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KIT Multi-scale thermal–hydraulic coupling methods for improved simulation of nuclear power plants

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ABSTRACT

In a Nuclear Power Plant (NPP), the Thermal-Hydraulic (TH) phenomena take place at different scales in the core and the primary and secondary circuits. Thus different TH codes have been developed to describe the phenomena at the macro- and *meso*- scale (system, sub-channel, porous media codes). Besides, the use of general-purpose CFD codes for the analysis of specific local problems is rapidly increasing. To take full advantage of the code's strength, the multi-scale TH approach which couple those codes together is becoming a trend in recent years. At Karlsruhe Institute of Technology (KIT), those multi-scale TH approaches involve the system, sub-channel, and CFD codes: 1) the system code TRACE and the sub-channel code SubChanFlow (SCF) were coupled to improve the prediction of the core thermal hydraulics; 2) the system code TRACE and the open-source CFD code TrioCFD were also coupled to improve the prediction of the TH phenomena inside the Reactor Pressure Vessel (RPV). Those works are based on an Interface for Code Coupling (ICoCo) either with or without the SALOME platform. The current investigations demonstrate the potential of multi-scale TH coupling approaches for improved safety-related analysis of the NPP behavior under accidental conditions. In the future, the focus of KIT work is on multiscale coupling based on domain decomposition using both ICoCo and user define functions of commercial CFD codes.

1. Introduction

In a Nuclear Power Plant (NPP), Thermal-Hydraulic (TH) phenomena take place at different scales in the core, and in the primary/secondary circuits including both single and two-phase flow conditions. Different TH codes have been developed to describe these phenomena at macro- and *meso*- scale (system, sub-channel, porous media codes) for many decades. Extensive validation and code development work was done to improve the prediction accuracy of such codes. In recent years, the development and application of thermal–hydraulic codes with higher spatial resolution including physical models e.g. 3D porous media codes and CFD-codes in nuclear engineering increased continuously (Jeong et al., 2010); (Jauregui-Chavez et al., 2018).

System code is characterized by fast running and covering the complete boiling curve, but with coarse mesh. Sub-channel code also has good two-phase flow models and it is to improve the core TH prediction with better spatial resolution. CFD code currently is not yet mature for the analysis of the full range of the void fraction. Furthermore, the CFD simulations of a full reactor core with a detailed spatial resolution at the pin and sub-channel level for the prediction of local safety parameters are computationally intensive and are not yet practical in current High-Performance-Computing (HPC) computers. Nevertheless, some peculiarities of CFD codes are a versatile and precise description of the real geometries of the problem of interest thanks to the variable combination of different mesh sizes in one computational domain, the parallel capability, and the employment of robust numerical solvers. Hence, within a typical multi-scale TH simulation, the CFD code usually simulates the downcomer and lower plenum, while the core (fuel assemblies, fuel rods) is typically solved by sub-channel or porous media code, and the system code handles the remaining NPP system. There are many

Abbreviations: CHF, Critical Heat Flux; DIAS, Dynamic Implicit Additional Source; DNS, Direct Numerical Simulation; ECI, Exterior Communication Interface; ICoCo, Interface for Code Coupling; GUI, Graphical User Interface; LOCA, Loss of Coolant Accident; LOFT, Loss of Fluid Test; LES, Large Eddy Simulation; LOF, Loss of Flow; LWR, Light Water Reactor; MPI, Message Passing Interface; NPP, Nuclear Power Plant; OS, Operator Split; PVM, Parallel Virtual Machine; PWR, Pressurized Water Reactor; RPV, Reactor Pressure Vessel; RANS, Reynolds-Averaged Navier–Stokes; SCF, SubChanFlow; SFR, Sodium-cooled Fast Reactor; SMR, Small Modular Reactor; TH, Thermal-Hydraulic.

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multi-scale coupling approaches under development, which differ from each other by the kind of implementation, selection of the solvers to be coupled, etc. In (Zhang, 2019) a nice overview of current methodologies and approaches is summarized and discussed.

At KIT, the focus is on the development of different TH codes as well as the multi-scale TH approaches to describe the physical phenomena within NPP in a more accurate manner, by coupling different TH codes e.g. system (TRACE), sub-channel (SubChanFlow - SCF), and CFD-codes (TrioCFD) (Jauregui-Chavez et al., 2018); (Imke and Sanchez, 2012); (Zhang, 2019). The key aspect of such approaches is the selection of the most flexible and accurate coupling methodology taking the solvers' differences and the way they treat the spatial discretization of the computational domains into account. At KIT, different coupling methodologies e.g. ECI (Mahaffy, 2003); (Zhang and Sanchez-Espinoza, xxxx), and ICoCo (Zhang et al., 2019), were evaluated and implemented for different combinations of TH solvers. The goal is to combine the advantages of the codes on different TH scales and improve the performance of the code on the safety analysis of NPP.

Following the introduction, **Chapter 2** gives a short description of the involved TH codes. **Chapter 3** introduces the main features of the peculiarities of different coupling methods and codes. **Chapter 4** particularly explains the ICoCo interface which is the emphasis of the KIT work. **Chapter 5** discusses the ICoCo-based coupling of an open-source CFD code TrioCFD with a system code TRACE as well as the main coupling features, its first validation, and application. **Chapter 6** focuses on the implementation of the coupling of a sub-channel code SCF with TRACE using SALOME-YACS as a supervisor and its first application. Finally, **Chapter 7** summarizes the full paper and **Chapter 8** presents further work for the improvement of the coupling approaches and the practical use by different end-users (regulators, industry, utility) in the frame of safety evaluation of NPPs as well as for extensive validation.

2. Selected codes for multi-scale coupling

The following TH codes are selected for the implementation of multi-scale coupling at KIT: TRACE, SCF, and TrioCFD. Hereafter a short description of each code is provided.

2.1. The system code TRACE

TRACE (Nrc, 2016) is a best-estimate system code of the U.S. NRC for LWR and more recently extended for liquid–metal-cooled fast reactors. TRACE solves the static or time-dependent system of six conservation equations of a two-fluid mixture in 1D and 3D (Cartesian and Cylindrical coordinates) computational domain using the finite volume and donor-cell approach. Additional equations are formulated to describe the transport of boron in the liquid phase and of non-condensable gases in the gas phase. Thanks to its versatility, not only NPPs but also different experimental test sections or loops can be simulated with TRACE. A complete set of constitutive equations are formulated to close the balance equations describing the interphase and wall-to-fluid mass and heat transfer in all flow regimes of the boiling curve (i.e. pre- and post-CHF) for both horizontal and vertical flow conditions. In this approach, mechanical and thermal non-equilibrium situations are considered. Various models for components of an NPP e.g. pumps, valves, pipes, heat structures, as well as dedicated models for trips and control systems are also implemented in TRACE. Two numerical methods, a semi-implicit method, and the SETS method are implemented in TRACE to solve any kind of slow and fast transients (Nrc, 2016). It also has dedicated models to describe specific physical phenomena such as thermal stratification, point kinetics, critical flow, etc. TRACE is recently equipped with an Exterior Communication Interface (ECI) for internal or external coupling with any kind of solvers (Mahaffy, 2003). Typically, it was already coupled with 3D nodal diffusion solvers for the enhanced simulation of non-symmetrical transients in NPPs.

2.2. The sub-channel code SubChanFlow (SCF)

SCF (Imke et al., 2010) is developed for the simulation of reactor cores consisting of hexagonal and square fuel assemblies. It solves a system of three mixture equations (mass, momentum, and energy) including another one for the cross-flow at channel and subchannel levels. Additional constitutive relations are formulated to close the balance equations that describe the pressure drop, wall friction, boiling, and heat transfer models for the whole boiling curve (Imke and Sanchez, 2012). State equations for various coolants e.g. water (IAPWS 97), lead, Lead-Bismuth, Sodium, Helium, and CO_2 are implemented. The system of equations is solved for stationary or time-dependent flow conditions in mainly upward flow. SCF is widely used as stand-alone or coupled to different neutronic solvers (deterministic and Monte Carlo) as well as to a fuel performance code (Transuranus) (Basualdo and Sanchez, 2017). The validation work is mainly focused on Light Water Reactor (LWR) applications using tests e.g. from NUPEC PSBT and BFBT (Imke and Sanchez, 2012).

2.3. The open-source CFD code TrioCFD

The open-source CFD code TrioCFD is based on the TRUST platform (TRio_U Software for Thermo-hydraulics) being developed by CEA for nuclear applications (Bieder and Graffard, 2007). TrioCFD is an object-oriented computational fluid dynamics code written in C++ for massively parallel computing based on the MPI (Message Passing Interface) protocol. It includes models based on the Reynolds-Averaged Navier-Stokes (RANS), the Large Eddy Simulation (LES), and the Direct Numerical Simulation (DNS) for the solution of different fluid dynamic problems with flexible spatial discretization. Extensive verification and validation of TrioCFD are performed using various experimental data (Angeli et al., 2015). TrioCFD-applications in the nuclear industry are focused on 3D problems of NPPs such as boron transport, thermal mixing, mix-convection, etc. that may occur in case of accidental sequences such as boron dilution, main steam-line break, pressurized thermal shocks, etc. (Bieder and Graffard, 2007). In the past, TrioCFD was coupled with the system code CATHARE (Bavière et al., 2014) using the ICoCo methodology and applied for the analysis of LWR problems e.g. within the European NURISP and NURESAFE (Nuclear Reactor Safety Simulation Platform, 2019) projects.

3. Review of methodologies for multi-scale TH coupling

For many years, different research groups tried to implement multi-scale TH coupling schemes to increase the prediction capability regarding safety-relevant phenomena in NPPs. One of the first coupled codes was based on an internal coupling of TRAC and CobraTF (Frepoli et al., 2009), and RELAP5 and Cobra-TF (Jeong et al., 1997) to better predict Loss of Coolant Accident (LOCA) with reflood of the core and 2D/3D phenomena in the upper plenum of Pressurized Water Reactor (PWR) (LOFT, UPTF). Later on, the coupling of a porous-media 3D code (CUPID) with the 1D system code MARS was developed to improve the simulation of advanced Generation 3 reactors like APR+ (Cho et al., 2013). The increasing use of commercial and open-source CFD codes in the nuclear industry fostered also the development of coupling approaches involving the system and CFD codes for the simulation of different kinds of problems, where spatial effects play a key role and cannot be properly described by 1D or coarse 3D models of system codes (Scheuerer et al., 2005) in the primary/secondary circuit and the containment (Bieder and Graffard, 2007); (Böttcher and Krüßmann, 2010); (Yadigaroglu, 2005) (Hoehne et al., 2010); (Cheng et al., 2015).

Early developmental work on a multi-scale coupling approach was devoted to the domain decomposition approach. In (Aumiller et al., 2001) the explicit coupling of RELAP5-3D and CFX using the Parallel Virtual Machine (PVM) capabilities for the data transfer. A proof of concept by solving the Eduards O'Brien blowdown problem was

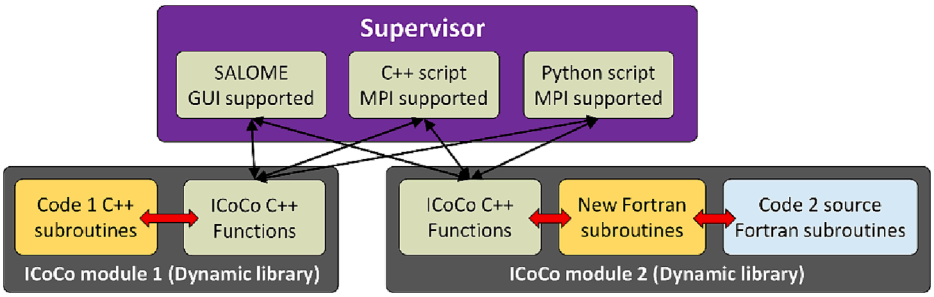

Fig. 1. The general architecture of the ICoCo-based coupling system.

demonstrated. At SCKEN (Toti et al., 2017), an explicit scheme and fixpoint iteration method are applied for the coupling of RELAP5-3D and FLUENT was realized and applied to assess the behavior of a pool-type research reactor in case of a loss of flow accident (LOF). At PSI (Bertolotto et al., 2009), an explicit and semi-implicit implementation of the coupling of TRACE and ANSYS CFX was developed and applied to a vertical pipe and a two-loop problem connected with a double *T*-junction, where user-defined subroutines in FORTRAN (Interface) were used for the manipulation of the CFX-code and PVM for the data exchange. The GRS (Georgios et al., 2014), describes a data-driven coupling approach for ATHLET and ANSYS CFX based on a general and user-friendly CFX-coupling prototype with external 1D codes. It can deal with explicit and semi-implicit coupling approaches. To demonstrate the new capabilities, a double *T*-Junction experiment, where 3D phenomena are important, is successfully solved.

In parallel, different domain overlapping coupling approaches were also developed and implemented in the last decades. The first domain-overlapping application was the multi-scale coupling of the thermal–hydraulic system code – CATHARE and the CFD code – TRIO_U for steady-state and transient simulations of e.g. Gas Fast Reactor (Perdu and Vandroux, 2008) and the analysis of the Phénix Sodium-cooled Fast Reactor (SFR) (Tenchine et al., 2012) (Bavière et al., 2014). There are also several other attempts to use the domain-overlapping method e.g. SAS4A/SASSYS-1/STAR-CD (Fanning and Thomas, 2010) and RELAP5/STAR-CCM+ (Jeltsov et al., 2013) (Papukchiev et al., 2015). The first time that the 3D CFD results are used to correlate the solution of a system thermal–hydraulic code in the entire overlapped domains was done by the coupling of RELAP5 and FLUENT. The "Closure-on-Demand" (Cadinu et al., 2008) or "Coupling-by-Closure" (Cadinu and Kudinov, 2009) method was developed to properly implement the domain-overlapping approach. In the two approaches above, they drop the convective pressure drop as well as the form-friction pressure drop from the system code's motion equation and use the total pressure drop from FLUENT to represent the two pressure drop items by imposing the two effects all into the form-friction loss coefficient. Following this basic idea, TRACE and STAR-CCM + were coupled. The fine coolant velocity and pressure fields from STAR-CCM + are used to calculate the new closure coefficients for TRACE. Thus, TRACE is expected to produce CFD-like hydraulic results in the entire overlapped domain. This coupled code works well for both 1D (Grunloh and Manera, 2016) and 3D (Grunloh, 2016; Grunloh and Manera, 2017) system models.

Besides the domain decomposition and overlapping methods, the codes can be coupled either internally or externally. For many years, internal coupling where a code acts as a library of the other code is the most common coupling approach thanks to its simplicity. Nowadays, modularity as well as efficiency is becoming increasingly important for a coupling system. Thus external coupling where each code is independent of others is becoming mainstream. There, a code interface is necessary and various of them were developed these years. In (Mahaffy, 2003) a new interface – ECI for TRACE coupling issues was developed. Based on ECI, the coupling of TRACE and SCF was implemented at KIT (Zhang and Sanchez-Espinoza, xxxx). In (Bavière et al., 2014); the coupling of CATHARE and Trio_U was implemented by CEA based on the ICoCo-methodology to simulate the natural circulation within the vessel of a Sodium Fast Reactor (SFR). Also based on ICoCo, at KIT, TRACE/TrioCFD (Zhang et al., 2020), TRACE/SCF (Zhang et al., 2021), and SCF/TrioCFD (Zhang et al., 2020) are developed with the traditional domain decomposition method or the overlapping method. This paper focuses more on the first two coupling implementations. For more information on the multi-scale TH coupling cases and methods, (Zhang, 2019) gives an extensive review of them.

4. Short description of the ICoCo methodology

ICoCo is the abbreviation of Interface for Code Coupling. It is a standard framework telling what functions should be implemented for code coupling. Some of the most common functions are:

1) setDataFile – define the input file and the relevant path;
2) initialize – perform the initialization;
3) computeTimeStep – get the current timestep size;
4) initTimeStep – set the current timestep size;
5) solveTimeStep – solve the current timestep;
6) getOutputMEDField – extract and export the field e.g. coolant density and coolant temperature, etc;
7) setInputMEDField – write the field from other code;
8) terminate – terminate the simulation.

The preconditions for the coupling of two solvers based on ICoCo are the modularization of the involved codes (to correspond to the ICoCo functions), the generation of meshes (for field interpolation and visualization) for each solver, and the development of an ICoCo-interface (implementation based on the ICoCo framework) for each code. The modified code, together with its ICoCo, will be compiled into a shared library (called the ICoCo module). Those modules will be called by a supervisor which controls the computation sequence and manipulation of data. Fig. 1 gives the general architecture of the ICoCo-based coupling system.

The supervisor could be scripts written in C++ or Python (MPI supported), as well as the open-source SALOME platform (GUI supported). Furthermore, ICoCo inherently uses the open-source MED or MEDCoupling library to manipulate mesh and fields (MED, 2019).

To sum up, the advantages of ICoCo over other methods mainly lie in the following two aspects: a) the standardization and modulization of the architecture, which makes the codes convenient for extension; b) the inherent application of MED functionalities, which solves the mesh and field translations (always a heavy workload and hurt point for code coupling) between codes.

5. Coupling of TRACE and TrioCFD based on ICoCo-approach

At KIT, a new ICoCo interface was developed for TRACE and the built-in ICoCo of TrioCFD was modified for better performance. A C++ script that employs the MPI functions was developed as the supervisor.

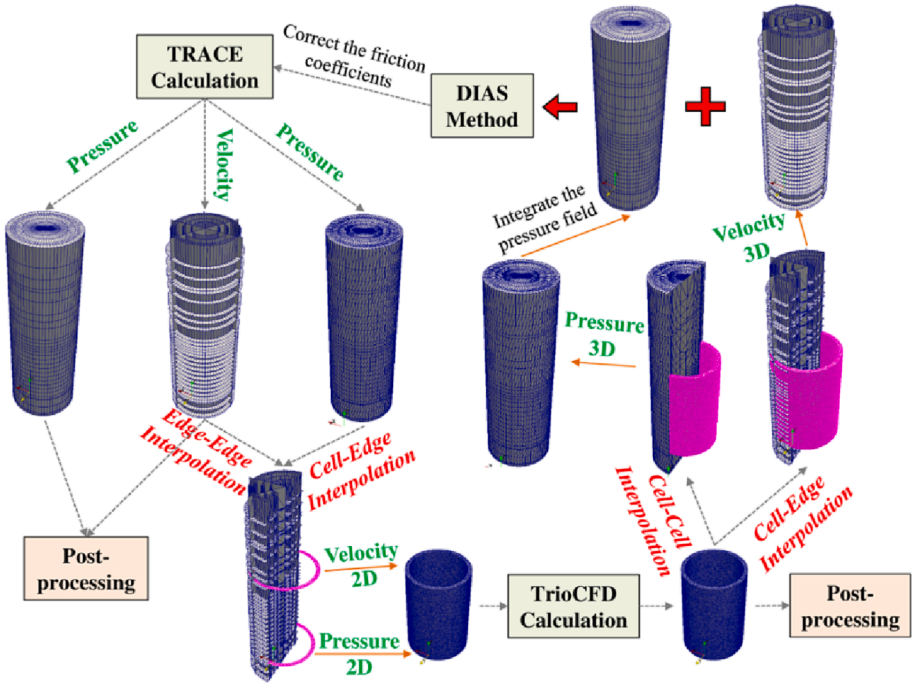

Fig. 2. Data flow between TRACE and TrioCFD based on the DIAS approach for the velocity and pressure based on the different meshing (Zhang et al., 2020).

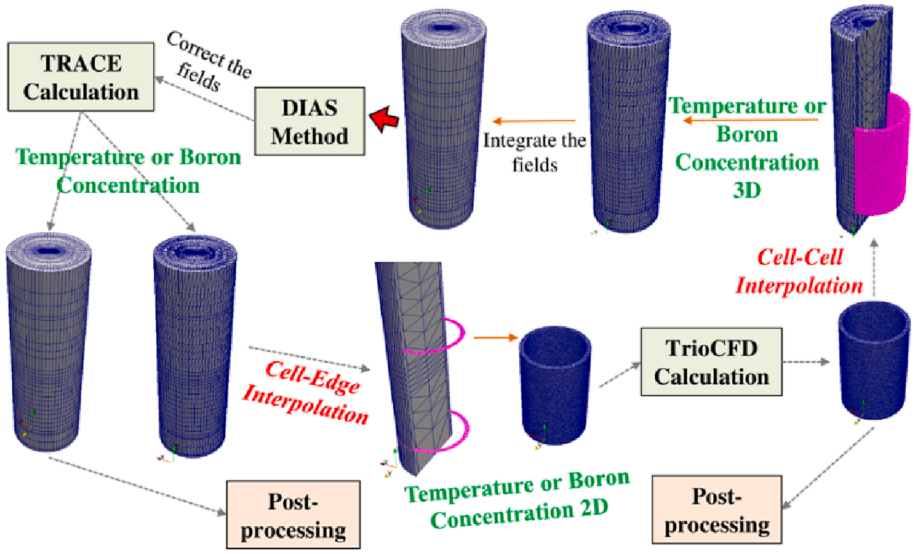

Fig. 3. Data flow between TRACE and TrioCFD based on the DIAS approach for the coolant temperature and boron concentration based on the different meshing (Zhang et al., 2020).

The domain overlapping approach applied here is based on the basic principles of the work performed for the coupling of RELAP5/FLUENT and TRACE/STAR-CCM +. There, the implemented domain overlapping method takes the 3D fine velocity and pressure fields from TrioCFD to correlate the friction coefficients at each overlapped edge of the TRACE computational domain. In doing so, TRACE is expected to calculate TH fields with a TrioCFD-like accuracy. In addition to that, the volumetric correlations are extended to include the coolant temperature and boron concentration fields. These correlations finally form the Dynamic Implicit Additional Source (DIAS) method, which is especially for the domain overlapping approach with 3D volumetric transfers.

5.1. The DIAS method

In (Zhang and Sanchez-Espinoza, 2020) the DIAS method is extensively presented and discussed. In the multi-scale coupling, DIAS is used to properly use the 3D volumetric fine data from TrioCFD to correlate the TRACE simulations. In short, the DIAS method can correlate four TRACE TH parameters in the entire TRACE overlapped domain using the high-resolution data predicted by TrioCFD:

- The coolant velocity and pressure. The fine pressure and coolant velocity fields predicted by TrioCFD are used to update the friction and form loss coefficient K for each edge located in the overlapped domains of TRACE. Hence, TRACE predicts TrioCFD-like hydraulic

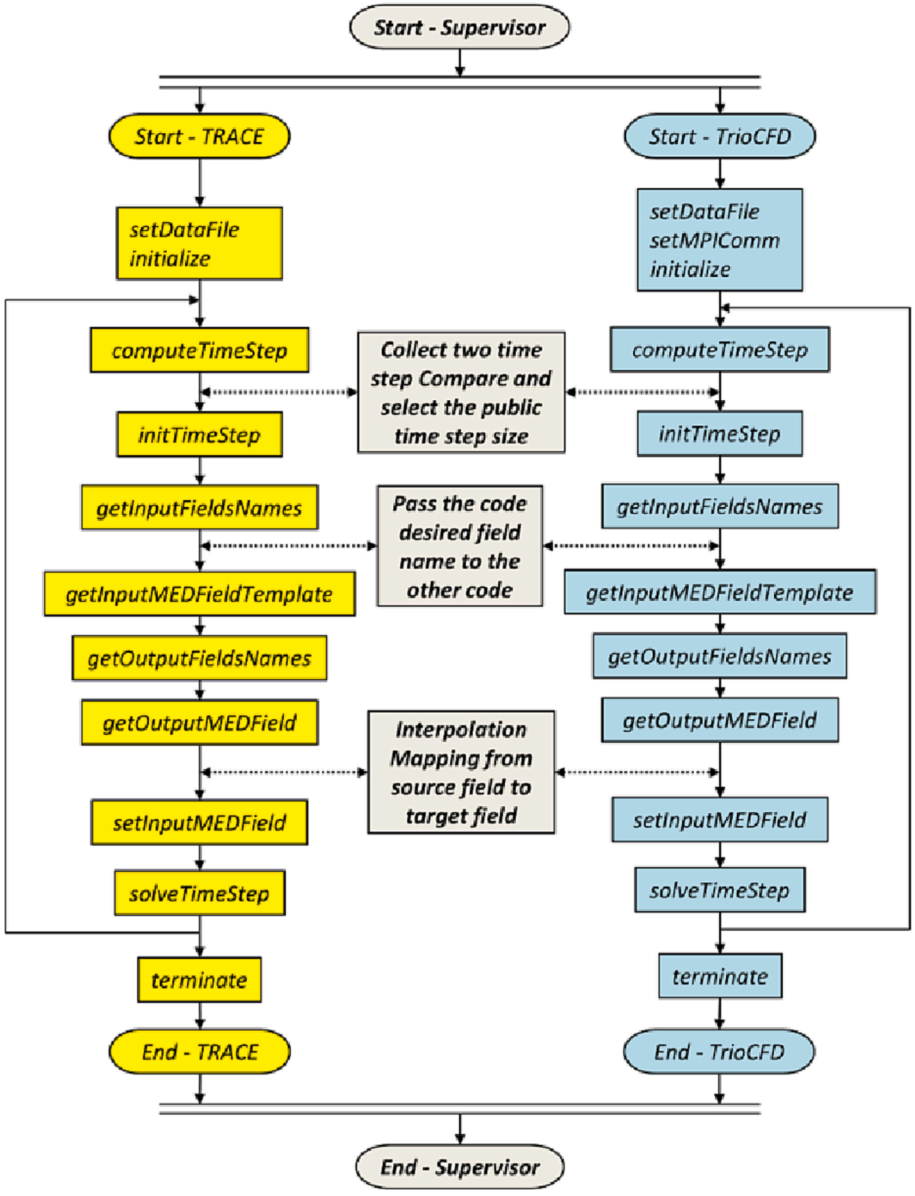

Fig. 4. The explicit temporal coupling scheme of TRACE/TrioCFD based on ICoCo (Zhang et al., 2020).

results. The two parameters are correlated together because they are tightly coupled in the momentum equation.

- The coolant temperature. The correlation goes deep into the TRACE-numerics i.e. the linearization process and appends an implicit additional heat source to the energy equation.
- The boron concentration. The correlation is implemented at the end of each time step and appends an implicit additional boron source to the boron equation.

It is worth emphasizing that the DIAS method for the correlation of key parameters between TrioCFD and TRACE does not imply that the refined TRACE fields in the overlapped domain are used for the final analysis. Since the fine TrioCFD result is already (SALOME-The Open Source Integration Platform for Numerical Simulation, 2019)in the overlapped domain, there is no gain to use the "coarse field" instead of the "fine field". Indeed, the overlapped-domain correlations to TRACE ensure the TrioCFD information at a "fine field" can be passed to TRACE and so let TRACE be able to give better predictions over the entire nuclear power system and provide better-refined boundary conditions to TrioCFD for the following time steps.

5.2. *Domain overlapping between TRACE and TrioCFD: Spatial mapping and data exchange*

Assume that TrioCFD simulates only the downcomer region of an RPV and TRACE simulates the full RPV. In this case, the overlapped region covers only the downcomer. Taking advantage of the meshes developed for TRACE at KIT (Zhang et al., 2019), two categories were developed for the spatial mapping and data exchange between TRACE and TrioCFD:

- Category 1: edge mesh and tetrahedron-cell mesh for the simultaneous correlations for the velocity and pressure, Fig. 2;
- Category 2: tetrahedron-cell mesh for the correlations of the coolant temperature and boron concentration, Fig. 3.

The spatial mapping is based on the mesh and field generated with the MEDCoupling libraries and the data transfer/utilization is performed based on the DIAS method.

Table 1
Main initial operating parameters before the test.

Parameter	*Initial State*	*Accuracy*
Thermal power, MW	281	± 60
Reactor inlet pressure, MPa	15.97	
Reactor pressure drop, MPa	0.418	±0.043
Coolant temperature at cold legs, K		± 1.5
Loop-1 &3 and 4:	541.75	
Loop-2:	541.85	
Coolant temperature at hot legs, K		± 2.0
Loop-1&2&4:	545	
Loop-3:	544.9	
Mass flow rates, kg/s		± 110
Loop-1:	4737	
Loop-2:	4718	
Loop-3:	4682	
Loop-4:	4834	

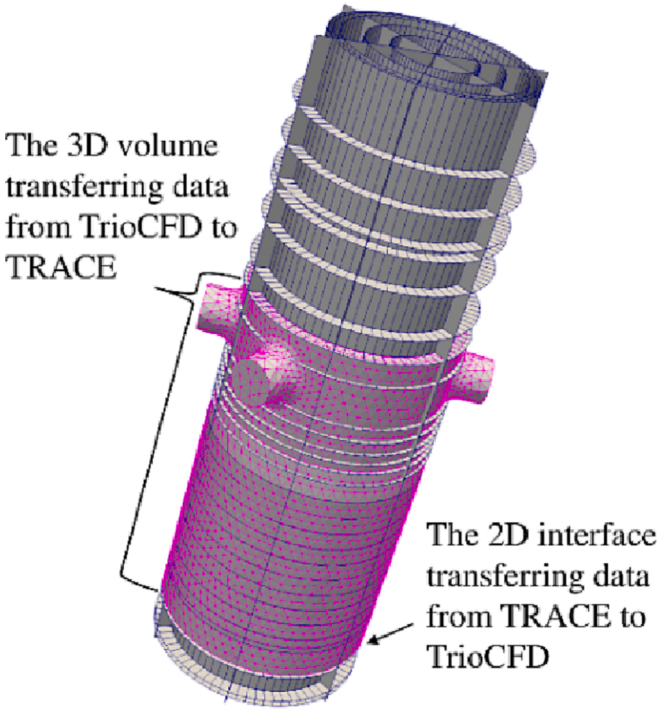

Fig. 5. The overlapped meshes of TRACE and TrioCFD for the analysis of the coolant mixing test (Zhang et al., 2020).

5.3. The explicit temporal coupling scheme

An explicit temporal coupling approach was implemented for this case. It is a server-client and parallel system controlled by a C++ supervisor, Fig. 4.

In this approach, the data synchronization during the time advancement of both solvers is based on an explicit Operator Splitting (OS) approach. The data transfer is only performed within each time step. The upgrading to a semi-implicit temporal coupling is not a significant task because only the supervisor script needs to be reorganized while the ICoCo functions remain untouched.

5.4. Validation of TRACE/TrioCFD-ICoCo

For the evaluation of the prediction capability of the TRACE/TrioCFD, the coolant mixing test performed at the VVER-1000 Kozloduy plant is analyzed (Kolev et al., 2004). The pre-test main initial operating parameters are summarized in Table 1.

The test is triggered by the closure of a main steam isolated valve on the secondary side of the SG-1 when the plant was operated at around 20 % of the nominal power. As a consequence, the heat transfer from the primary to the secondary loop-1 was perturbed, and hence, the coolant temperature of the cold leg of loop-1 increased by 14 K during the first 500 s. Consequently, a coolant mixing took place in the downcomer, and the mixing patterns propagate through the lower plenum into the core. The challenge is to predict the heat out of coolant temperature within the core and hot legs and the resulting mixing pattern.

For the domain overlapping approach, a TrioCFD-model of the downcomer and a TRACE model of the full RPV was developed for the simulation of the coolant mixing tests. The overlapped meshes are presented in Fig. 5. There, the TRACE-edge mesh and TrioCFD-mesh overlap in the downcomer region. The inlet boundary condition of TrioCFD is pre-defined in the input file. The outlet boundary condition of TrioCFD comes automatically from TRACE through the 2D interface plane, where mesh interpolation and field mapping is done by the MEDCoupling library. The 3D volumetric fields of TrioCFD are translated by MEDCoupling and passed to the TRACE-mesh to correlate its corresponding fields according to the DIAS method.

It must be pointed out that the four loops of the Kozloduy plant are not symmetrically arranged. This will impact the simulation of the test with the coupled TrioCFD/TRACE code since this arrangement cannot be represented accurately.

A coupled simulation of the coolant mixing test was performed with TrioCFD/TRACE and important parameters such as coolant temperature, pressure, and coolant velocity have been predicted. In Fig. 6, the coolant temperature matching between TRACE and TrioCFD is evident, which indicates the temperature translation is executed correctly. It can be observed that the hot coolant enters the downcomer from one loop and gradually diffuses over a larger area along the main flow direction.

A comparison of the coolant temperature at the hot legs of loop-1 and- 4 as predicted by TRACE and TRACE/TrioCFD and the measured data is given in Fig. 7. For the hot-leg-1, the coupled code improves the prediction of the coolant outlet temperature compared to the stand-alone code. On the contrary, the coolant temperature of the hot-leg-4 is over-predicted by TRACE/TrioCFD and under-predicted by TRACE. The coolant temperature of the hot leg of loop-2 is also over-predicted by TRACE/TrioCFD and is a little bit better than the one predicted by TRACE. But, for the coolant temperature of the hot-leg-3, which connects to a downcomer sector, not in the direct neighborhood of the affected sector, all predictions are not satisfactory. Further investigations are necessary to find out the main reasons for this behavior. One reason could be the inability of TRACE to represent the non-symmetrical arrangement of the loops connected with the domain overlapping approach and the DIAS method.

6. ICoCo coupling of TRACE and SCF based on domain overlapping

Based on the work performed for the coupling of TRACE and TrioCFD, a domain overlapping coupling approach for SCF and TRACE was implemented. Here, the YACS module of the SALOME platform supervises the computational route and data synchronization during the time advancement of the explicit temporal coupling for steady-state and transient simulations. Furthermore, this coupled code was upgraded to be able to run under a domain decomposition mode recently at KIT (a similar approach as the ECI-based coupling (Zhang and Sanchez-Espinoza, xxxx). This function was tested and verified to produce consistent results with the domain overlapping method. Anyway, this paper focuses on the description of the coupling and the verification with the domain overlapping approach.

6.1. Coupling methodology

SALOME as the supervisor also takes profit from the powerful interpolation functions for code coupling (SALOME-The Open Source

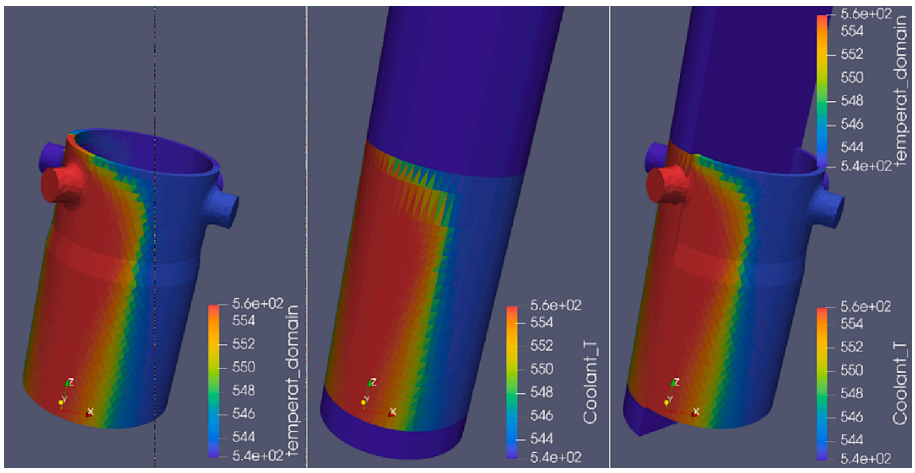

Fig. 6. The coolant temperature distributions (left-TrioCFD, middle-TRACE, right-overlapped meshes) in the downcomer as predicted by the different solvers and the correlated ones based on the DIAS method (Zhang et al., 2020).

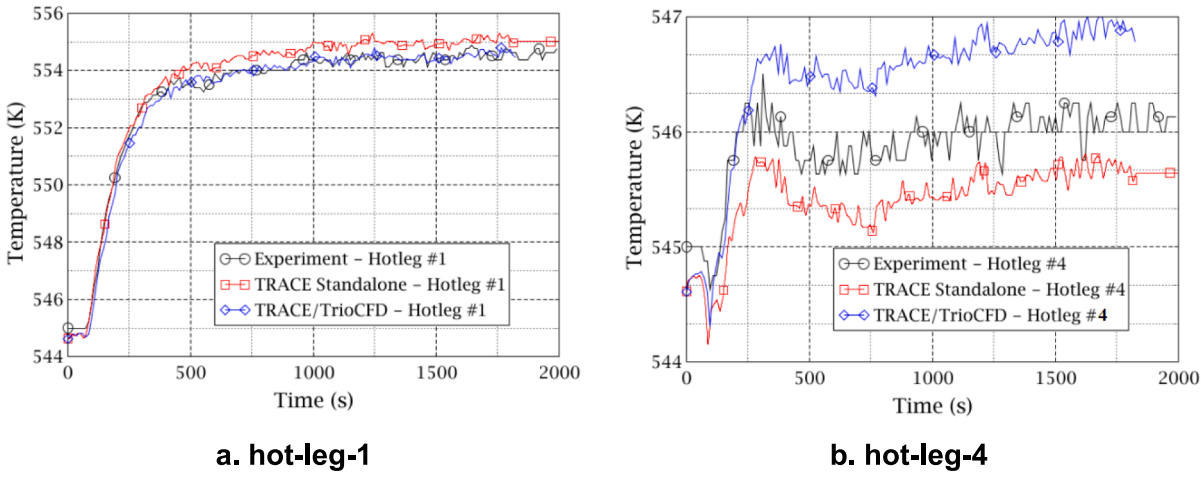

Fig. 7. Comparison of the coolant temperatures predicted by TRACE and TRACE/TrioCFD with the measured data (Zhang et al., 2020).

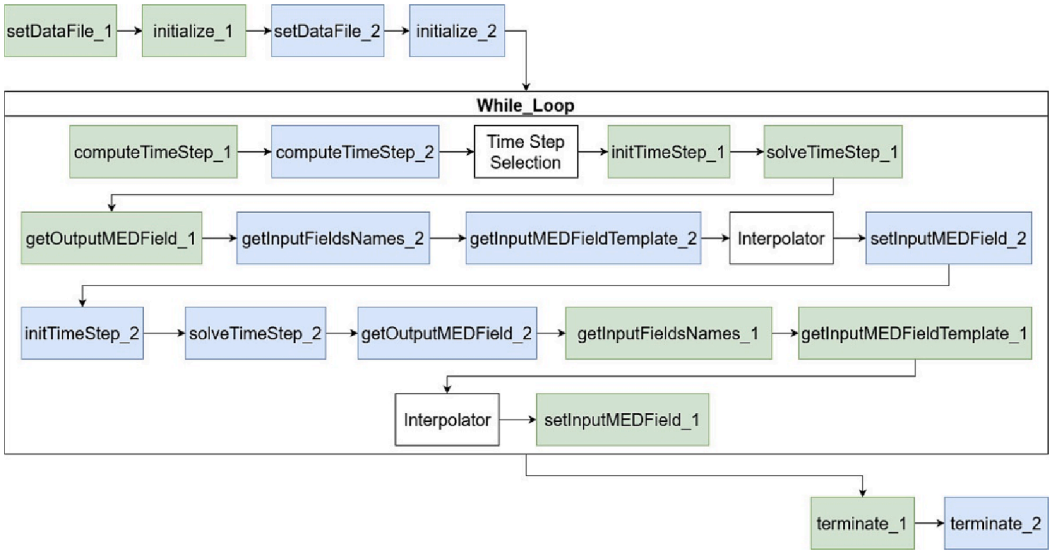

Fig. 8. Computational route for the coupling code TRACE/SCF inside the SALOME platform based on ICoCo (1-TRACE, 2-SCF).

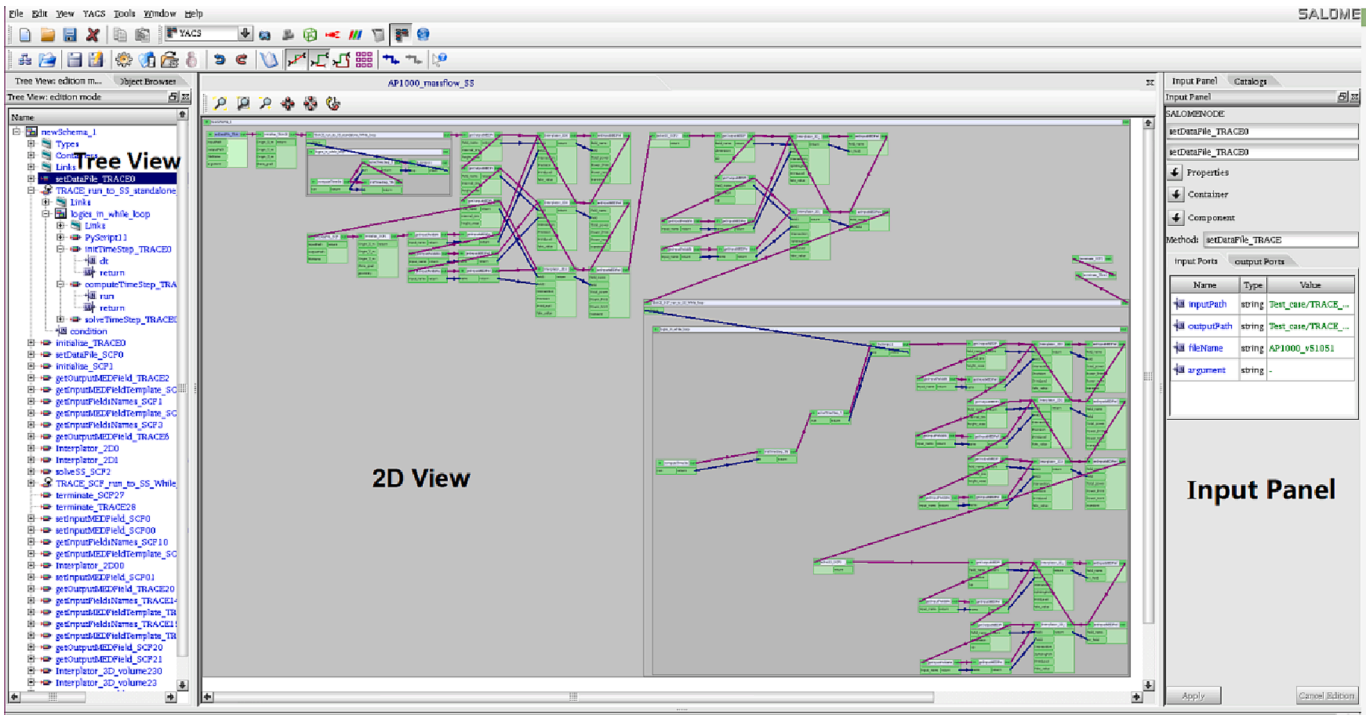

Fig. 9. The SALOME YACS GUI for the TRACE/SCF-ICoCo simulations.

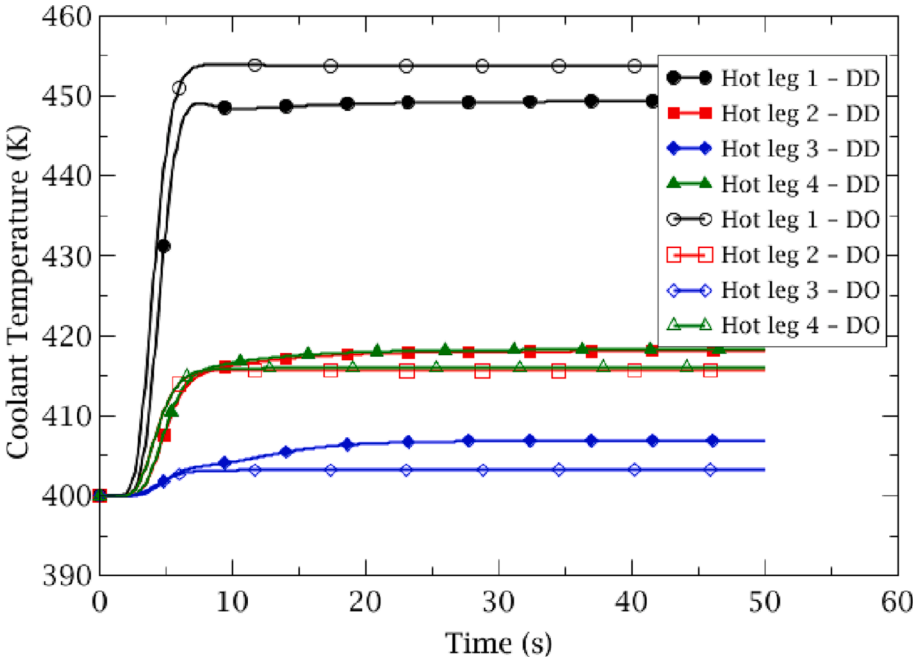

Fig. 10. The comparison of the coolant temperature at the hot legs predicted by TRACE/SCD-ICoCo-SALOME with domain decomposition (DD) and domain overlapping (DO) method.

Integration Platform for Numerical Simulation, 2019) embedded in the MEDCoupling library (embedded in SALOME). The other highlight of SALOME is the built-in module named YACS (SALOME - YACS module, 2019). It offers a Graphic User Interface (GUI) to define the calculation routes just by "drag" and "click". It is worth mentioning that SALOME is the best option for less CPU-intensive solvers and it offers online monitoring of the running processes. Besides, this work builds on the ICoCo-module developed for SCF to couple it with 3D diffusion solver and Monte Carlo codes (García et al., 2020) on one hand and the ICoCo-module developed for TRACE in (Zhang et al., 2019) on the other hand.

In (Campos, 2020), the details of this coupling of TRACE with SCF inside the SALOME platform are given. Modifications of the ICoCo-interfaces for both codes were necessary and are documented in (Zhang, 2017). Currently, the ICoCo Interface for TRACE and SCF as well as their simulation sequence are shown in Fig. 8.

In this approach, the exchange of the fields between TRACE and SCF is based on the inherent interpolations capabilities that are quite similar to the coupling case of TRACE and TrioCFD:

Table 2
Main initial operating parameters before the test (Zhang et al., 2020).

Parameter	*Initial State*	*Accuracy*
Thermal power, MW	281	± 60
Reactor inlet pressure, MPa	15.97	
Reactor pressure drop, MPa	0.418	±0.043
Coolant temperature at cold-legs, K #1–541.75; #2–541.85; #3–541.75; #4–541.75		± 1.5
Coolant temperature at hot-legs, K #1–545; #2–545; #3–544.9; #4–545		± 2.0
Mass flow rates, kg/s #1–4737; #2–4718; #3–4682; #4–4834		± 110

- 2D fields interpolation: map two-dimensional fields, for boundary conditions from TRACE to SCF;
- 3D edge field interpolation: map three-dimensional surface-based fields like the coolant velocity, from SCF to TRACE;
- 3D cell field interpolation: map three-dimensional cell-centered fields like the coolant temperature, from SCF to TRACE.

In Fig. 9 a screen capture of the coupling simulation in the SALOME YACS GUI is shown, where TRACE and SCF can be loaded as components for code coupling. Each code is characterized by its meshing and the functional modules e.g. for the initialization, steady-state solution, transient solution, convergence checking, etc. YACS allows graphically to define connections between the different modular parts of the codes. In this approach, it is worth mentioning, that key data is stored in fields defined in meshes. Hence, by automatic mesh superposition, the MED-coupling library allows the exchange of data among the solvers. In YACS, computational routes e.g. for the stand-alone solvers integrated as "components" in SALOME or for a coupled steady-state or transient solution can be defined. Besides, the coupled simulations are started from the GUI and the changes in the key parameters can be monitored on-the-fly.

As mentioned above, this coupled code was recently expanded with the domain decomposition method. With a simple testing case, the first result is obtained. This is a coolant mixing case that is described in (Zhang and Sanchez-Espinoza, xxxx). There, the reactor has four loops corresponding to four cold legs and four hot legs. In the beginning, the coolant temperature in the RPV and the hot and cold legs is 400 K. Then cold leg 1 will experience a temperature rise from 400 K to 500 K in 10 s, while others remain 400 K. Fig. 10 plots the coolant temperature evolution at the hot legs predicted by TRACE/SCF with domain decomposition and domain overlapping methods. The difference is obvious. The former method predicts a more strong coolant mixing in the core area. Further work about the domain decomposition method for the ICoCo- and SALOME-based TRACE/SCF will be performed and the relevant result will be published.

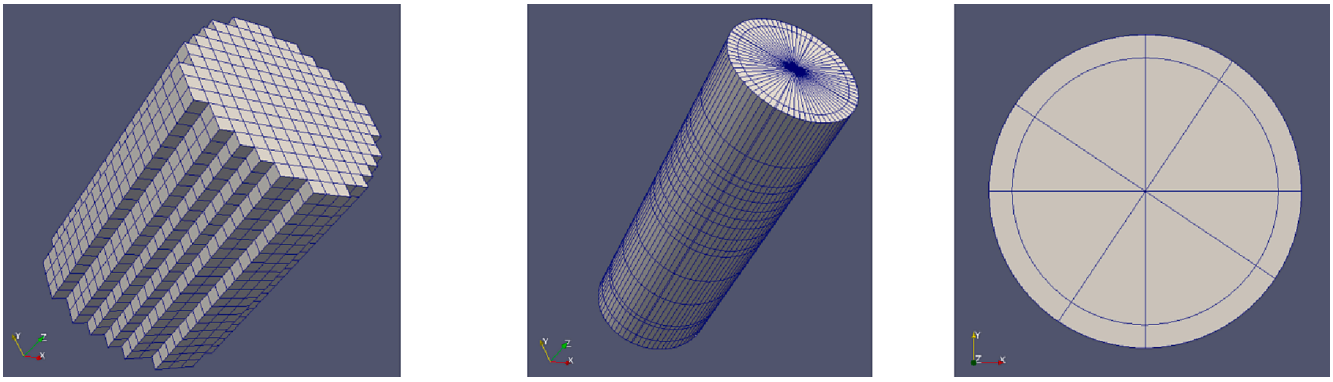

Fig. 11. Meshing of the SubChanFlow and TRACE thermal–hydraulic codes to represent the core and the RPV.

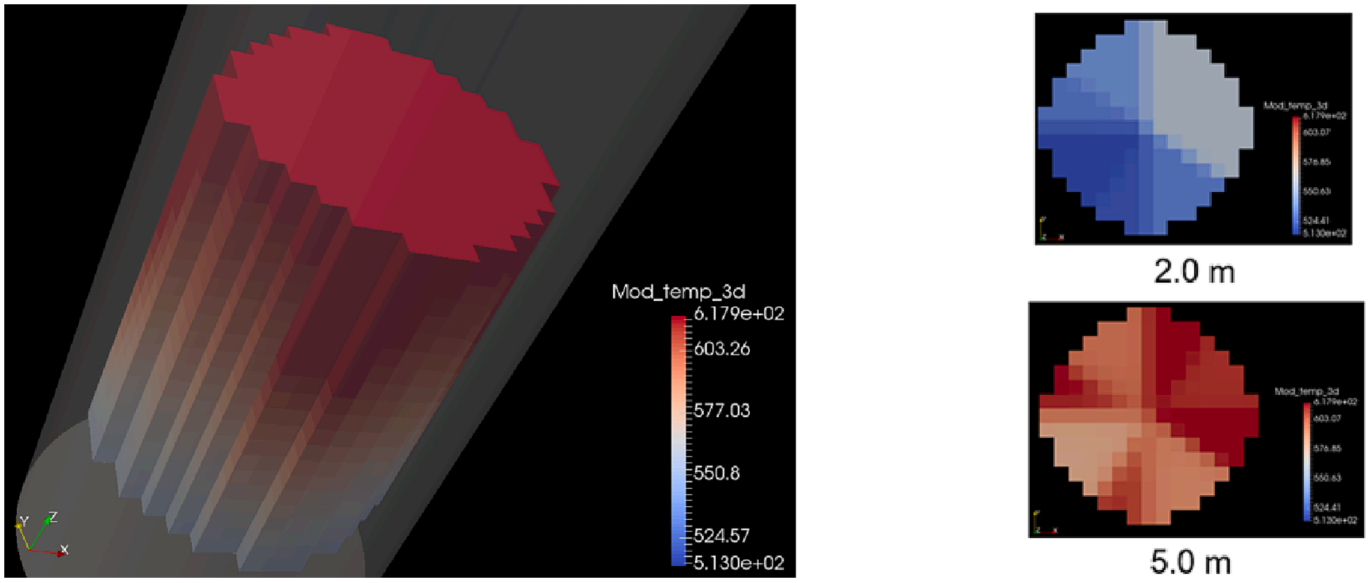

Fig. 12. AP-1000 Predicted moderator temperature at times 0 and 20 s.

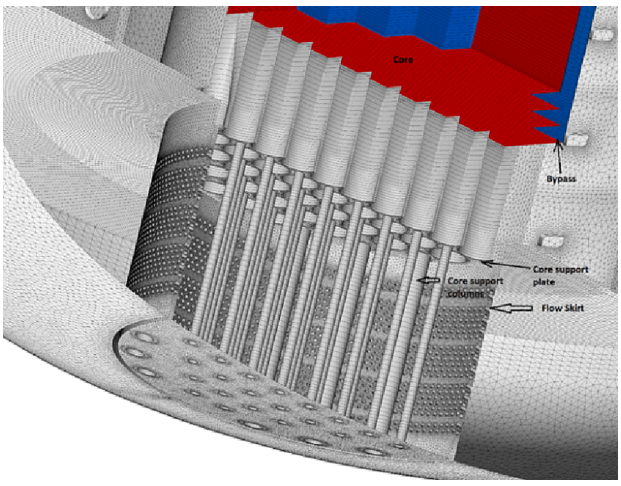

Fig. 13. The CFD mesh in the lower plenum of the SMART RPV (Böttcher and Sanchez-Espinoza, 2022).

6.2. First application of the coupled code TRACE/SCF-ICoCo

To demonstrate the prediction capability of the coupled code, the TH behavior of the AP-1000 RPV is evaluated. This NPP has four loops which correspond to four cold legs and hot legs. The initial state of the reactor is given in Table 2.

During the transient, the coolant temperature of one loop is reduced within 10 s from 553.7 K to 503.7 K, and the reactor is operating at the nominal power. For this purpose, a TRACE model of the AP-1000 reactor developed in (Di, 2017) was modified to evaluate only the RPV and core behavior. Besides, the assembly-wise SCF model of the core was developed, where each fuel assembly is represented by one TH channel. In Fig. 11 the meshes of the two thermal–hydraulic solvers are represented. Besides, TRACE also has a tetrahedron and an edge-face mesh.

In Fig. 12, the moderator temperature predicted with TRACE/SubChanFlow using the point kinetics models of SubChanflow for a coolant temperature transient is shown. The results seem to be consistent.

7. Summary and conclusions

In this paper, the current developments at KIT focusing on multi-scale TH are presented, and the first results for consistency checking and validation are discussed. The combination of the best capability of different thermal–hydraulic solvers in a multi-scale approach paves the way for a more physical prediction of the safety parameters of reactor systems.

Based on the implementation of the ICoCo coupling approaches, it can be stated that the ICoCo-concept is a very versatile and appropriate methodology that is independent of the involved solvers (compared to the KIT activities on the development with ECI). Other interfaces e.g. ECI is also powerful but it requires a deep understanding of the data and programming structure of TRACE. Based on the performed work, it can be also concluded that the domain overlapping approach is not the most practical approach to be followed in the future because it requires the introduction of correlations between the fine mesh solution of a CFD

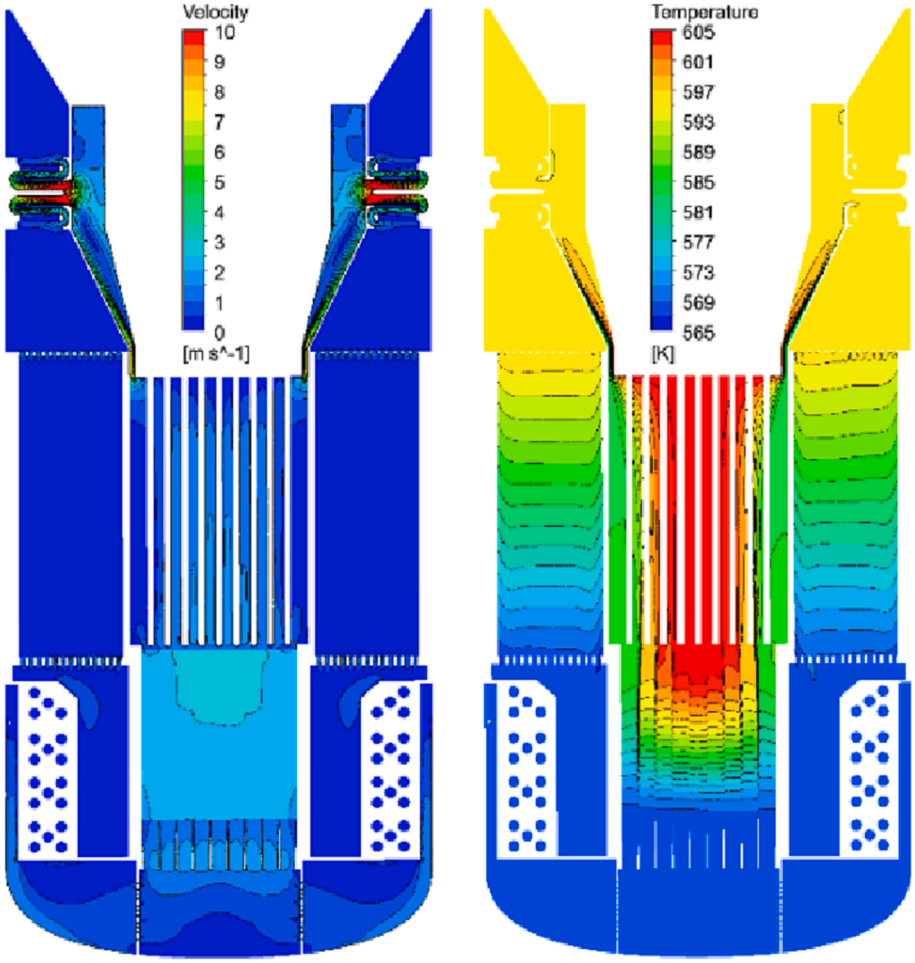

Fig. 14. Velocity and coolant temperature distribution predicted by ANSYS CFX (Böttcher and Sanchez-Espinoza, 2022).

code and a coarse mesh solution of the system code.

The inherent functionalities of the SALOME platform on which ICoCo relies i.e. the 3rd-party MEDCoupling library are very powerful to perform mesh interpolation and field mapping between different domains. The two coupling approaches presented and discussed needs further improvements and optimization as well as extensive validation using experimental data. A by-product of these developments is the fact that now the TRACE and SubChanFlow versions have nice and powerful post-processing with open-source tools such as ParaView or inside SALOME.

8. Outlook

Since the new tools will be able to solve the computational domains e.g. core, downcomer, lower plenum, and upper plenum with different degrees of details (CFD, subchannels, system TH: *meso*, component, and macro-scale), well-instrumented test facilities and/or test in nuclear power plants are required. Moreover, information on the uncertainties of measured data may be necessary when assessing the code's uncertainty. Hence, new experiments shall provide the measurement error of each measurement device. If repetitive tests are performed and different parameters are measured, this data could be also used to derive a probability distribution function of the parameters of interest when performing uncertainty quantifications.

The past work at KIT makes evident the limitations of the domain overlapping multi-scale coupling approach. Consequently, KIT is exploring the domain decomposition coupling approach since it offers more flexibility when applied to solve 3D phenomena in the reactor pressure vessel of NPPs of different types (PWR Gen-2 and − 3, SMR). At the moment, besides TRACE, SCF, and TrioCFD, other TH codes e.g. the porous media two-phase flow code TwoPorflow –developed at KIT- and TRACE are being coupled with OpenFOAM using ICoCo and the domain decomposition approach. Alternatively, the coupling of system TH codes with commercial CFD-codes e.g. ANSYS CFX, and FLUENT which are based in user define functions is worth to be followed. For this purpose, KIT is developing ANSYS CFX models for the integrated RPV of Small Modular Reactors (SMR). In Fig. 13, the lower part of the SMART RPV meshing is shown. First steady-state results for the SMART nominal conditions were obtained with ANSYS-CFX. In Fig. 14, the velocity and temperature distribution of the coolant in the integrated SMART RPV can be observed (Böttcher and Sanchez-Espinoza, 2022). These results are very promising and pave the way for alternative multi-scale coupling based on commercial CFD codes, which are numerically robust and stable in solving large complex problems.

CRediT authorship contribution statement

Victor Hugo Sanchez-Espinoza: Conceptualization, Investigation, Validation. **Kanglong Zhang:** Writing – original draft, Investigation, Writing – review & editing, Validation. **Alejandro Campos Muñoz:** Writing – original draft, Writing – review & editing. **Michael Böttcher:** Writing – original draft, Writing – review & editing, Validation.

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.

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