social media, newsletters, and popular science presentations/videos).

Acknowledgements

The authors would like to acknowledge all researchers involved in the projects mentioned in this paper, which summarizes some of the results of the collective efforts undertaken within each consortium.

Conflict of interests

The authors declare that they have no competing interests to report.

Funding

The CORTEX project was funded by the Euratom Research and Training Programme 2014–2018 under grant agreement number 754316. The McSAFER project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement number 945063. The METIS project has received funding from the Horizon 2020 program under grant agreement number 945121.

Data availability statement

This article has no associated data generated and/or analyzed / Data associated with this article cannot be disclosed due to legal/ethical/other reason.

Author contribution statement

C. Demazière, V.H. Sanchez-Espinoza and I. Zentner wrote and reviewed the manuscript.

References

1. International Atomic Energy Agency, Advanced surveillance, diagnostic and prognostic techniques in monitoring structures, systems and components in nuclear power plants, IAEA Nuclear Energy Series, No. NP-T-3.14 (2013)
2. I. Pázsit, C. Demazière, Noise techniques in nuclear systems, in *Handbook of Nuclear Engineering*, edited by D. Cacuci (Springer, 2010), Vol. 3
3. C. Demazière, P. Vinai, M. Hursin, S. Kollias, J. Herb, Overview of the CORTEX project, in *Proceedings of the International Conference on the Physics of Reactors – Reactor Physics paving the way towards more efficient systems (PHYSOR2018), Cancun, Mexico, April 22–26, 2018* (2018)
4. A. Durrant, G. Leontidis, S. Kollias, L.A. Torres, C. Montalvo, A. Mylonakis, C. Demazière, P. Vinai, Detection and localisation of multiple in-core perturbations with neutron noise-based self-supervised domain adaptation, in *Proceedings of the International Conference in Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C2021), online, October 3–7, 2021* (American Nuclear Society, 2021)
5. G. Ioannou, T. Tasakos, A. Mylonakis, G. Alexandridis, C. Demazière, P. Vinai, A. Stafylopatis, Feature extraction and identification techniques for the alignment of perturbation simulations with power plant measurements, in *Proceedings of the International Conference in Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C2021), online, October 3–7, 2021* (American Nuclear Society, 2021)
6. T. Tasakos, G. Ioannou, V. Verma, G. Alexandridis, A. Dokhane, A. Stafylopatis, Deep learning-based anomaly detection in nuclear reactor cores, in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C2021), online, October 3–7, 2021* (American Nuclear Society, 2021)
7. V. Sanchez-Espinoza, S. Gabriel, H. Suikkanen, J. Telkkä, V. Valtavirta, The H2020 McSAFER project: main goals, technical work, program, and status, Energies **14**, 6348 (2021)
8. C.A. Cornell, Engineering seismic risk analysis, Bull. Seismol. Soc. Am. **58**, 1583 (1968)
9. R.P. Kennedy, C.A. Cornell, R.D. Campbell, S. Kaplan, H.F. Perla, Probabilistic seismic safety of an existing nuclear power plant, Nuclear Eng. Design **59**, 315 (1980)
10. C.B. Haselton, J. Baker, J.P. Stewart, A. Whittaker, N. Luco, A. Fry, R. Hamburger, R. Zimmerman, Response-history analysis for the design of new buildings in the NEHRP provisions and ASCE/SEI 7 standard: Part I – overview and specification of ground motions, Earthq. Spectra **33**, 373 (2017)
11. C. Blaesius, J. Herb, J. Sievers, A. Knospe, C. Lange, Modelling of FSIs for reactor vessel internals, CORTEX deliverable D1.2 (2020)
12. Openquake platform https://platform.openquake.org/
13. Code_aster FEM code https://www.code-aster.org
14. B.W. Boehm, *Software Engineering Economics* (Prentice-Hall, Saddle River, NJ, USA, 1981)
15. W.L. Oberkampf, T.G. Trucano, Verification and validation benchmarks, Nucl. Eng. Des. **238**, 716 (2008)
16. W.L. Oberkampf, T.G. Trucano, C. Hirsch, Verification, validation, and predictive capability in computational engineering and physics, Appl. Mech. Rev. **57**, 345 (2004)
17. K. Ivanov, M. Avramova, S. Kamerow, I. Kodeli, E. Sartori, E. Ivanov, O. Cabellos, Benchmarks for Uncertainty Analysis in Modelling (UAM) for the design, operation and safety analysis of LWRs – Volume I: specification and support data for neutronics case (Phase I), report NEA/NSC/DOC(2013)7, OECD/NEA (2013)
18. C. Demazière, A. Rouchon, A. Zoia, Understanding the neutron noise induced by fuel assembly vibrations in linear theory, in *Proceedings of the International Conference on Mathematics and Computational Methods Applied*

to Nuclear Science and Engineering (M&C2021), online, October 3–7, 2021 (American Nuclear Society, 2021)
19. P. Vinai, H. Yi, A. Mylonakis, C. Demazière, B. Gasse, A. Rouchon, A. Zoia, A. Vidàl-Ferràndiz, D. Ginestar, G. Verdú, T. Yamamoto, Comparison of neutron noise solvers based on numerical benchmarks in a 2-D simplified UOX fuel assembly, in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C2021), online, October 3–7, 2021* (American Nuclear Society, 2021)
20. V. Lamirand, A. Rais, S. Hübner, C. Lange, J. Pohlus, U. Paquee, C. Pohl, O. Pakari, P. Frajtag, D. Godat, M. Hursin, A. Laureau, G. Perret, C. Fiorina, A. Pautz, Neutron noise experiments in the AKR-2 and CROCUS reactors for the European project CORTEX, EPJ Web Conf. **225**, 04023 (2020)
21. P. Vinai, K. Ambrozic, A. Brighenti, C. Demazière, B. Gasse, D. Ginestar, M. Hursin, S. Hübner, A. Knospe, V. Lamirand, C. Lange, A. Laureau, R. Macian, A. Mylonakis, O. Pakari, A. Rais, A. Rouchon, S. Santandrea, Z. Stankovski, G. Verdú, A. Vidal-Ferràndiz, T. Yamamoto, H. Yi, S. Yum, I. Zmijarevic, A. Zoia, Final validation report, CORTEX deliverable D2.5 (2021)
22. M. Kloos, E. Hofer, SUSA – PC, a personal computer version of the program system for uncertainty and sensitivity analysis of results from computer models, version 3.2, User's guide and tutorial, Gesellschaft für Anlagen- und Reaktorsicherheit, Garching, Germany (1999)
23. S. Yum, R. Macian, P. Vinai, Methodology for uncertainty and sensitivity analysis, CORTEX deliverable D1.1 (2019)
24. S. Yum, M. Hursin, A. Vasiliev, P. Vinai, A.G. Mylonakis, C. Demazière, R. Macián-Juan, Uncertainty analyses of neutron noise simulations in a zero-power reactor, Ann. Nucl. Energy **174**, 109157 (2022)
25. K. Tielinen, J. Telkkä, E. Kotro, V. Kouhia, H. Suikkanen, Description of the MOTEL facility and instrumentation, McSAFER deliverable 2.4, Helsinki (2021)
26. D. Grishchenko, HWAT experimental setup and test matrix for first test series, McSAFER deliverable number 2.7, Stockholm (2021)
27. S. Gabriel, G. Albrecht, W. Heiler, F. Heineken, COSMOS-H experimental setup and tests, McSAFER deliverable number 2.1, Karlsruhe (2021)
28. J. Telkkä, A. Räsänen, E. Kotro, H. Suikkanen, Results of the MOTEL helical coil steam generator behaviour experiments, McSAFER deliverable number 2.5, Helsinki (2021)
29. V. Ville, F. Anthime, F. Emil, L. Héctor, M. Luigi, Specifications for the reactivity transients scenarios in the four SMR cores, McSAFER deliverable number 3.1, Helsinki (2021)
30. E. Fridman, D. Ferraro, V. Valtavirta, H. Lestani, L. Mercatali, R. Vocka, Y. Bilodid, M. Seidl, A. Fard, Group constant generation for the state-of-the-art codes, McSAFER deliverable number 3.2, Dresden (2021)
31. E. Fridman, J. Blanco, H. Lestani, A. Farda, V. Valtavirtta, State-of-the-art solutions for the transient scenarios in the four SMR cores, McSAFER deliverable number 3.4, Karlsruhe (2022)
32. L. Amiradable et al., Analysis of NUSCALE plant with 1D system code and intercomparing between codes, McSAFER deliverable number 4.2, Petten (2022)
33. TRACTEBEL, Analysis of SMART plant with 1D system TH Codes, McSAFER deliverable number 4.1, Brussels (2022)
34. V. Jammot, N. Palmas, Status of WP4 and WP5 Tractebel Contributions, McSAFER Status Meeting WP4 and WP5, McSAFER, 20 July 2021 (2021)
35. M. Bencik, Multiscale RPV analysis methodologies for SMR, McSAFER Progress Meeting, McSAFER, 20 July 2021 (2021)
36. A. Grahn, CFD simulations of NuScale downcomer, McSAFER Progress Meeting on WPs 4 and 5, McSAFER, 20 July 2021 (2021)
37. M. Böttcher, Analysis of stationary plant conditions of SMART with Ansys CFX, McSAFER internal report, Karlsruhe (2021)
38. M. Korres, F. Lopez-Caballero, V. Alves Fernandes, F. Gatti, I. Zentner, F. Voldoire, D. Clouteau, D. Castro-Cruz, Enhanced seismic response prediction of critical structures via 3D regional scale physics-based earthquake simulation. J. Earthq. Eng. (2021), DOI: 10.1080/13632469.2021.2009061
39. I. Zentner, J. Berger, M. Caudron, An integrated approach for the transfer of seismic load from bedrock to the structure based on RVT and CMS, in *Proceedings of the 17th World Conference on Earthquake Engineering (17WCEE), September 27-October 2, 2021, Sendai, Japan* (2021)
40. A. Durrant, G. Leontidis, S. Kollias, 3D convolutional and recurrent neural networks for reactor perturbation unfolding and anomaly detection, EPJ Nucl. **5**, 20 (2019)
41. https://digital-strategy.ec.europa.eu/en/policies/plan-ai

Cite this article as: Christophe Demazière, Victor Hugo Sanchez-espinoza, and Irmela Zentner. Advanced numerical simulation and modeling for reactor safety – contributions from the CORTEX, McSAFER, and METIS projects, EPJ Nuclear Sci. Technol. **8**, 29 (2022)