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Development and application in multiscale and multiphysics methodologies in Spain: Present and future trends

Sergio Gallardo [a,*], Francisco Álvarez-Velarde [b], Teresa Barrachina [a], Óscar Cabellos [c], Emilio Castro [c], Max Casamor [d], Diana Cuervo [c], Alberto Escrivá [e], Jordi Freixa [d], Nuria García-Herranz [c], Victor Martinez-Quiroga [d], Rafael Miró [a], César Queral [c], Yago Rivera [e], Jorge Sánchez-Torrijos [f], Amparo Soler [f]

[a] *Instituto Universitario de Seguridad Industrial, Radiofísica y Medioambiental (ISIRYM), Universitat Politècnica de València, Camí de Vera s/n, 46022 València, Spain*
[b] *Departamento de Fisión Nuclear, Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT), Avda Complutense 40, 28040 Madrid, Spain*
[c] *Universidad Politécnica de Madrid (UPM), Ramiro de Maeztu 7, 28040 Madrid, Spain*
[d] *Advanced Nuclear Technologies, Universitat Politècnica de Catalunya, Av. Diagonal 647, 08028 Barcelona, Spain*
[e] *Instituto Universitario de Investigación de Ingeniería Energética (IIE), Universitat Politècnica de València, Camí de Vera s/n, 46022 València, Spain*
[f] *NFQ Group, Nuclear Department, Calle de O'Donnell 34, 28009, Madrid, Spain*

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ABSTRACT

In the field of reactor physics analysis, the coupling of multiple physics phenomena plays a crucial role in enhancing the accuracy of predictions and understanding complex systems. Multiphysics refers to the study and analysis of physical phenomena that involve multiple interconnected physical processes occurring simultaneously in a nuclear system to ensure essential aspects of reactor design, safety analysis, and optimization, among others. Multiphysics encompasses various domains of physics, such as Thermal-Hydraulics, Neutronics, Structural Mechanics, Radiation Transport, Chemistry, and Materials Science. On the other hand, the Multiscale approach involves combining high-fidelity models with lower-fidelity ones to accurately capture the relevant physical phenomena in a Nuclear Power Plant (NPP). Multiscale involves three main scales: system level, core level, and detailed analysis scale. This paper presents an overview of the main research performed by Spanish groups in the field of multiphysics and multiscale calculations, particularly on thermal–hydraulic analysis. This revision is focused mainly on two key aspects: thermal–hydraulic multiscale coupling and thermal–hydraulic / neutronic coupling. The paper also includes the expected future trends in this field.

1. Introduction

Multiphysics refers to the study and analysis of physical phenomena that involve multiple interconnected physical processes occurring simultaneously in a nuclear system. These processes can encompass various domains of physics, such as Thermal-Hydraulics (TH), Neutronics (NK), Structural Mechanics, Radiation Transport, Chemistry, and Materials Science. Integration (or coupling) of multiphysics provides a comprehensive framework to analyze and understand nuclear systems, including thermal characteristics, coolant flow, and material deformation. This coupling enables a more accurate representation of complex interactions within reactors, ensuring that essential aspects of reactor design, safety analysis, and optimization are addressed. In this frame, Zhang (2020) points out the importance of considering various scales (Multiscale), including system level, subchannel or subassembly level, and pin-by-pin level, to accurately capture the physical phenomena in a Nuclear Power Plant (NPP). Concerning thermal-hydraulics aspects, to achieve reliable and efficient calculations, system TH codes like RELAP5 (Nuclear Regulatory Commission, 1995), TRACE (Nuclear Regulatory Commission, 2016); and ATHLET (Lerchl et al., 2012) use 1D or 3D coarse-meshes. Subchannel codes such as COBRA-TF (Salko et al., 2015) divide the core region into groups of channels for accurate modeling of thermal–hydraulic operating limits and safety margins at a sub-channel level. To capture 3D effects, CFD codes like ANSYS-CFX (ANSYS, Inc., 2021) and OpenFOAM (OpenFoam Foundation, 2019) are employed, particularly for addressing single-phase problems in primary and secondary circuits.

Some examples of coupling between system TH and subchannel

* Corresponding author.
E-mail address: sergalbe@iqn.upv.es (S. Gallardo).

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codes are the following. The Pacific Northwest National Laboratory (Thurgood et al., 1983) developed a TRAC/COBRA-TF coupling, however, it has not been maintained or updated with the new versions of COBRA or TRAC. Later in 1992, KAERI developed a coupling between COBRA-TF and RELAP5/MOD3.2 (Lee, et al., 1992). Both codes run in parallel on different processors and the exchange of information is carried out using Inter-Process Communication (IPC) techniques. KAERI continued developing the coupling between RELAP5 and COBRA-TF and, in 1996, developed MARS (Jeong et al., 1999), which uses a serial computation model that includes 1-D (RELAP5) and 3D (COBRA-TF) modules to simulate multi-dimensional two-phase flow transients. Weaver et al., (2002) developed a RELAP5-3D/COBRA-TF coupled code using the semi-implicit numerical methodology. In this case, both codes are compiled separately, using the Parallel Virtual Machine (PVM) software package for communication between the programs.

Regarding the coupling between System TH and CFD codes, the following examples can be found in the literature: RELAP5/FLUENT (Yan et al., 2008); RELAP5-3D/FLUENT (SCK-CEN) (Toti et al., 2018) RELAP5-3D/CFX (University of Pisa) (Mengali et al., 2012); ATHLET/FLUENT (UJV-Rez) (Vyskocil and Macek, 2014); ATHLET/OpenFOAM (Karlsruher Institut für Technologie, KIT) (Huber et al., 2013); TRACE/CFX (Paul Scherrer Institute) (Bertolotto et al., 2009) and TRACE/FLUENT (National Tsing Hua University) (Ku et al., 2015). The coupling of computational domains in thermal–hydraulic solvers (system, subchannel, and CFD) is crucial. Meshes used in these codes have varying spatial resolutions, which necessitates proper translation of data between them. Using a third-party mesh-processing toolkit, such as the SALOME platform (Cascade, 2023), may be necessary for accurate translation and data transfer between different meshes.

Multiscale simulation provides a detailed understanding of the interactions between different scales. This enables a deeper characterization of complex systems that would not be possible with single-scale simulations, leading to better predictions of the reactor's behavior. On the other hand, multiscale simulations can be highly complex, requiring advanced numerical techniques and computational resources. Validating multiscale simulations is challenging due to the need for experimental data at multiple scales. Obtaining accurate experimental data across different scales is difficult, limiting the ability to validate and refine multiscale models effectively. Maintaining stability throughout the simulation process is crucial for obtaining reliable results, but it is difficult to achieve across diverse scales. Finally, developing multiscale simulation models is time-consuming. The process of verifying and validating multiscale models often requires iterative adjustments, contributing to longer times compared to single-scale simulations.

The interaction between TH and NK has an essential role in reactor design and safety analysis. According to Wang et al., (2020), TH/NK coupling can be categorized into tight and loose coupling. Loose coupling involves solving the neutron transport equation and conservation equations of thermal hydraulics separately (decoupled). On the other hand, tight coupling involves developing new calculation codes to solve the neutron transport equation without decoupling both TH and NK codes. Loose coupling benefits from well-established NK and TH codes, where deterministic and stochastic methods like Monte Carlo can be employed for the neutronic part. High-fidelity methods are currently available for modeling neutronics, thermal-hydraulics, and thermal-mechanics, but practical coupling for transient analysis remains challenging.

Multiphysics computational platforms are being developed to couple 3D neutron kinetics transport or diffusion codes with system, subchannel, or CFD TH codes. Such coupling enables the analysis of core kinetics behavior with plant dynamics. In the literature, different deterministic or stochastic neutronic codes can be found, used in TH/NK loose coupling approaches. Examples of deterministic codes are PARCS from the Nuclear Regulatory Commission (USNRC) (Downar et al., 2012), COBAYA developed by the Universidad Politécnica de Madrid (COBAYA team, 2015), and DeCART developed by the Korea Atomic Energy Research Institute (Joo et al., 2004).

Concerning stochastic or Monte Carlo codes, examples are MCNP developed by Los Alamos National Laboratory (MCNP team, 2014) and Serpent from VTT Technical Research Centre (Leppänen et al., 2015). Other examples of Monte Carlo codes are the following: OpenMC from the Massachusetts Institute of Technology (Romano and Forget, 2013) and TRIPOLI-4 developed by the Commissariat à l'Energie Atomique -France- (Jaboulay et al., 2014).

Some examples of the resulting TH/NK coupled systems are the following: COBAYA4/COBRA-TF by Universidad Politécnica de Madrid (García-Herranz et al., 2017); PARCS/COBRA-EN (Noori-Kalkhoran et al., 2014); PARCS/RELAP5 (Kouidri et al., 2015) and DeCART/TRACE (Hursin et al., 2012), among others.

Multiphysics enables the simultaneous modeling of multiple physical phenomena in different domains within the same simulation framework. This allows for a comprehensive understanding of complex systems where different physics interact, such as, e.g., fluid dynamics, heat transfer, and chemical reactions. By capturing the interactions between different physics phenomena, multiphysics leads to more accurate simulations that better reflect actual conditions. Furthermore, multiphysics facilitates the integrated design of complex systems by considering the mutual influences of different physics phenomena on system performance. However, multiphysics is computationally intensive, requiring significant computational resources to solve coupled equations accurately. Coupling physics phenomena can lead to numerical instabilities. Managing these instabilities requires careful selection of numerical methods, discretization schemes, and solver settings to ensure robust and accurate solutions. Furthermore, multiphysics can be more difficult to set up and validate due to the increased complexity of the models and their interactions. Integrating multiple physics phenomena requires expertise in various disciplines to ensure the accuracy and reliability of the simulations.

In Spain, several research groups are actively engaged in the development and application of multiscale and multiphysics coupling. This paper compiles the experiences in this field from the following institutions and research groups:

- Advanced Nuclear Technologies (Universitat Politècnica de Catalunya, UPC).
- Nuclear Innovation (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, CIEMAT).
- Department of Energy Engineering (Universidad Politécnica de Madrid, UPM).
- Engineering School of Mining and Energy (Universidad Politécnica de Madrid, UPM).
- Nuclear Safety and Bioengineering of Ionizing Radiation group (SENUBIO), Instituto Universitario de Seguridad Industrial, Radiofísica y Medioambiental (Universitat Politècnica de València, UPV-ISIRYM).
- Instituto Universitario de Investigación de Ingeniería Energética (Universitat Politècnica de València, UPV-IIE).
- NFQ Group.

Next, a description of the main research areas of each group is provided.

The "Advanced Nuclear Technology" (ANT) research group (Universitat Politècnica de Catalunya, UPC) works in different lines with simulation tools at different scales and degrees of detail (neutron transport code and radiation through Monte Carlo techniques – MCNPX, GEANT4, FLUKA-, CFD codes with MHD simulation capabilities, TH codes at different scales with coupling to reactor kinetics codes. The combination of these capabilities allows the ANT group to deal with complex problems that require an interdisciplinary computational platform. In the field of thermal hydraulics, the R&D activity of the research team has been focused on technology transfer to the industry and regulatory bodies. ANT participates in many international OECD projects featuring experimental TH facilities of different sizes. The final goal is to obtain high-fidelity multiphysics and multiscale results to predict accurately the behavior of a NPP.

The research group "Nuclear Innovation" (Centro Investigaciones Energéticas, Medioambientales y Tecnológicas, CIEMAT) started more than 20 years ago, focused on the neutronics of current and advanced nuclear reactors, including aspects of design, fuel cycle, and the performance of experiments for better measurement of the reaction cross sections. Later, multiphysics was included in the research areas by coupling TH and NK codes, forming the COUNTHER code. This activity has been performed in EU projects for the analysis of transients in thermal and fast reactors, and for a better estimation of the temperature and power maps of the core.

The research group "Science and Technology of Advanced Nuclear Fission Systems" (Universidad Politécnica de Madrid, UPM) includes Reactor Physics -neutronics, thermal-hydraulics, and multiphysics for both current generations and Generation-IV fast reactors- among their research areas of interest.

The research in Reactor Physics focuses on the development of beyond-state-of-the-art methods and computer codes for multiphysics and multiscale steady-state and transient reactor analysis, including cross section generation and coupling algorithms. The final goal is to address the current demands for more accurate and efficient calculations, which directly relate to the safety of current and next generations of nuclear reactors.

The research group from the Engineering School of Mining and Energy (Universidad Politécnica de Madrid, ETSIME-UPM) has more than 30 years of experience in nuclear safety analyses. During that period, the group has performed different safety analysis applications using different codes, such as TRACE, MELCOR, RELAP5, MAAP, HIPA, TRETA, TIZONA, TRANSURANUS, RiskSpectrum, to PWR, BWR, VVER, AP1000, SMRs-LWR, and fusion facilities. Those tools have been applied following different approaches like best-estimate, conservative, BEPU, dynamic PSA, E-BEPU, and severe accident. Regarding multiscale and multiphysics activities, most of the activities performed by the ETSIME-UPM has been developed within the H2020 'High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors' (McSAFER) European project.

The group "Nuclear Safety and Bioengineering of Ionizing Radiation", SENUBIO, is a research group of the research institute ISIRYM (Universitat Politècnica de València, UPV). Among the objectives of this multidisciplinary group, stands out the development of a multiphysics platform to perform complex transient analysis in NPPs using coupled codes. For that purpose, in recent years the group has developed different couplings TH-TH and TH-NK. The TH codes used are TRACE, TRAC/BF1, RELAP5 and COBRA-TF. The NK neutronics codes are VALKIN3D and VALKIN-FVM owned by ISIRYM, and the commercial codes NEM and PARCS. The couplings developed include the following codes: TRACE/CTF, TRAC-BF1/NEM, TRAC-BF1/PARCS, RELAP5/PARCS, CTF/PARCS, TRACE/CTF/PARCS/FRAPCON-FRAPTRAN. The group has applied these developments to the analysis of RIA (Reactivity-Initiated Accidents) and analysis of instabilities, together with the simulation of ATWs (Anticipated Transient Without Scram), Rod Ejection Accident, Control Rod Drop Accident, etc. Another line in which the group works is in the development of neutronic codes. The neutronics code VALKIN3D was the first and later the code VALKIN-FVM-Sn was developed.

The research lines within the "Thermal-hydraulics and Nuclear Energy" group (Universitat Politècnica de València, UPV-IIE) are focused on the exploration of nuclear engineering disciplines and cover the field of thermal-hydraulics and safety. The multifaceted approach integrates computational simulations using advanced software like RELAP5, TRACE, and CFX, and experimental investigations through state-of-the-art laboratory equipment, such as Planar Laser-Induced Fluorescence (PLIF), Particle Image Velocimetry (PIV), Laser Doppler Velocimetry (LDV) and high-speed cameras. The group actively engages in nuclear safety analysis, focusing on reactor stability, criticality calculations, and radiological consequences and has the expertise to support fuel reload licensing and has conducted extensive work on the Code Scaling Applicability and Uncertainty methodology. Furthermore, it participates in international benchmarks and collaborations with prominent organizations like the USNRC, Spanish Nuclear Safety Council (CSN), the IBERDROLA group, UNESA, CIEMAT, Trillo NPP and Leibstadt NPP.

Formerly known as Nfoque Advisory Services, NFQ Group stands as a Spanish consultancy firm headquartered in Madrid (Spain), with broad experience in the nuclear sector. The main expertise is related to providing support in nuclear design, reactor license calculations, monitoring of the operating cycle, neutronic noise calculation, development of best-estimate methodologies for nuclear safety calculations with TH and NK coupled codes, and development and maintenance of NPP license simulation codes. NFQ group is also participating in several international benchmarks related to Generation III + NPPs and advanced fuel designs such as ATFs.

This work is structured as follows: in section 2 general aspects of multiscale coupling are exposed. Section 3 is devoted to multiphysics coupling, including TH-NK coupling and applications; fluid dynamics / thermo-mechanics coupling and simulation platforms. Finally, in Section 4 the future trends in the research of multiphysics and multiscale are exposed.

2. Multiscale coupling

2.1. Multiscale approach

Nuclear reactors are installations that include a high level of heterogeneity and where the physical phenomena must be analyzed at different scales as they usually have origin as local effects but eventually impact the whole plant. With the tools that are available nowadays, the same system can be described with different levels of fidelity. The higher fidelity models represent better the physical processes than the lower fidelity ones, but they require more computational resources and time. Therefore, a combination of both types of tools may result in the optimum solution for the problem.

Three main scales are considered when modeling TH systems: (1) the full system scale carried out with system codes allows for the analysis of system behavior; (2) the subchannel scale for representing the physics taking place in between fuel rods and (3) the detailed analysis of specific regions that can be carried out by CFD codes.

The codes that can work at the system scale include the ability to model plant components such as pipes, heat exchangers, pumps, valves, and their associated control systems. In most cases, they use rather coarse models for the core and simple reactivity models that determine the power distribution. In some cases, these codes may include 3D components to model the reactor vessel but the level of detail of the set of equations and correlations is not as specific as in subchannel codes, which are associated with the modeling of the reactor core and fuel bundles at a subchannel level. In this case, the 3D formulation is used, and they can achieve a great level of detail when predicting key parameters such as the critical heat flux and Departure from Nucleate Boiling Ratio (DNBR). CFD codes use finer 3D meshings and more complex physical models. Considering the limitations of each of the three approaches in TH, it is evident that coupling is needed to provide high fidelity simulations.

The possible applications of TH-TH coupling are:

- System codes coupling with subchannel codes to evaluate in detail the cladding performance.
- System codes coupling with CFD codes to account for mixing phenomena taking place in large open areas and complex geometries.

In TH-TH coupling for licensing simulations, the coupling method can be simplified to the off-line transfer of some boundary conditions from one code to the other (off-line coupling). The off-line coupling is fast and sufficiently accurate in many situations. In a typical TH-TH off-line coupling, the core outlet pressure would be imposed from the system code to the subchannel, while temperature and mass flow rate would be imposed at the core inlet.

In other cases, more complex coupling methods between system and subchannel codes are achieved by applying on-line coupling methods. This is achieved by compiling the two codes together or by the use of a software to interconnect them such as Parallel Virtual Machine (PVM). In this case, the core is usually only modeled by the subchannel code since a separate domain scheme is used. These methods imply coherent boundary conditions between codes in all the domains. One example of this scheme is the coupling between the TRACE (system) and CTF (subchannel) codes. This coupling allows to improve the predictive capacity of the TRACE code in the reactor core. The 3D characteristics and the greater detail in the geometric representation of the fuel elements, together with the use of three fields in the representation of the two-phase fluid and some advanced physical models, make the subchannel code the ideal complement for the detailed representation of the reactor core. This TH tool is implicitly designed for the detailed analysis of LWR cores. It uses two phases and three fields (continuous liquid, dispersed liquid droplets in certain boiling regimes, and vapor) as an approximation to the two-phase fluid whose conservation equations are solved in a 3D orthogonal mesh.

2.2. Coupling methods

The semi-implicit method is one of the most used in TH computational codes because it combines some good convergence and acceptable levels of diffusion and numerical stability. In this type of scheme, the values of some variables are taken from the previous time-step and combined with others in which the new time-step is used. The coupled codes are based on the replacement of part of the model of one code by the domain simulated by the other, with real-time feedback existing between both codes, that is, maintaining the necessary synchronization between both codes. This is the most used in TH-TH coupling.

To implement this type of coupling the following assumptions are made:

- One code is defined as the main process, and therefore it is always responsible for solving the system of equations associated with the connection driver between codes.
- It is assumed that the secondary code is always used to simulate parts of the whole domain.
- Apart from these two assumptions, to properly solve the system formed by the union of two simulated domains, it is necessary to implement a communication scheme between codes. In this scheme, the variables necessary for the simulation to be synchronized must be communicated: time, current time step, logical variables to indicate convergence or need for backup, etc.
- To do this, the secondary code must be compiled as a static library that links to the executable of the main code project. Once the joint compilation project has been prepared, all the necessary subroutines and functions have been programmed so that secondary code can communicate internally with the master code, exchanging the necessary information at each stage of the internal coupling process.
- It is also necessary to exchange, for instance in TH-TH coupling, the state variables of the fluid and the solid to reconstruct the conservation equations of the adjacent cells of different processes: geometric variables, velocities/flows, temperatures, densities, phase fractions, etc.

The domain modeled with the main code represents the entire system that is pretended to simulate except for the component(s) that you want to analyze in greater detail using the slave (reactor core, for instance). Both domains are coupled through a driver component defined in both codes, as shown in Fig. 1.

As seen in Fig. 2, the meshes of both codes should overlap in the center of a cell of the mesh of both codes (and therefore between the faces of the conservation mesh). The transport of variables and quantities through the interface of the meshes of both codes is carried out through the external type unions defined within external components connected at this point of the mesh. For the coupling to function correctly, the conservation of the different variables at the mesh interconnection points must be ensured.

The control of the time step is done by the leader code (master code). If both codes use semi-implicit methods for temporal discretization, their selected time step must comply with the Courant limit to ensure numerical stability. The time step of the coupled code must be unique. Therefore, the most restrictive of the codes is the one that marks the size of the time step in each temporal advance.

In contraposition to implicit couplings, an internal explicit coupling scheme can be performed. This type of coupling is temporally explicit because the two domain (physics) equations are not solved at the same time, using a joint scheme. The codes only exchange the values necessary to provide boundary conditions for each other at each time step. Each code solves its system of equations and the convergence of both is ensured for each time step through the coupling feedforward control scheme. Temporally it is equivalent to the typical explicit coupling scheme in a leader/follower code system (master/slave) like the one in Fig. 3.

The transfer of information between codes is carried out through internal communication. This is possible when both codes are included in the same compilation project, thanks to this the possibility of mutual transfer of information within the same joint execution is enabled. That is, one is embedded in the other with bidirectional data transfer between the codes. It is necessary to implement effective communication for the correct functioning of the coupled code. As mentioned above, internal communication avoids the need to use additional external libraries and protocols for communication. This type of communication implies that both codes should be included in a single compilation project and a single executable is obtained in which the coupled code is integrated.

2.3. TH– TH coupling and applications

In Spain, there is extensive experience in coupling codes in TH multiscale. Spanish research groups developed a series of studies and applications, in which coupling between system and subchannel codes have been performed. Regarding system codes, notable efforts have been made with RELAP5 and TRACE. Concerning subchannel codes, it is worth noting the coupling with CTF and SUBCHANFLOW (Fig. 4). The following is a review of the main works in multiscale coupling.

TRACE / CTF. In 2017, Abarca (Abarca, 2017) from UPV, developed a coupling between TRACE and CTF. This coupling was programmed using the parallelization and communication components between processes presented by the TRACE code through the Exterior Communications Interface (ECI). For this purpose, small modifications had to be made to the TRACE source code. A substantial modification of CTF was necessary to program the entire communication interface with TRACE, implementing the semi-implicit coupling equations and the pressure correction terms within its resolution scheme. This code has been tested and qualified against PWR and BWR steady state and transient scenarios, including even 3D neutronics, as a real control rod insertion operational transient in a KWU reactor and the turbine trip Peach Bottom 2 Benchmark.

RELAP5 / CTF. The UPC in collaboration with North Carolina State University (NCST) and the CSN developed a semi-implicit coupling between RELAP5 and CTF codes Casamor et al. (2022). The coupling was implemented by applying the methodology presented by (Weaver et al., 2002) which was also used by (Soler, 2011) for the semi-implicit thermal–hydraulic coupling of advanced subchannel and system codes for

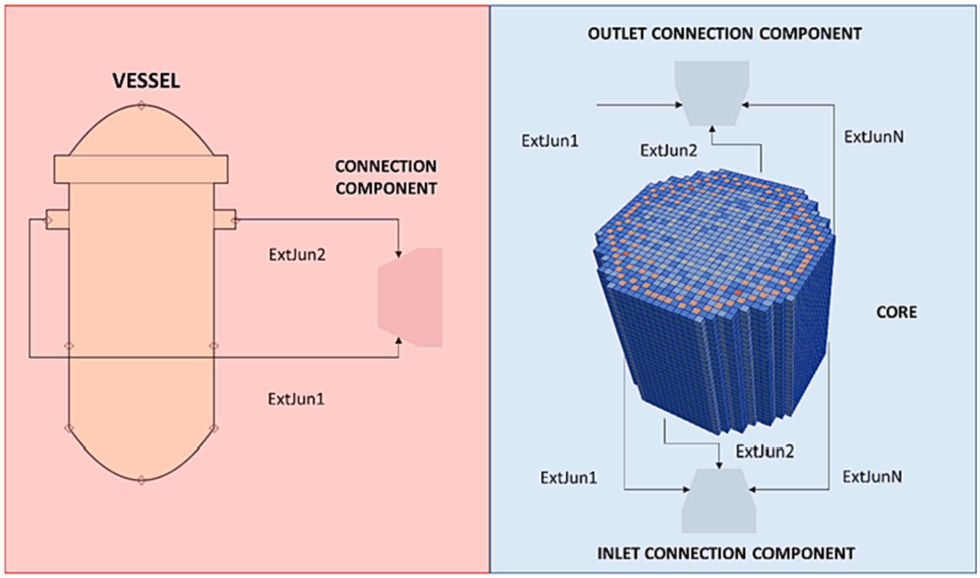

Fig. 1. Example of two TH coupled domains.

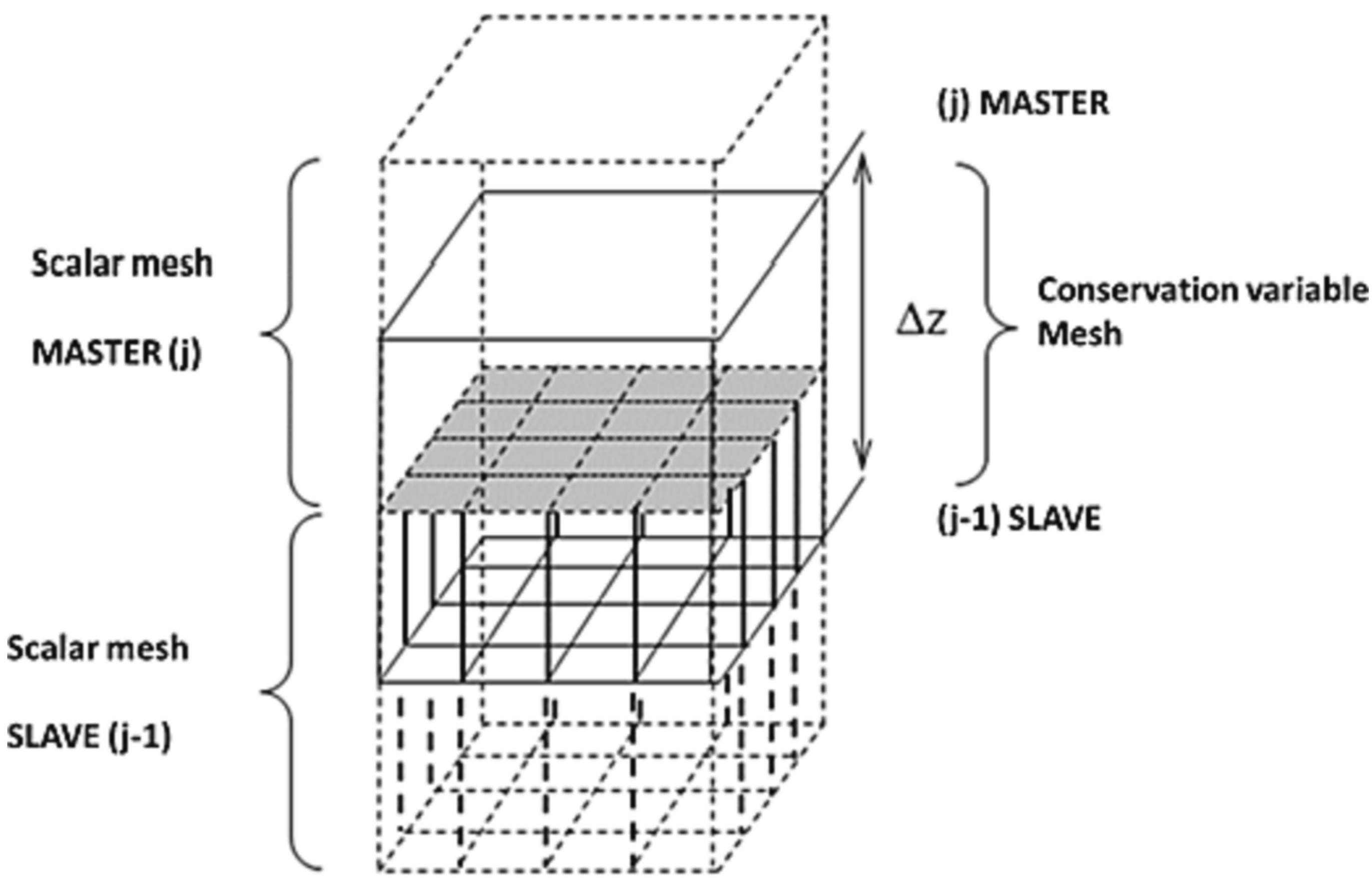

Fig. 2. Scheme of a 1:16 mesh between two subdomains.

PWR transient applications using Fortran 77 versions of RELAP5-3D and COBRA-TF at The Pennsylvania State University (PSU). The main contribution of this study was the development of improved general coupling interfaces, which were designed to perform axial and lateral coupling between two codes while accounting for the differences in the code models as well as improving the stability and numerics of the coupled scheme.

In addition to the coupling, a two-scale subchannel approach was implemented for simulating some fuel assemblies with a single channel (assembly-level approach) and some fuel assemblies at a subchannel level. The two approaches were performed together and in combination with the system analysis. The developed coupled tool provided detailed results of the fuel response to failures or malfunctions of system-related components. On the other hand, the tool presented some important

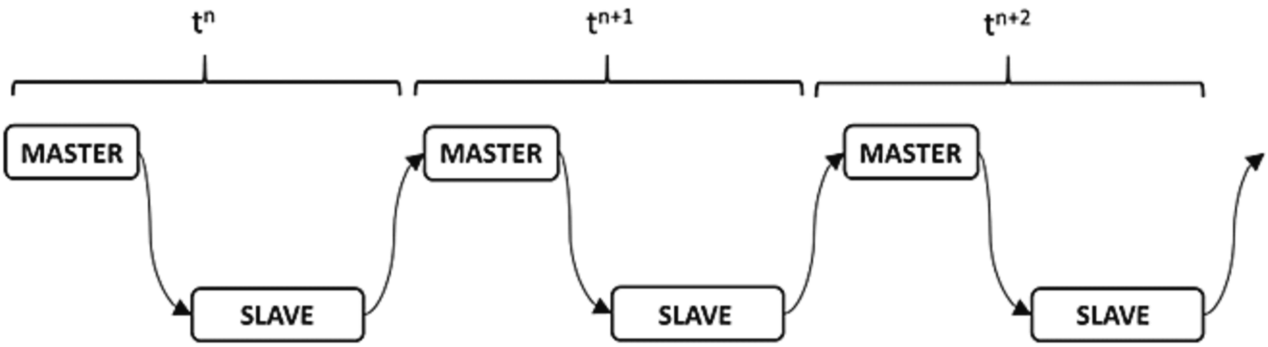

Fig. 3. Explicit coupling scheme.

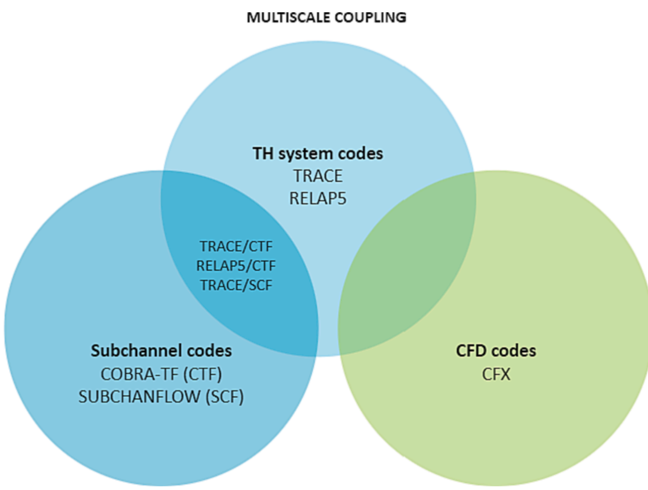

Fig. 4. Multiscale coupling.

limitations because it was generated for the study of specific cases related to the DNBR (Fig. 5). In this sense, the tool only was tested for liquid phase and upward flows and cannot be used for transients involving two-phase flow conditions at the core inlet. However, it is worth recalling that CTF is mostly used in safety analysis to predict the cladding response, i.e., the critical heat flux and DNBR, and this analysis is, in general, applied when the flow enters the core from the bottom and in subcooled conditions. In his Ph.D. thesis (Casamor, 2022) provided a comparison between conservative and BEPU approaches and the implications of the different coupling approaches (off-line and on-line).

TRACE / SUBCHANFLOW (SCF). In the framework of the H2020 European McSAFER project and as a result of the collaboration between the research groups from the UPM and the Karlsruhe Institute of Technology (KIT), an application of the coupling TRACE and SUBCHANFLOW (SCF) was performed. A comparison of the results obtained using the TRACE standalone (1D and 3D modeling approach) and the multiscale TRACE/SCF calculations of the boron dilution transient in a NuScale-like reactor can be found in (Sánchez-Torrijos, 2023). The TRACE/SCF coupled tool was developed by the KIT research group, and it takes profit from the Interface for Code Coupling (ICoCo) methods and MEDCoupling library capabilities to perform the data exchange using a domain decomposition coupling approach along with the SALOME platform (Zhang, 2021). It should be noted that data exchange between both codes was performed at the core inlet and core outlet region using FILLs and BREAKs components to introduce the data from SCF as boundary conditions in the TRACE model at each time step and vice versa.

3. Multiphysics coupling

3.1. Thermal-hydraulics / neutronics

Numerous publications conclude that 3D TH-NK coupled codes are the only ones that allow to practically describe, in a reasonable computing time and with precision, the phenomena that take place in the reactor core and the interaction with the rest of the plant dynamics (Uhle and Aktas, 2000). In addition, it has also been shown that high-performance computing techniques can provide the degree of development necessary to make possible a substantial decrease in computing time for this type of problem (Ivanov et al., 2000). The use of multiphysics platforms in which TH and NK are jointly simulated in Nuclear Safety is supported by the conclusions drawn after the publication of the CSNI Integral Test Facility Validation Matrix for the Assessment of Thermal-Hydraulic codes for LWR LOCA and Transients (OCDE NEA, 1996). This document indicates that to obtain adequate results in numerous transients in LWRs it is necessary to use a multidimensional NK model coupled to a TH model. The usual scheme is based on leader/follower communication between the TH code and the 3D NK code. The TH acts as the leading code in the coupling, and therefore is responsible for controlling the progress of the joint simulation and making the necessary calls to neutronics code. As can be seen in the coupling diagram in Fig. 6, the TH code provides the 3D NK module with the thermal–hydraulic values of the core. These values must correspond to the parameterization made in the cross-section tables. These are generally the fuel Doppler temperature, moderator density, and boron concentration. Using these boundary conditions and cross-section tables, the diffusion equation at the nodes of the 3D mesh representing the reactor core is solved. The nodal power obtained by the 3D NK code is then communicated to the TH code. The power values are used as the thermal boundary condition in the heat structures that represent the fuel rods in the TH code.

Spanish research groups have extensive experience in coupling TH-NK codes, both in system thermal-hydraulics with neutronics and in core thermal-hydraulics with neutronics. The expertise is very relevant in different system TH codes such as RELAP5 and TRACE and subchannel codes such as CTF and SUBCHANFLOW. There is also experience in coupling these with neutronic codes such as PARCS, SIMTRAN, VALKIN, COBAYA, SCDAPSIM, and MCNP (Fig. 7). The following provides a description of the main works carried out in the coupling of system codes with neutronics and core codes with neutronics.

3.1.1. System thermal-hydraulics / neutronics

RELAP5 / PARCS, TRACE / PARCS, RELAP5 / VALKIN, TRAC-BF1 / PARCS. The UPV-ISIRYM Senubio group has extensive experience in developing, improving, and use of coupled TH-NK codes. Some of the improvements made in these codes have been adopted by the developers. This experience includes RELAP5/PARCS, TRACE/PARCS, RELAP5/VALKIN, and TRAC-BF1/PARCS, as well as the necessary

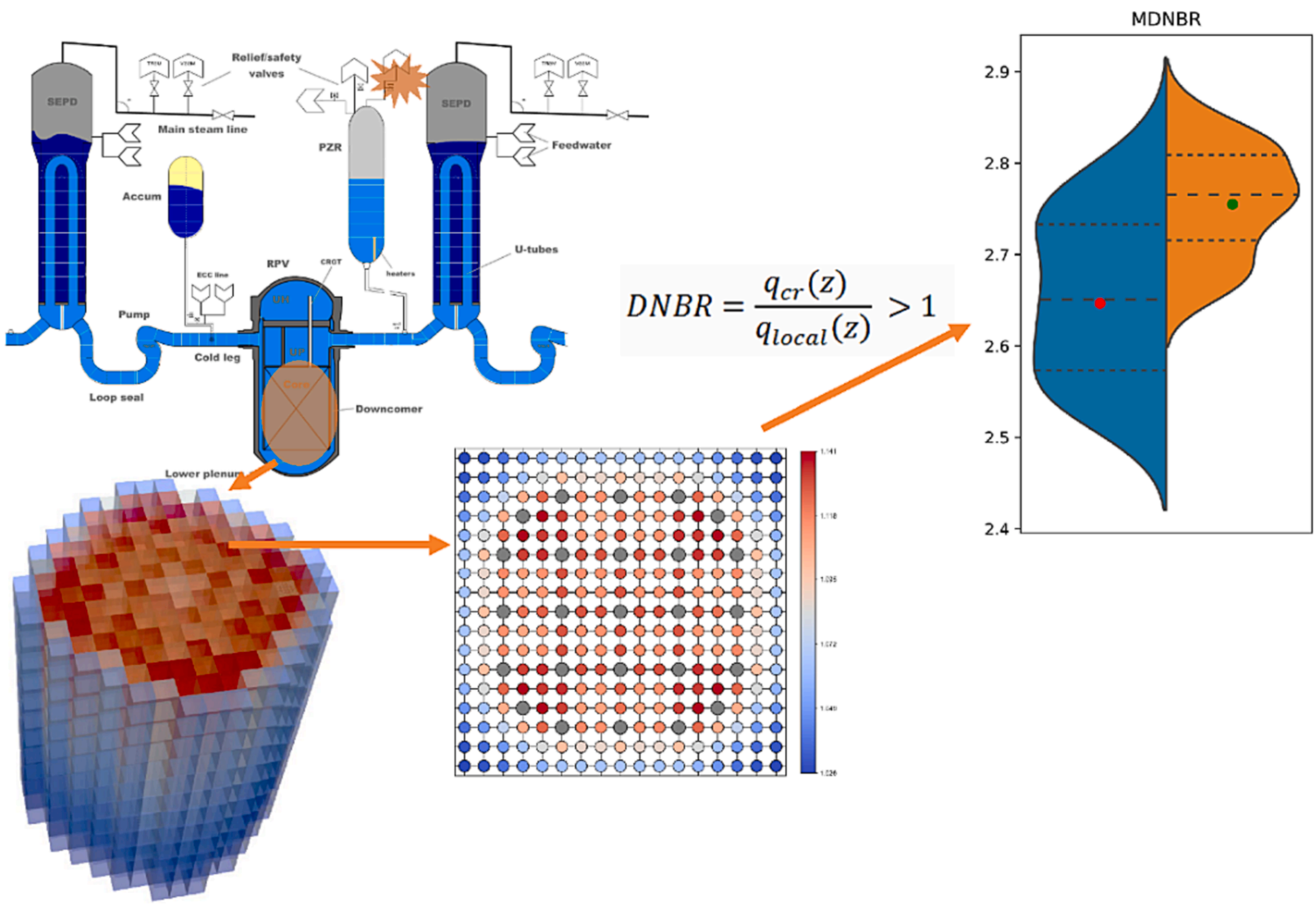

Fig. 5. UPC TH-TH coupling application for the determination of DNBR in BEPU calculations.

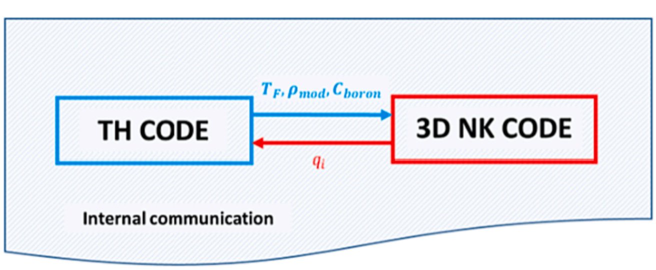

Fig. 6. General scheme of a TH/3D NK coupled code.

neutron parameters methodologies to feed the neutron kinetics modules of these codes. As a matter of example, the coupling between TRAC-BF1/MOD1 and PARCS codes, in which TRAC-BF1 is used in BWR NPP for licensing analysis. With this set of coupled codes diverse analyses in facilities using distinct TH and NK models were carried out to verify and qualify the coupling. Results confirmed the couplings were capable of simulating licensing transients. Different transient and accidental scenarios were analyzed and most of them were validated with these codes (for both PWR and BWR reactors) as control rod drop test, full scope of rod ejection accidents, neutron flux fluctuations in PWR, BWR stability, BWR turbine trip accidents, BWR ATWS, partial SCRAM accident in a BWR, Boron dilution in PWR, Xenon transients in PWR, pump malfunction, PWR flexible operation, etc.

The UPV-IIE group applied the coupling TRACE/PARCS to simulate the behavior of the Cofrentes NPP in the event of transients (Escrivá et al., 2015; Escrivá et al., 2017). Models were developed for the Cofrentes NPP considering the 624 fuel elements, that is, without collapsing the nuclear fuel. CASMO cross sections were provided for each fuel lattice configuration that compose the fuel loaded in this core. The CASMO cross sections were converted to PMAXS format using the branch structure recommended in NUREG-CR-7164 (Wang et al., 2013). This work was carried out by NFQ Group. Simulations were carried out for transients where abundant reference data was available, to verify and validate the model and the results obtained. Moreover, steady-state data calculated by TRACE/PARCS was benchmarked successfully against (a) measured traveling in-core probes (TIPs) data, and (b) 3D power distributions provided by the plant core-follow computer (Fig. 8). Data points for the steady state benchmarks include the complete depletion of the cycle at full power, but with different flow, control rod patterns, and inlet subcooling. Steady-state operating conditions during a control rod sequence exchange were also benchmarked against the 3D power shapes calculated by the core-follow plant computer, which is regularly adapted by the plant to reproduce the TIP and LPRM measured data. The purpose of this study is to validate the ability of TRACE/PARCS to calculate 3D power distributions for real reactor operating conditions with modern fuel features. This work was developed by NFQ Group together with Iberdrola, Michigan University, and Oak Ridge National Lab.

RELAP / SIMTRAN. The research group "Science and Technology of Advanced Nuclear Fission Systems" (UPM) developed the coupling RELAP/SIMTRAN. The resulting coupling interface SIMTRAN-RELAP was named SIMREL (Aragonés et al., 2004). This interface was developed for participation in the transient analysis of the OECD/NEA – PWR-MSLB Benchmark – Exercise III (Todorova et al., 2003). Results for core integral parameters and power distributions at different times of the transient were compared with PARCS-RELAP (Miller et al., 1999)

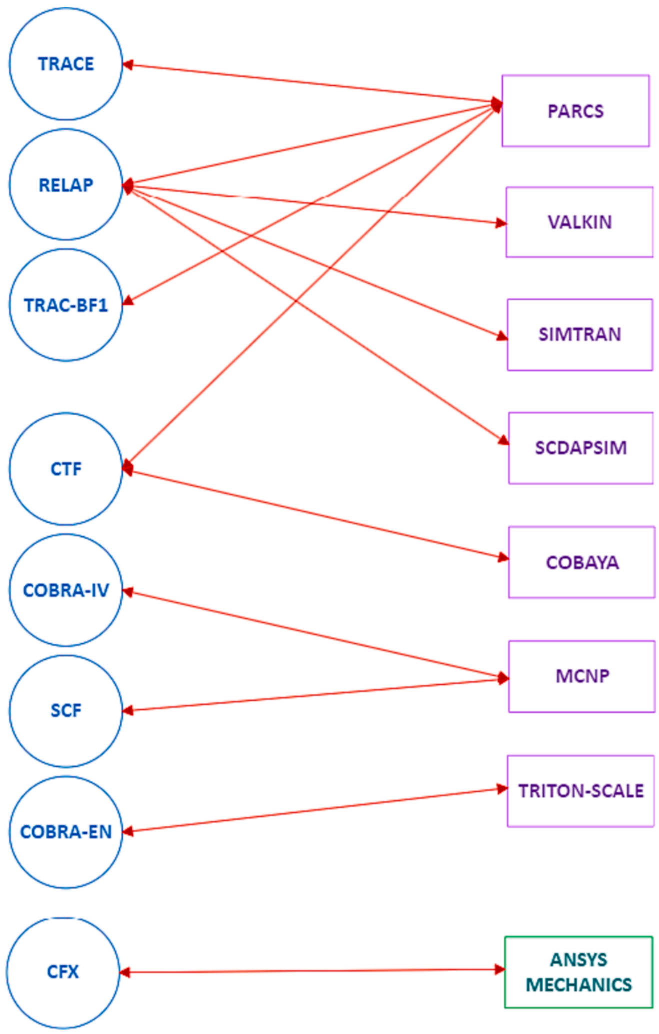

Fig. 7. Examples of multiphysics coupling.

showing a general good agreement within the acceptance criteria of nuclear design and safety margins. An example of these results is shown in Table 1 which provides values at the initial steady state and at the time of maximum power before the trip. The evolution of the reactivity calculated by SIMTRAN and PARCS was very close in the different scenarios of the Benchmark, with some systematic differences attributed to the different ways of calculating the dynamical reactivity, SIMTRAN uses inverse point kinetics, and PARCS a perturbation method with separated effects (Aragonés et al., 2004).

RELAP / SCDAPSIM. The Spanish company Nortuen S.L. together with Innovative Systems Software developed different software capabilities (NIRK3D and 3DKIN) for integrating neutron kinetics codes within RELAP/SCDAPSIM system code (Martínez-Quiroga et al., 2016). The advantage of using RELAP/SCDAPSIM code in TH-NK coupling is the potential use of SCDAPSIM code for a wider range of transients including the gradual extension to severe accident conditions. NIRK3D is a neutronic interface developed for RELAP/SCDAPSIM code. NIRK3D allows to integration and compiling of neutron kinetics codes as DLLs of RELAP/SCDAPSIM. With NIRK3D, TH-NK codes are coupled in series, by following a semi-implicit time management approach. Hence, no external software or intermediate blocks and parameters are necessary. It greatly simplifies the coupling process and allows numerically efficient and robust coupled TH-NK calculations using user-developed or widely used 3D kinetics packages. 3DKIN is a nodal kinetics package based on models and correlations of NESTLE 5.2.1 (North Carolina State University, 2003). The architecture of NESTLE code was modified and reprogrammed in FORTRAN 90/95/2000 standards to keep the implicit solution of the neutron diffusion equation as an internal library of RELAP/SCDAPSIM codes. New input cards were added to RELAP/SCDAPSIM codes for user-friendly mapping of LWRs Cartesian geometries. The software was tested in the Ph. D thesis of Sabahattin Akbas (Akbas et al., 2019; Akbas et al., 2015; Martínez-Quiroga et al., 2015) by simulating case D1 of the NEACRP LWR core transients benchmark (Finnemann and Galati, 1992), a BWR transient with an unexpected injection of subcooled water. Despite the differences between the results of the OECD benchmark's participants and the limitations of the meshing modeling in the supplied RELAP5 input decks, RS-3DKIN results (Fig. 9) showed that the transient simulations are within the range of the simulations of the other participants.

3.1.2. Core thermal-hydraulics / neutronics

CTF / PARCS. UPV-ISIRYM Senubio group developed a coupling between the CTF subchannel code and PARCS 3D v3.2 (PARCSv3.2). In this coupling, the logic of the explicit internal coupling between neutronics and TH was followed. The objective of this coupling is to include 3D kinetics in CTF to feedback to the code with the power obtained from the neutronics. The PARCS code, which is available within the TRACE source codes as it is internally coupled with that code, was slightly modified to facilitate the communication and data exchange with CTF. It is worth mentioning that the CTF starting version lacked a coupling interface with neutron kinetic codes therefore a new interface was completely programmed by the UPV-ISIRYM group. The coupling was performed with the goal of making the minimum possible modifications to the PARCS source code therefore the bulk of the necessary modifications were made in CTF source code. In the developed CTF/PARCS coupling, the TH code acts as a director. This role implies that CTF oversees making calls to PARCS so that it completes part (or all) of its calculation scheme. The initial power (heat) conditions in CTF are read from the input file and are usually provided by power profiles calculated by running PARCS alone. There is only one communication point that is bidirectional; CTF must provide PARCS with the necessary TH values so that it can, in turn, calculate the powers that CTF includes as a restriction in its heat structures. The overlap between the different physics modeled with both codes occurs when calculating the heat transfer term with the wall. In nuclear reactors, energy is generated inside the solid nuclear fuel rods, due to fissions, and is transferred to the coolant that circulates outside. The link between the power applied to the heat structure and the wall temperature is propagated through the equation for heat conduction in a solid medium. Energy is transferred from the thermal structure to the fluid by a heat flow boundary condition. Energy is deposited into the fuel by the neutron kinetics code through the rate of heat generation per unit volume. Finally, the calculation of temperatures inside the solid ends up having consequences on the heat transfer term with the wall included in the energy conservation equation for each phase of the fluid. This closure equation is originally semi-implicit, but when coupled with PARCS the wall temperature calculation is no longer implicit. This is because the heat generation rate per unit volume calculated by PARCS is used to calculate thermal conduction through the solid. This rate of heat generation due to fissions has been calculated using TH variables of the previous time-step and is therefore explicit with time. Thus, the heat transfer closure term with the wall included in the energy conservation equation calculates all its terms referring to the previous time-step, except for the temperature of the fluid phase in contact with the wall.

CTF / COBAYA. The UPM multiphysics platform, from Universidad Politécnica de Madrid, was developed through the participation of the developer's team in several European Projects. This platform is devoted to the analysis of LWR cores using Best Estimate and Uncertainty Methodologies using different codes integrated into a computational platform based on SALOME software and Python. The main codes integrated into this platform are the in-house neutronic code COBAYA, the lattice code SCALE, and the TH code CTF. COBAYA is a neutronic code

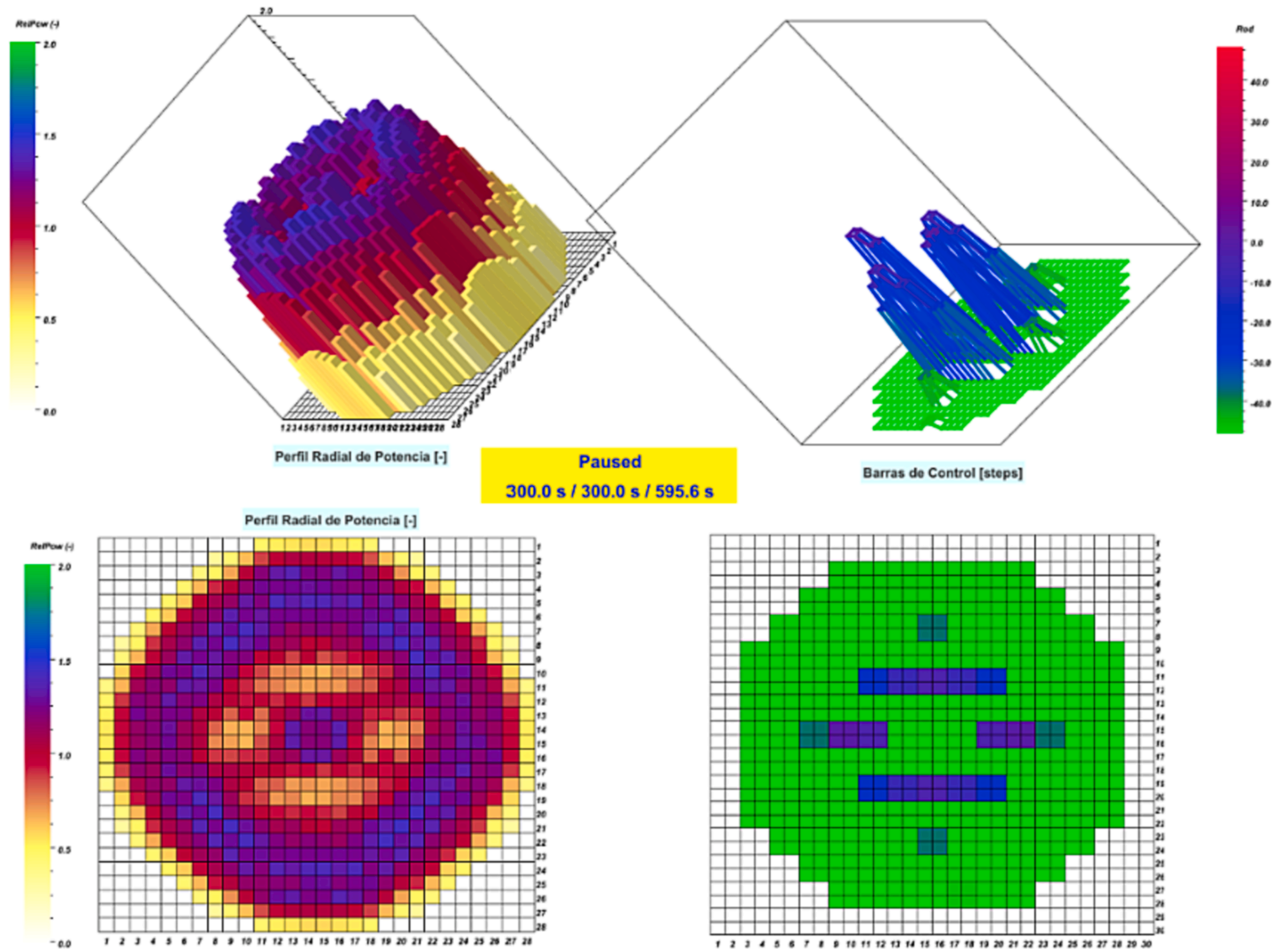

Fig. 8. Radial power profile and control rod positions.

Table 1
Initial steady state at full power and at the time of maximum power before the trip.

Integral parameter	RELAP5 / SIMTRAN	RELAP5 / PARCS
Power at initial state (in %)	100	100
Multiplication factor (keff)	1.00479	1.00528
Radial assembly power factor (F_{xy})	1.326	1.332
Axial power factor (Fz)	1.062	1.070
Axial offset of core power (%)	−0.39	+0.47
Power just before trip (%)	118.61	118.12
Radial assembly power factor (F_{xy})	1.460	1.464
Axial power factor (Fz)	1.091	1.072
Axial offset of core power (%)	−2.72	−1.82

based on the diffusion approximation that can solve the reactor core at nodal and pin-by-pin level using 2, 4, and 8 energy groups. It can compute steady-state and space–time kinetics problems. The nodal solver employed in COBAYA (Lozano et al., 2008) is based on the Analytic Coarse-Mesh Finite-Difference Method (ACMFD) (Aragonés et al., 2007). The ACMFD method combines a classical transverse leakage integration procedure with an analytical 1D solution of the diffusion equation on each of the spatial directions and can deal with 3D Cartesian and hexagonal-Z geometries (Lozano et al., 2010). The pin-by-pin solver included in COBAYA is based on the transport-corrected Finite-Mesh Finite-Difference (FMFD) diffusion method. This solver can be used to solve full core problems. Both methods have been extensively validated

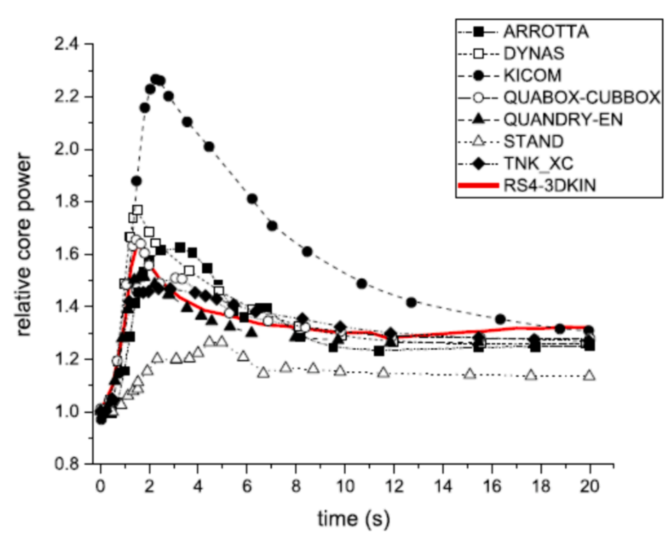

Fig. 9. Core power of transient problem.

for several numerical benchmarks. COBAYA can be applied for steady state and transient calculations originated by control rod movement, boron concentration changes, or evolutions of the coolant conditions. Transients can initiate from critical or subcritical conditions. To compute the necessary macroscopic cross sections and discontinuity factors needed by COBAYA to reproduce the transport solution for the core at nodal and pin-by-pin level, the platform integrates the system SCALE using the codes NEWT and ORIGEN (that are included in the sequence TRITON). NEWTtoNEMTAB is the module in charge of extracting the necessary information from NEWT output and build the cross section libraries needed by COBAYA to perform nodal or pin-by-pin simulations. Another module included in the platform is MUSIC. This consists of a set of Python subroutines that can generate coherently the necessary inputs for the codes integrated into the platform. In this way, the inputs for COBAYA, CTF, and the SCALE system are generated from the same specifications for the core and the fuel assembly avoiding the user effect very common in this type of approach and simplifying the initialization process for the codes. A graphic of the modules included in the platform can be seen in Fig. 10.

The UPM multiphysics platform has been applied to the analysis of steady states and transients of cores of PWR, VVER, and SMR as part of the verification and validation process of the platform. As part of the European Projects, it was applied to the analysis of a Main Steam Line Break (MSLB) at 4-loop Westinghouse PWR ZION-type reactor and compared with other participants in the benchmark (Kliem et al., 2017). Also, an analysis of the differences between nodal and pin-by-pin analysis was performed to consider multiscale effects (García-Herranz et al., 2017; Sabater et al., 2016). It has also been applied to an MSLB at a VVER reactor including the comparison with other participants (Spasov et al., 2017). Concerning SMR, some analysis has been performed to analyze the applicability to a Rod Ejection Accident in NuScale reactor (Durán-Vinuesa et al., 2022).

COBRA-IV / MCNP, SUBCHANFLOW (SCF) / MCNP. COUNTHER is one of the second-generation TH-NK coupled codes that implements the coupling with stochastic codes instead of deterministic ones. COUNTHER was developed by the "División Fisión Nuclear" from CIEMAT. MCNP was chosen for neutronic analysis, and two different subchannel codes were available for TH: COBRA-IV and SUBCHANFLOW (SCF).

The methodology of COUNTHER consists of a coupling scheme based on loose coupling where individual codes perform their calculations before sharing some important results with the rest of the codes. This coupling scheme can be implemented for both a steady state and a transient analysis. For the latter, at each time step a looped steady state calculation is needed before advancing in time. The coupling scheme for the steady state estimation consists of a first calculation of MCNP to obtain the neutron flux profile of the reactor, and therefore, the 3D power distribution, which is used as input data in the TH code. After the simulation of COBRA or SCF, the temperature profile of the different materials and the density profile of the coolant are employed to update the MCNP input, changing the cross sections and density profiles. This process is repeated until a convergence level for the fuel temperature in two consecutive steps is reached. This code was verified for BWR operating conditions through the NURISP (Nuclear Reactor Integrated Simulation Project) benchmark and for fast reactors through the simulation of transients of the MYRRHA concept.

COBRA-EN / TRITON-SCALE (depletion code). Within the framework of the project between the UPM and the CSN on Criticality Safety Assessment in Burnup Credit Calculations (2009–2013), the UPM developed a 2D depletion (TRITON/SCALE) + 3D thermal–hydraulic (COBRA-EN) tool (Fig. 11) aiming at estimating better agreement between calculations and measurements in Post Irradiation Experiments (PIE) in BWR burnup samples. In this frame, the isotopic content of eight irradiated samples extracted from different axial positions of a rod in a GE14 10x10 fuel assembly in the Swedish boiling water reactor Forsmark Unit 3 is computed. These samples with an initial enrichment of 3.95 wt% U-235 were irradiated during five cycles under changing moderator density conditions and surrounded by a highly heterogeneous arrangement of fuel cells, including different enrichments and burnable absorbers. The fuel rod attained an average burnup of 41 MWd/kgU (Conde et al., 2006). By coupling TRITON depletion code and the subchannel thermal–hydraulic code COBRA-EN for a given time dependent-axial power profile, the radial and axial time-dependent void fractions, fuel temperature and specific power for the rods and sample are provided by the code. Then, the isotopic results in the sample are obtained with more realistic radial and axial distributions in fuel bundles.

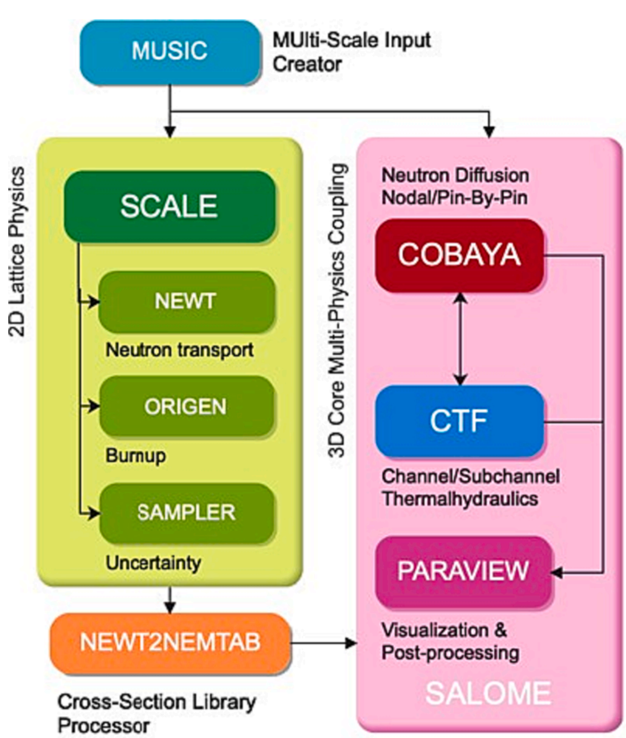

Fig. 10. UPM core simulation platform.

3.2. Fluid dynamics – Thermomechanics

CFD facilitates studying processes involving interconnected phenomena such as fluid motion, interaction with structures, heat transfer, or chemical reactions. CFD codes are often limited by the computational power required, but with the evolution of computing systems and High-performance Computing (HPC) centers, code coupling has become increasingly important (NEA-CSNI-R20, 2017). Mechanical codes, such

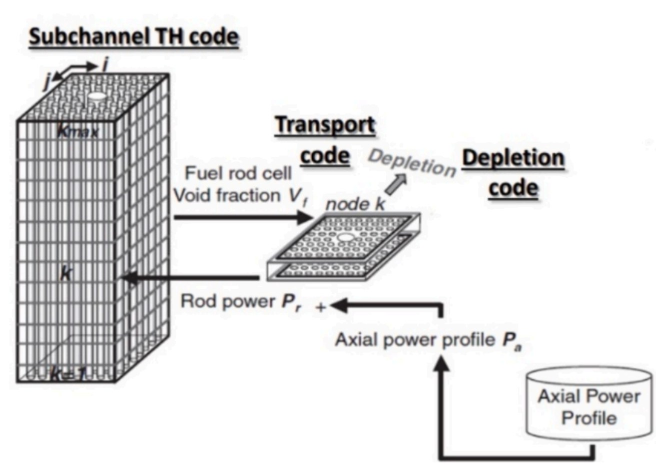

Fig. 11. Coupling subchannel code – depletion code to predict isotopic content in Boiling Water Reactor Fuel Bundles (Ikehara et al., 2008).

as Finite Element Analysis (FEA) or Computational Structural Mechanics (CSM), complement CFD by providing detailed analysis of structural behavior, stress distribution, and response to external forces. This integration allows for a comprehensive evaluation of the mechanical integrity of reactor components, including fuel rods, pressure vessels, and piping systems.

The research conducted by the UPV-IIE, in collaboration with the CSN, focuses on coupling CFD codes with FEA codes to explore the interaction between fluids and the surrounding environment. This investigation is part of the "Advanced Thermo-Hydraulics and Uncertainty Treatment in Nuclear Safety" project, jointly financed by UPV-IIE and CSN. A crucial component of this research involves participation in an international benchmark organized and sponsored by the OECD/NEA and the Committee on the Safety of Nuclear Installations (CSNI) (OECD Nuclear Energy Agency, 1996).

A specific benchmark exercise was conducted to assess induced vibration from water current over two vertically aligned cylinders fixed at the bottom of a rectangular channel in the experimental facility. As the water flow passes through the structure, it generates a repetitive hydrodynamic process known as vortex shedding, which induces motion in the cylinders. The structural features of the facility enable a comprehensive understanding of structural excitation, including both the induced and natural frequencies. The motivation behind the benchmark initiative stems from the need to address the hydrodynamic forces exerted by coolants on various structures within a nuclear reactor (IAEA-TECDOC-1454, 2004), leading to the occurrence of vibrations. These vibrations, if not adequately understood and managed, can give rise to a range of issues, including fuel-clad fretting, fatigue in steam generator tubes, wearing of control rod guiding tubes, and fluid elastic instabilities.

In terms of CFD-FEA code coupling, two approaches have been considered. The first approach is the one-way coupling, where the communication is unidirectional, allowing the transmission of hydrodynamic force information from the fluid to the cylinder tandem. However, the induced motion in the cylinders is not fed back to the CFD code. This approach is more efficient regarding computational cost, as it eliminates the need to recalculate the CFD domain mesh at each time step and the communication process between codes. Alternatively, the second approach is the two-way coupling, characterized by bidirectional communication between the codes at each time step or a defined number of time steps. In this configuration, the two-way coupling accounts for the cylinder oscillations and can potentially capture the lock-in mode resonance between the vortex shedding frequency (or its harmonics) and the natural oscillation frequency of the structure. However, the calculations required in this mode are computationally intensive and typically require the support of large HPC centers. For that reason, in general, a bidirectional coupling between CFD and FEA is entirely limited by the case under study - strong requirements justifying the need, such as the lock-in mode - and the available computational resources.

The UPV-IIE/CSN employed the one-way coupling approach, which provided satisfactory results closely aligned with the experimental data for cases where the lock-in mode was absent. Ansys CFX and Ansys Mechanical codes were employed within the Workbench platform to establish a coupled simulation framework. It is worth mentioning that, despite all the effort, none of the twelve worldwide groups participating in the exercise could predict the lock-in mode, including those using a two-way coupling.

Fig. 12 illustrates a simple scheme of the one-way coupling process followed. The simulations of the CFD code are performed initially, obtaining the main hydrodynamic features of the flow and storing the pressure field information for each timestep at the cylinders' surface. This data is then imported into the FEA simulation to calculate the induced vibrations.

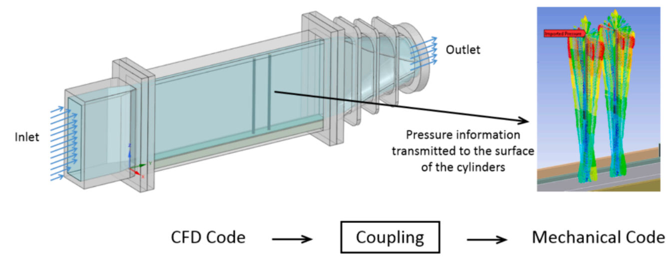

Fig. 12. CFD-FEA one-way coupling scheme.

3.3. Simulation platforms

In recent years computer tools are being developed through which it is possible to obtain a detailed description of the phenomena that take place in the core of nuclear reactors. The purpose of these new tools is to perform safety analysis in nuclear reactors using best estimate techniques.

In this frame, computer platforms are being developed to integrate computer codes that cover most of the physics which take place in nuclear reactors. For the integration of the different feedback phenomena between thermal-hydraulics, neutronics, mechanics and heat transmission, a series of couplings between the codes that make up the platform have been developed. All the developments carried out are aimed at realistically representing the design and behavior of the nuclear facility, including the control system, the fuel elements, and fuel rods.

Two simulation platforms have been used by the Spanish research groups: SALOME and NUC-Multphys. A brief description of both platforms is presented in this section.

SALOME. At UPM, a multiphysics platform was developed based on SALOME open-source software to facilitate the coupling of codes required for the simulation of the physical phenomena involved in power nuclear reactors. The platform also makes easy the pre- and post-processing of the numerical calculations (Chauliac et al., 2011; Chanaron, 2017).

The UPM core simulator COBAYA4 (3D NK), and the subchannel code CTF (TH), were first integrated into the platform to take advantage of one of the platform simulation capabilities, the med-coupling structures (SALOME6.6, 2016). Those structures allow the exchange of fields between meshes corresponding to different physics, overcoming the limitations of a tight coupling approach. To integrate COBAYA4 in the SALOME platform, versions 6.6 and 7, ICoCo standard functions were implemented (Crouzet, 2015).

ICoCo (Interfase COde COupling) is a set of C++ functions defined to be used by the codes integrated into SALOME to execute different steps of the calculation. Integration of CTF was carried out by Gesellschaft für Anlagen- und Reaktorsicherheit in the framework of 7FP EU NURESAFE project (Périn, 2017). Once integrated with the platform, codes can be run in a modular way and be coupled through the ICoCo functions using different resolutions for the NK and TH solvers. That is, a neutronics nodal or pin-by-pin calculation can be performed using one TH channel per assembly or a subchannel among four fuel rods. The interpolation tool incorporated in SALOME takes care of transferring the fields between the TH and NK meshes without having to explicitly indicate the cells' connection.

It is also possible to use different types of interpolations for the physical quantities depending on the nature of the fields that are going to be transferred, delegating all the interpolation aspects in an external tool. The logical control of the COBAYA4/CTF coupling is in a python script. First, the script generates the NK and TH meshes depending on the desired level of refinement. Then, it adjusts both meshes as necessary to fit them in scale, position, and angle. Finally, the script takes care of the execution of the ICoCo functions to carry out the different steps in steady state and transient calculations according to the coupling scheme established by the user. A graphical description of this new coupling approach is in Fig. 13. In summary, the use of a platform like SALOME offers an environment to facilitate the coupling of computing codes providing a generic user-friendly interface. This type of coupling facilitates the maintenance of codes, that can be updated to a new version with few modifications and no influence on the coupling scheme.

NUC-Multphys. The NUC-Multphys computer tool has been developed at the UPV-ISIRYM to provide a detailed description of the phenomena occurring in nuclear power plants, particularly in the core (Abarca, 2017). The final purpose of these new tools is to perform safety analyses with best-estimate coupled codes that join the simulation of the physical processes that occur in a nuclear reactor related to neutron transport, fluid mechanics, heat transfer, and material resistance. All these processes have a strong dependence between them, so thanks to the joint analysis sufficient standards of precision can be achieved to give credit to the prediction made.

One of the main goals of the SENUBIO research group of the ISIRYM was to create a computer platform that includes the coupling of some of the latest generation codes for the analysis of the NPP. In the thermo-hydraulic plane, the code formed by the semi-implicit coupling between TRACE code and a parallelized CTF code is implemented. To perform transient simulations with 3D NK calculations, the explicit coupling between PARCS and CTF was developed, although the coupling between TRACE and PARCS continues to be available.

An internal explicit coupling scheme like the one currently existing between PARCS and TRACE has been used for the CTF/PARCS. The coupling is temporally explicit because the neutron and TH equations are not solved at the same time, using a joint scheme. The codes only exchange the values necessary to provide each other with boundary conditions at each time step. Each code solves its system of equations and ensures the convergence of both for each time step using the coupling advance control scheme.

A coupling between the CTF subchannel code and the FRAPTRAN nuclear fuel behavior analysis code was also developed (Fig. 14). The coupling is based on the internal exchange of data. There is no need for external communication interfaces between both codes. The implemented coupling is temporally explicit. This means that there is no real coupling between the equations of both codes, so they are only fed back with the boundary conditions generated by the other code. The current coupling has the limitation that the analysis of only a single rod can be carried out by the computational process.

4. Future trends

The multiscale and multiphysics coupling is and will be a topic of special relevance in nuclear safety. Below are some brief headlines on possible topics that will be addressed in the future, and Spanish research groups will focus a significant part of their efforts on these.

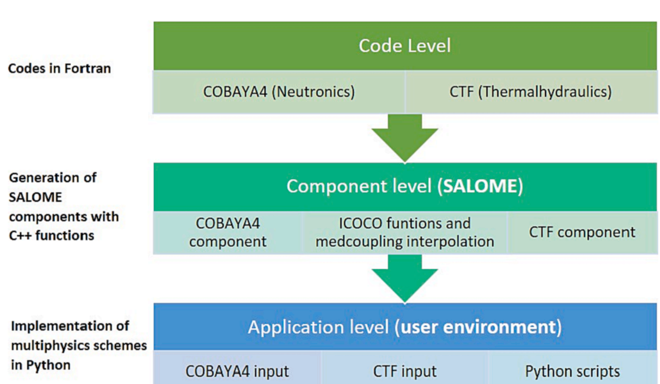

Fig. 13. Description of the different layers that are included in the integration of COBAYA4 and CTF in the SALOME platform.

- In multiscale coupling for thermal-hydraulics, and specifically in the coupling between system codes and subchannel codes where the main goal is the detailed evaluation of the DNBR, efforts are needed for the analysis of asymmetrical scenarios where velocity profiles at the core inlet play a significant role. For this type of cases the coupling of system code and subchannel may not be sufficient to provide high fidelity results and additional studies are needed to predict the correct velocity profiles at the subchannel code inlet, this could be calculated or estimated by surrogate CFD models.
- The evaluation of uncertainties in high fidelity multi-scale multi-physics will require further research as all the sources of uncertainties and their interdependence need to be evaluated. Several works have been done in this direction but still, some of the input uncertainties are derived from expert judgment and not with more advanced methods in the realm of Inverse Uncertainty Quantification.
- In the multiphysics platforms development the trend in the future research is based on the inclusion of different codes able to simulate the new Gen reactors, especially Small Modular Reactors (SMR) design and licensing analyses, which require 3D NK codes with the capability of solving the neutron transport equation or SP3 approximation.
- CFD coupling with neutronics codes. It would be interesting to continue fostering improvements in the coupling between thermal-hydraulic phenomena at CFD small-scale with neutronics codes for precise control of thermal loads in the rod bundles. Initial steps have been done outside of Spain, but usually limited geometries or relatively simple transients.
- CFD coupling with structural codes. Two main interactions are identified for future works, mainly related to pressure forces and heat transfer. Simplified activities have been done for both types of interaction. However, more validation exercises must be fostered to ensure accurate prediction in complex geometries, as well as separate and integral effects.
- CFD coupling with system codes. Integrating the small-scale resolution of CFD codes into system codes allows for a noteworthy representation of the phenomena in specific components where small-scale might considerably affect the prediction capabilities. This coupling also allows for the inclusion of other phenomena in the CFD simulation, such as chemistry or fire propagation for specific scenarios.

5. Conclusions

The utilization of multiscale, multiphysics and coupling methodologies is essential in comprehensively understanding and simulating the complex behavior of nuclear reactors. Nuclear reactors involving different physical effects occurring at different scales, and the multiscale approach allows for a balanced compromise between accuracy and computational efficiency. This approach is particularly valuable in solving reactor core-related problems, such as neutron transport, power distribution, and thermal–hydraulic and thermo-mechanical analyses. Coupling methods play a crucial role in integrating different codes and models to simulate the interactions between various physical phenomena within nuclear reactors.

In Spain, different research groups actively work in this field: Advanced Nuclear Technologies (Universitat Politècnica de Catalunya); Nuclear Innovation (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, CIEMAT); Department of Energy Engineering (Universidad Politécnica de Madrid); Engineering School of Mining and Energy (Universidad Politécnica de Madrid); Nuclear Safety and Bioengineering of Ionizing Radiation group from Instituto Universitario de Seguridad Industrial, Radiofísica y Medioambiente (Universitat Politècnica de València); Instituto Universitario de Investigación de Ingeniería Energética (Universitat Politècnica de València) and NFQ group, among others.

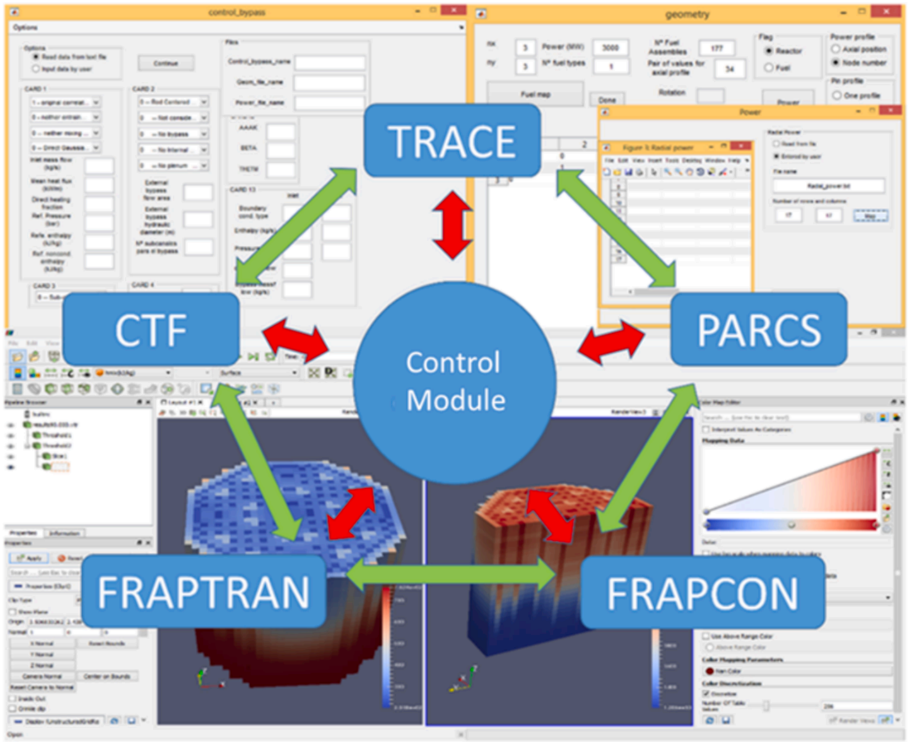

Fig. 14. Flowchart of the computing platform.

These groups have developed and applied different TH/TH coupling, for example: RELAP5/3D-CTF; RELAP5/CTF; TRACE/CTF and TRACE/SCF. Various research groups have experience in developing and improving coupled system thermal–hydraulic and neutronics codes for safety analysis. Examples of this coupling are RELAP5/PARCS, TRACE/PARCS, RELAP5/VALKIN, and TRAC-BF1/PARCS, which have been used for analyzing different transient and accidental scenarios in both PWRs and BWRs. These studies have been valuable for understanding reactor behavior and safety margins. With regard core thermal-hydraulics and neutronics, different couplings have been developed including CTF/PARCS; CTF/COBAYA; and COUNTHER (COBRA-IV or SUBCHANFLOW)/MCNP.

For detailed analysis of specific regions, CFD codes are coupled with structural codes such as Ansys CFX and Ansys Mechanical to explore the interaction between fluids and their surrounding environment. These coupling efforts enhance the prediction capabilities of nuclear safety analysis tools and contribute to a deeper understanding of reactor behavior under diverse operating conditions.

Furthermore, the development of simulation platforms, such as the one based on SALOME open-source software and the NUC-Multphys tool, facilitates the integration and coupling of codes, streamlining the simulation process for nuclear reactor analyses.

Overall, the combination of multiscale approaches and coupling methodologies, along with the development of simulation platforms, significantly contributes to the safe and efficient operation of nuclear reactors and the advancement of nuclear science and technology.

CRediT authorship contribution statement

Sergio Gallardo: Writing – review & editing, Writing – original draft, Conceptualization. **Francisco Álvarez-Velarde:** Writing – original draft, Methodology, Conceptualization. **Teresa Barrachina:** Writing – original draft, Methodology. **Óscar Cabellos:** Writing – original draft, Methodology, Conceptualization. **Emilio Castro:** Writing – original draft, Methodology. **Max Casamor:** Writing – original draft, Methodology. **Diana Cuervo:** Writing – original draft, Methodology, Conceptualization. **Alberto Escrivá:** Writing – original draft, Methodology, Conceptualization. **Jordi Freixa:** Writing – original draft, Methodology, Conceptualization. **Nuria García-Herranz:** Writing – original draft, Methodology, Conceptualization. **Victor Martinez-Quiroga:** Writing – original draft, Methodology. **Rafael Miró:** Writing – original draft, Methodology, Conceptualization. **César Queral:** Writing – original draft, Methodology, Conceptualization. **Yago Rivera:** Writing – original draft, Methodology. **Jorge Sánchez-Torrijos:** Writing – original draft, Methodology. **Amparo Soler:** Writing – original draft, Methodology, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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