Multiscale thermal-hydraulic methods for improved simulation of nuclear power plants

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Abstract

In a Nuclear Power Plant (NPP), several thermal-hydraulic phenomena take place at different scales in the core and the primary and secondary circuits. Different thermal-hydraulic codes have been developed to describe the phenomena at meso- and macro-scale (sub-channel, porous media, and system thermal-hydraulic codes). Besides, the use of general-purpose CFD-codes for the analysis of the specific problem of nuclear power plants is rapidly increasing. At present, system thermal-hydraulic codes and some sub-channel codes are characterized by very good two-phase flow models covering the complete boiling curve while CFD codes are very good for analysis of single-phase flow. But, there is no way to resolve the full core with CFD codes at the spatial scale needed for the prediction of local safety parameters since it will not fit in the memory of current computers.

Based on those considerations, KIT is involved in the development of multi-scale coupling approaches to describe the physical phenomena more accurately than applying single codes. The approaches combine the three types of thermal-hydraulic codes: sub-channel, system, and CFD codes with each other.

The first step in this direction is the coupling of a system thermal-hydraulic codes with a sub-channel or porous-media code to improve the prediction of the core thermal-hydraulic phenomena. A subsequent step is to couple a system code with a CFD code to improve the simulation of 3D phenomena inside the Reactor Pressure Vessel (RPV). It is also feasible to couple a sub-channel code with a CFD-code to improve the core and RPV thermal hydraulics.

This paper will describe the different coupling methods realized based on an Interface for Code Coupling (ICoCo) applied for the coupling of a system code, a sub-channel code, and a CFD code. The first validation of such coupling approaches and further work is also described. It can be stated that the ICoCo-based multi-scale coupling approaches developed here are very powerful and promising.

1. Introduction

In a nuclear power plant, thermal-hydraulic phenomena take place at different scales in the core, and in the primary/secondary circuits including both single and two-phase flow conditions. Different thermal-hydraulic codes have been developed to describe these phenomena at meso- and macro-scale (sub-channel, and system thermal-hydraulic codes) for many decades. Extensive validation and code developmentwork were done to improve the prediction accuracy of such codes. It became evident, that the 1D/3D coarse-mesh approach (of system codes), as well as the quasi 3D-approach (of subchannel codes) implemented in the frame of two-fluid and in some cases in the two-fluid three-field flow models, contain limitations. Hence, 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 increases continuously [1], [2].

System thermal-hydraulic and sub-channel codes are characterized by very good covering the complete boiling curve, while CFD codes are very good for analysis of single-phase flow but not yet mature for the analysis of the full range of the void fraction. Some peculiarities of CFD-codes are a versatile and precise description of the real geometries of the problem of interest due to the variable combination of different mesh sizes in one computational domain, the parallel capability, and the employment of robust numerical solvers. Moreover, the CFD-simulations of a full reactor core with a detailed spatial resolution at the pin and sub-channel level as needed for the prediction of local safety parameters need a huge memory demand not yet available in current HPC-computer. Hence, the thermal-hydraulic description of the core (fuel assemblies, fuel rods) is typically solved by means of a porous media approach while the remaining regions of the RPV such as downcomer, lower plenum, upper plenum, circuits, etc. are treated with higher spatial resolution.

There are many 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 [3] a nice overview of current methodologies and approaches is summarized and discussed.

At KIT, the focus on a research area is the development of different thermal-hydraulic codes together with multi-scale coupling approaches to describe the physical phenomena within NPP in a more accurate manner than applying single codes, by combining different thermal-hydraulic codes e.g. sub-channel, system, and CFD-codes [2], [4], [5].

A key aspect of such multi-scale coupling is the selection of the most flexible and accurate coupling methodology taking into account the difference of the solvers and how they treat the spatial discretization of the computational domains to solve the thermal-hydraulic/fluid dynamic problem. At KIT, different coupling methodologies e.g. ECI [6], [7], and the ICoCo [8], were evaluated and implemented for different combinations of thermal-hydraulic solvers.

Chapter 2 gives a short description of the involved thermal-hydraulic codes for completeness. In **Chapter 3** of this paper, the main features of peculiarities of different coupling methods e.g. ECI and ICoCo are e presented and discussed in light of their implementation. The main focus of **Chapter 4** is the introduction of the ICoCo-based coupling of an open-source CFD-code (TrioCFD) with a system thermal-hydraulic code (TRACE) as well as the main coupling features, it first validation, and application. In **Chapter 5**, the implementation of the coupling of a subchannel code (SubChanFlow) with a system code (TRACE) using SALOME-YACS as a supervisor and a first application is briefly described and discussed.

Finally, **Chapter 6** presents the further work needed for the improvement of the developed coupling approaches and the practical use by the different end-users (regulators, industry, utility) in the frame of safety evaluation of NPPs as well as for an extensive validation.

2. Selected codes for multi-scale coupling

The following thermal-hydraulic codes are selected for the implementation of multi-scale coupling for reactor analysis: SubChanFlow, TRACE, and TrioCFD. Hereafter a short description of each one is provided.

2.1 The subchannel code SubChanFlow

The sub-channel code SubChanflow 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 level. Additional constitutive relations

are formulated to close the balance equations that describe the pressure drop, wall friction, boiling, heat transfer models for the whole boiling curve [4]. State equations for various coolants e.g. water (IAPWS 97), lead, Lead-Bismuth, Sodium, Helium, CO_2 are implemented. The system of equations is solved for stationary or time-dependent flow conditions in mainly upward flow. SubChanFlow 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). The validation work is mainly focused on LWR-applications using test e.g. from NUPEC PSBT and BFBT [4].

2.2 The system code TRACE

The system thermal-hydraulic code TRACE [9] is a best-estimate system code of the U.S. NRC for the analysis of Light Water Reactor (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. Due 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 [9]. Dedicated models describe specific physical phenomena such as thermal stratification, point kinetics, critical flow, etc. TRACE is recently equipped with an Exterior Communication Interface (ECI) for the coupling with any kind of solvers [ECI]. Typically, system codes such as TRACE are coupled 3D nodal diffusion solvers for the enhanced simulation of non-symmetrical transients in NPPs.

2.3 The open-source 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 [10]. 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 [11]. 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. [10]. In the past, TrioCFD was coupled with the system thermal-hydraulic code CATHARE [12] using the ICoCo methodology and applied for the analysis of LWR-problems e.g. within the European NURISP and NURESAFE [13] projects.

3. Methodologies for multi-scale thermal-hydraulic coupling

For many years, different research groups tried to implement multi-scale thermal-hydraulic coupling schemes to increase the prediction capability regarding safety-relevant phenomena in NPPs. One of the first

coupled codes were based on an internal coupling of TRAC and CobraTF [14], and RELAP5 and Cobra-TF [15] 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 thermal-hydraulic code MARS was developed to improve the simulation of advanced Generation 3 reactors like APR+ [16]. The increasing use of commercial and open-source CFD-codes in the nuclear industry fostered also the development of coupling approaches for system thermal-hydraulic and CFD-code aiming the simulation of different kind of problems, where spatial effects play a key role and cannot be properly described by 1D codes or coarse 3D models of system codes [17] in the primary/secondary circuit and the containment, [10], [18], [19] [20], [21]. In [6] a new interface – ECI for coupling of TRACE with other codes was developed. The key feature of ECI is the capability to parallelize the computational route of the coupling system in a random way. However, its implementation requires a deep knowledge of the code structure and numerics and the control of the synchronization of the data exchange among the involved solvers. Latter means to assure that the "right data" is transferred at the "right place" and at the "right time" among the codes in a multi-tasking parallel system. At KIT, an ECI-based coupling of TRACE and SubChanFlow was implemented for which an ECI-module for SCF was developed [7]. For this purpose, the SCF-source code was re-organized and modularized. This coupling approach was applied to simulate the thermal-hydraulics of an RPV, where SCF describes the core and TRACE, the remaining portions of the RPV being modelled by mans of the 3D VESSEL-component. Early developmental work on a multi-scale coupling approach was devoted to the domain decomposition (DD) approach. In [22] 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 demonstrated. At SCKEN [23], 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 [24], 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 [25], describes a data-driven coupling approach for ATHLET and ANSYS CFX based on 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 (DO) 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 [26] and the analysis of the Phénix Sodium-cooled Fast Reactor (SFR) [27] [12]. There are also several other attempts to use the domain-overlapping method e.g. SAS4A/SASSYS-1/STAR-CD [28] and RELAP5/STAR-CCM+ [29] [30]. 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" [31] or "Coupling-by-Closure" [32] 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 uses 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 [33] and 3D [34] system models.

In [12], 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). At the University of Michigan [35], [34], a domain overlapping method is implemented for the coupling of STAR-CCM+ and TRACE; it is applied for LWR applications, especially of flow inside the RPV e.g. downcomer and lower plenum where the 3D flow is expected in some transient scenarios.

Recently, at KIT [5], [8] a domain overlapping approach for the coupling of TRACE with the opensource code TrioCFD was developed based on the ICoCo-methodology and applied for the improved simulation of a coolant mixing test in a VVER-1000 reactor. Details of this coupling approach will be discussed in Chapter 5. Following this approach, in [36] of TrioCFD and SubChanFlow based on the ICoCo-methodology and domain decomposition approach was developed and applied to an academic problem consisting of a pipe, a core, and a plenum. An extensive review of the different multi-scale coupling approaches for thermal-hydraulic codes is given in [3].

4. ICoCo-based coupling of TRACE with TrioCFD

A precondition for the coupling of two solvers based on the ICoCo-concept is the modularization of the involved codes, the generation of meshes for each solver, and the development of an ICoCo-interface for each code. The open-source code TrioCFD is already equipped with an ICoCo-interface. Merely, a new interface was developed for TRACE. ICoCo contains the basic functions and provides different methods e.g. to insert various input /output ports to the solvers needed for flexible and convenient data exchange between them. In this concept, the supervisor program controls the data flow, calculational route, and data exchange. In **Figure 1**, the general scheme of the coupled system TrioCFD-TRACE is shown. Note that ICoCo is a cross-language interface since TRACE is written in Fortran and TrioCFD is in C++.

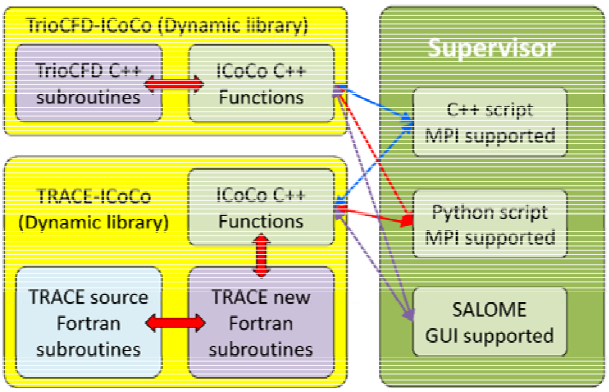


Figure 1: The coupled codes TRACE/TrioCFD with ICoCo coordinated by the supervisor

The supervisor can be implemented on C++ / Python scripts or in the open-source platform SALOME. To assure the parallel functionality of TrioCFD, the supervisor should be either a C++ script or a Python script that supports MPI. Central elements of any coupling of different solvers are the spatial mapping for a consistent data transfer and the temporal coupling that assure the proper synchronization of the solver during the time advancement. Here, the domain-overlapping approach based on the MEDCoupling library

that offers the mesh interpolation and field mapping functionalities, and the explicit temporal scheme was selected.

4.1 Domain-overlapping approach and the role of the DIAS-method

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+. Hence, the implemented domain-overlapping method takes the 3D fine velocity and pressure fields from TrioCFD to correlate the friction coefficients at each overlapped edges of the TRACE computational domain. In doing so, TRACE is expected to calculate thermal-hydraulic 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 form the Dynamic Implicit Additional Source (DIAS) method, which is especially for the domain-overlapping approach with 3D volumetric transfers.

Short description of the DIAS-method

In [37] 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 and introduce the effects sufficiently to TRACE. In short, the DIAS-method can correlate four TRACE thermal-hydraulic parameters in the entire TRACE overlapped domain using the high-resolution data predicted by TrioCFD. These parameters are listed below:

- 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 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. This method assures that the coolant temperature in the TRACE overlapped domains are a hundred percent consistent with ones of TrioCFD.
- The boron concentration. The correlation is implemented at the end of each time step and append an implicit additional boron source to the boron equation. This method assures that the boron concentration in TRACE overlapped domains is a hundred percent consistent with the ones of TrioCFD.

Figure 2 shows the TRACE overall solution approach and where the correlations are introduced by DIAS. 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 available 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.

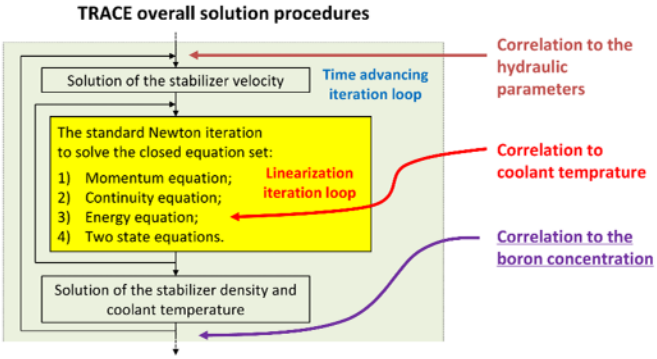


Figure 2: DIAS-Method: correlation of hydraulic, temperature, and boron fields for TRACE

4.2 Spatial mapping for consistent data exchange between TRACE and TrioCFD

Assume that TrioCFD simulates only the downcomer region of an RPV and TRACE the full RPV of a reactor e.g. a VVER RPV. In this case, the overlapped region covers only the downcomer. For illustration, a simplified downcomer model of TrioCFD is shown in **Figure 3**. For TRACE a normal 3D cell mesh and edge mesh was created for the coupling purposes [5].

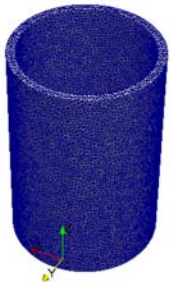


Figure 3 TrioCFD: VVER-1000 downcomer model

In the frame of the DIAS-method, where correlations to four system parameters in the overlapped domain e.g. the coolant velocity, the pressure, the coolant temperature, and the boron concentration are defined, the data transfers between the domains are specified by the following categories:

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

In **Figure 4**, the data flow for the correlations of the hydraulic parameters of TrioCFD/TRACE is shown.

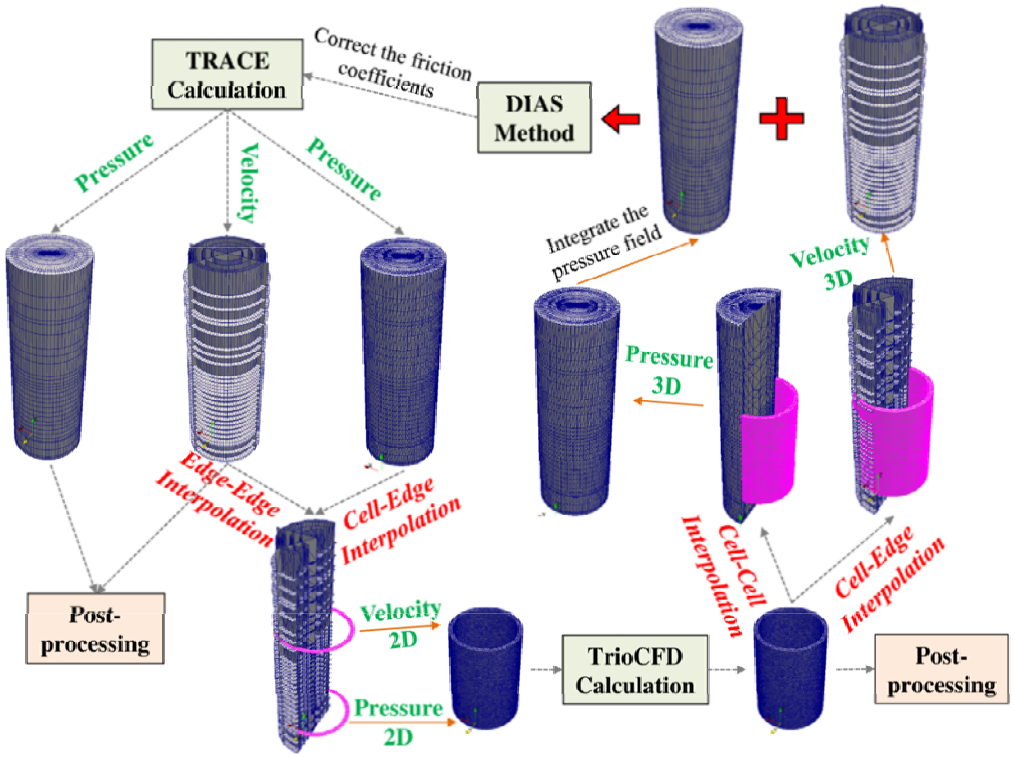


Figure 4: Data flow between TRACE and TrioCFD based on the DIAS-approach for the velocity and pressure based on the different meshing

The data flow follows the procedures listed below for the hydraulic parameter correlations and data exchange using the MEDCoupling library.

- Fist, TRACE solves a time step, saves the 3D-pressure fields in the normal-cell mesh (for post-processing), and in the tetrahedron-cell mesh (for the field mapping) to be used in the next time step. Similarly, the three-dimensional coolant velocity fields are stored in the edge mesh for both post-processing and field mapping purposes.
- The MEDCoupling library transfers the upper boundary 2D edge mesh of TrioCFD to the TRACE's edge mesh and derives the desired inlet velocity boundary conditions for TrioCFD by the edge-to-edge mesh interpolation. Then, it inserts the lower boundary 2D edge mesh of TrioCFD into the TRACE's tetrahedron-cell mesh and it derives the outlet pressure boundary conditions for TrioCFD by a cell-edge mesh interpolation. The transfer of the boundary conditions from TRACE to TrioCFD is exhibited in **Figure 5**a.
- TrioCFD runs another step using the updated boundary conditions and writes all of the calculated fields into the mesh.
- TRACE transfer the data of the tetrahedron-cell and edge mesh to the TrioCFD 3D mesh. The 3D pressure and velocity fields are extracted and written to the tetrahedron-cell and edge meshes. These steps from TrioCFD to TRACE are shown in **Figure 5**b and **Figure 5**c.
- Since the tetrahedron-cell mesh does not represent the real TRACE cells, the pressure field stored in it are integrated and then written to the normal-cell mesh.
- The pressure field in the normal-cell mesh is used to calculate the pressure drop across each edge first. Then the pressure drop field together with the velocity field is used by the DIAS method to correct the friction and form losses coefficients at the edges.
- With the updated parameters, TRACE moves a step forward and generates the fresh new fields.

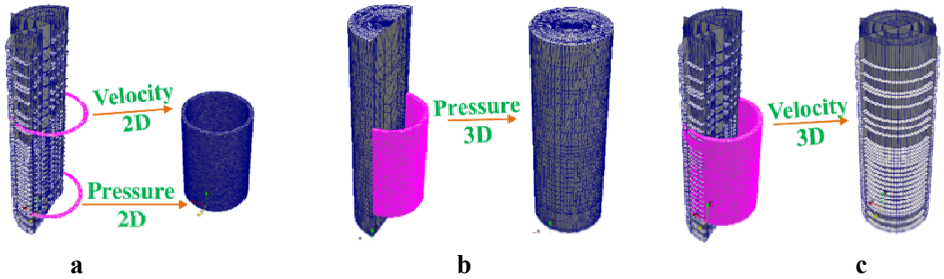


Figure 5: Hydraulic data transfer between TRACE and TrioCFD based on MEDCoupling library

Besides, the exchange of the coolant temperature and boron concentration data stored in the different meshes of the codes involved in the coupling and needed by the DIAS-method is given in **Figure 6**. The single steps are described hereafter:

- TRACE calculates a time step and stores the 3D coolant temperature and boron concentration fields in the normal-cell mesh (for post-processing) and the tetrahedron-cell mesh (for the field mapping) that can be used in the next step.
- The MEDCoupling library inserts the upper boundary 2D edge mesh of TrioCFD into the TRACE's edge mesh and derives the inlet coolant temperature and born concentration boundary conditions for TrioCFD using the cell-edge mesh interpolation functionalities, see **Figure 7**a.
- TrioCFD runs a time step and writes all of the fields in its mesh considering the updated inlet boundary condition.
- TRACE assemblies its tetrahedron-cell mesh to the TrioCFD 3D mesh. The 3D coolant temperature and boron concentration fields are derived and written to the tetrahedron-cell mesh, see **Figure 7**b.
- The information stored in the tetrahedron-cell mesh (no real TRACE cell) i.e. the coolant temperature, born concentration fields are first integrated and then written to the normal-cell mesh of TRACE.
- DIAS uses the coolant temperature / born concentration stored in the cell field to correct the TRACE-fields at each cell within the entire overlapped domain.
- Finally, TRACE moves a step forward and generates the new fields using the updated parameters.

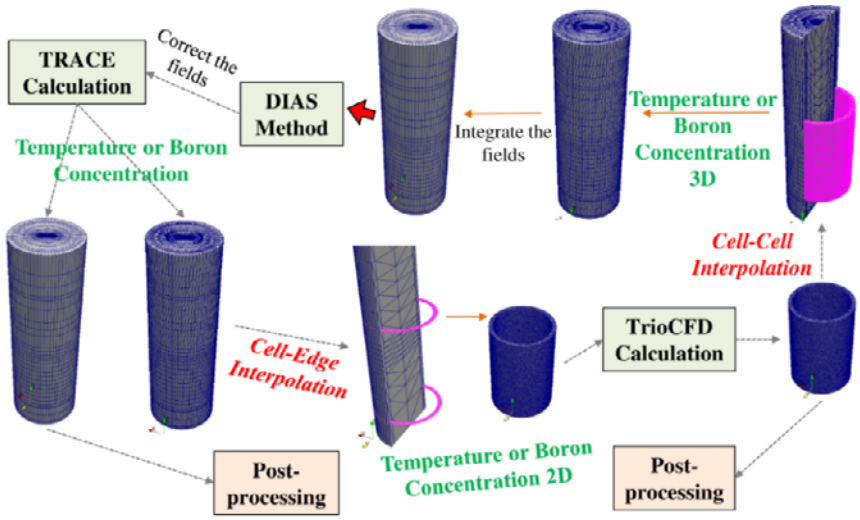


Figure 6: The data flow for coolant temperature and boron concentration correlations between TRACE and TrioCFD within the coupling system

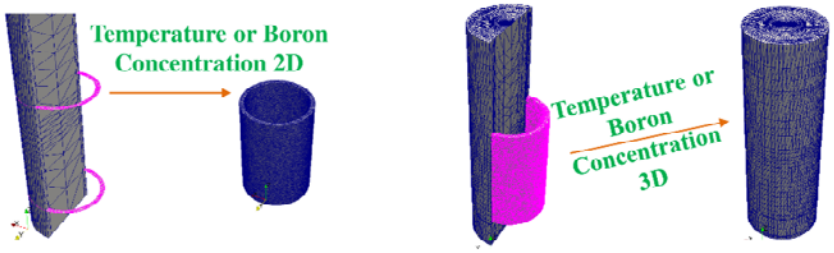


Figure 7: Data transfer (coolant temperature and boron concentration) between TRACE and TrioCFD using the MEDCoupling library

4.3 The explicit temporal coupling scheme

An explicit temporal coupling approach was implemented for the ICoCo-based coupling of TRACE and TrioCFD, which is a server-client system controlled by a C++ supervisor, **Figure 8**. In this approach, the data synchronization during the time advancement of both solvers based on an explicit Operator Splitting (OS) approach. According to it, the calculation procedure supervised by the C++ program performs the following tasks:

- The C++ supervisor launches both TRACE and TrioCFD codes.
- The two codes read in their input file and do the initialization at the same time. The MPI sett-up is finalized if necessary.
- The two codes advance their time step loops and they calculate first their time step size. Then, the supervisor gathers the two-time step size, selects the smaller one, and sends the “public time step” back to the two codes. With that, the two codes reset their current time step.
- The codes inform the supervisor about the field they are expecting from each other and prepare specific templates for the mesh-interpolation / field-mapping processes. The supervisor sends the requested fields’ names to the involved solvers.
- The codes recognize and check the fields’ names from the other code and depending on the names, the corresponding fields are extracted from the current codes’ memories. The supervisor receives the physical fields and interpolates them with the already-prepared templates thus generating the final fields. Then they are sent to the destinations.
- The codes receive their desired fields from the supervisor and use them to update the conditions for the current time step.
- The codes calculate their current time step and iterate unless the problem time is achieved.
- Once the problem time is achieved, the supervisor ends both TRACE and TrioCFD runs and with it, the whole execution is terminated.

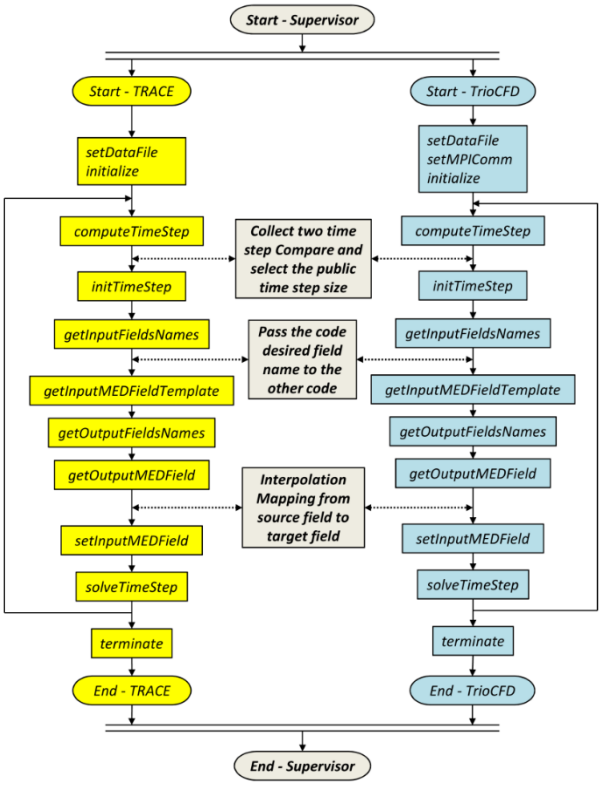


Figure 8: The explicit temporal coupling scheme of TRACE/TrioCFD based on ICoCo

In this explicit temporal coupling 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 re-organized while the ICoCo functions remain untouched.

4.4 Validation of the coupled system TRACE/TrioCFD

For the evaluation of the prediction capability of the TRACE/TrioCFD, the coolant mixing test performed at the VVER-1000 Kozloduy plant is analyzed [38]. The main initial operating parameters before the test are summarized in Table 1.

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		
Loop-1 &3 and 4: Loop-2:	541.75 541.85	± 1.5
Coolant temperature at hot-legs, K Loop-1&2&4: Loop-3:	 545 544.9	± 2.0
Mass flow rates, kg/s Loop-1: Loop-2: Loop-3: Loop-4:	 4737 4718 4682 4834	± 110

The test is triggered by the closure of an MSIV 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 patter.

Short description of the thermal-hydraulic models of TRACE and TrioCFD

For the domain overlapping approach, a TrioCFD-model of the downcomer, **Figure 9**, and a TRACE-model of the full RVP, **Figure 10**, was developed to the simulation of the coolant mixing tests. More details of the models are given in [5].

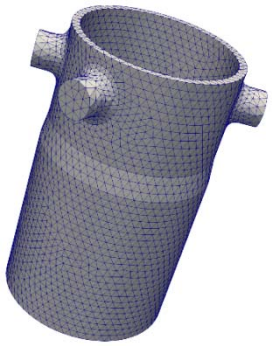


Figure 9: TrioCFD downcomer-mesh of the VVER-1000 RPV

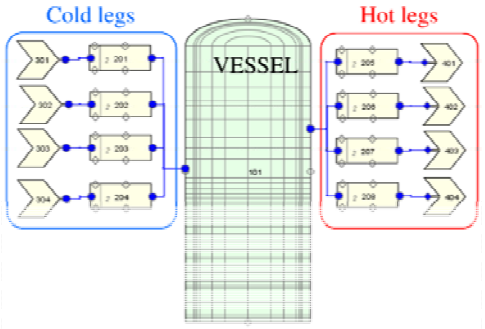


Figure 10: TRACE model of the VVER-1000 RPV

In **Figure 11**, the TRACE-edge mesh and TrioCFD-mesh that with the overlapping downcomer region are shown. 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 a 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. The details of the data exchange among the two domains are described in the former subchapter.

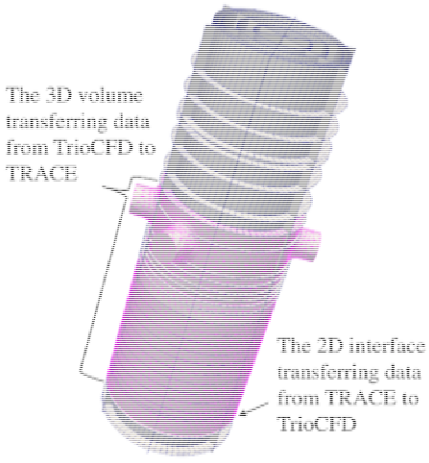


Figure 11: The assembled meshes of TRACE and TrioCFD for the analysis of the coolant mixing test

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.

Discussion of the selected results

A coupled simulation of the coolant mixing test was performed with TrioCFD/TRACE by using the models described before. Based on the DIAS-approach, important parameters such as coolant temperature, pressure, and coolant velocity have been predicted. In **Figure 12**, the coolant temperature distributions on the fine TrioCFD-mesh of the downcomer, on the TRACE-mesh, and the overlapped meshes are shown. The coolant temperature matching between TRACE and TrioCFD is evident, indicating 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.

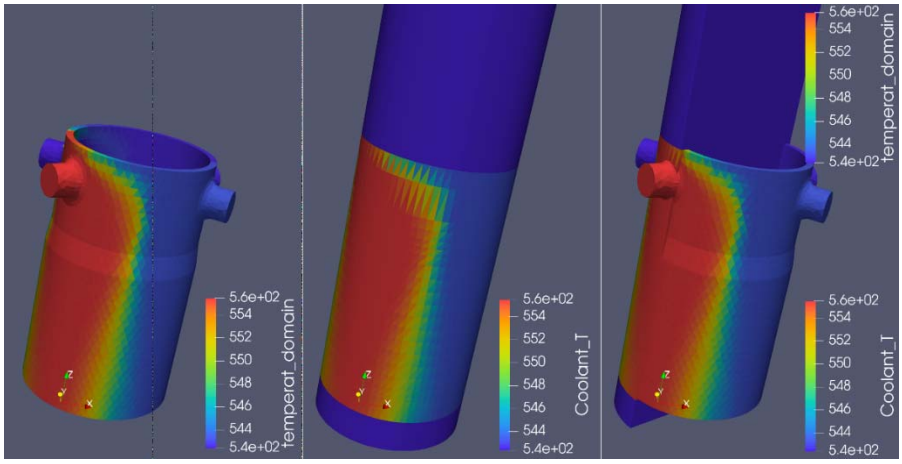
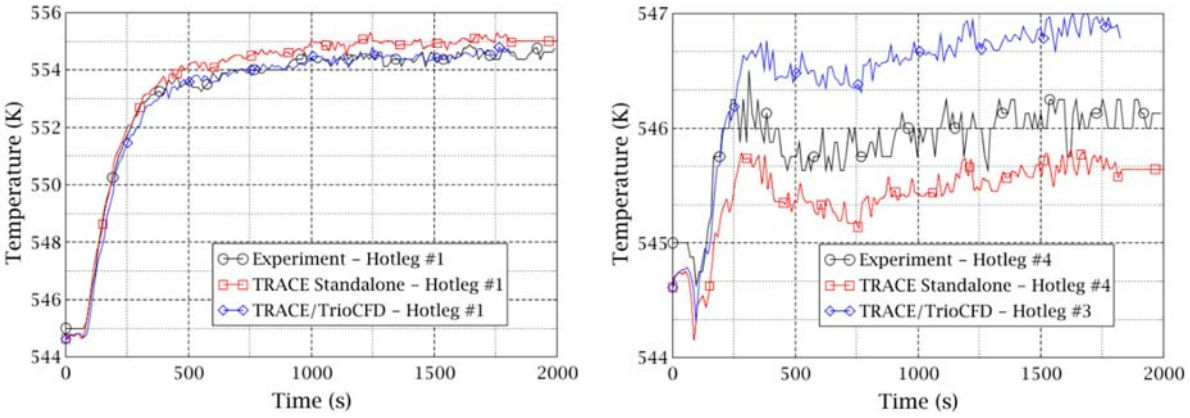


Figure 12: The coolant temperature distribution in the downcomer as predicted by the different solvers and the correlated ones based on DIAS-method

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 **Figure 13**. For the hot-leg-1, the coupled code improves the prediction of the coolant outlet temperature compare 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.



a. hot-leg-1 **b. hot-leg-4**

Figure 13: Comparison of the coolant temperatures predicted by TRACE and TRACE/TrioCFD with the measured data

5. ICoCo-based coupling of SubChanFlow and TRACE

Based on the work performed for the coupling of TRACE and TrioCFD, a domain overlapping coupling approach for SubChanFlow and TRACE was implemented using the YACS-module of SALOME for the supervision of the computational route and data synchronization during the time advancement of the explicit temporal coupling for steady-state and transient simulations. Hereafter a short description of the coupling methodology and an application case is described and discussed.

5.1 Coupling methodology

The coupling methodology is based on the sketch shown in **Figure 1**, where the TrioCFD code can be replaced by SubChanFlow and the supervisor is done by SALOME-tools, see **Figure 14**. SALOME also takes profit from the powerful interpolation functions for code coupling [39] embedded in the MEDCoupling library (the library is embedded in SALOME). The other highlight of SALOME is the built-in module named YACS [40]. 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 SubChanFlow to couple it with 3D diffusion solver and Monte Carlo codes [41] on one hand and the ICoCo-module developed for TRACE in [8] on the other hand.

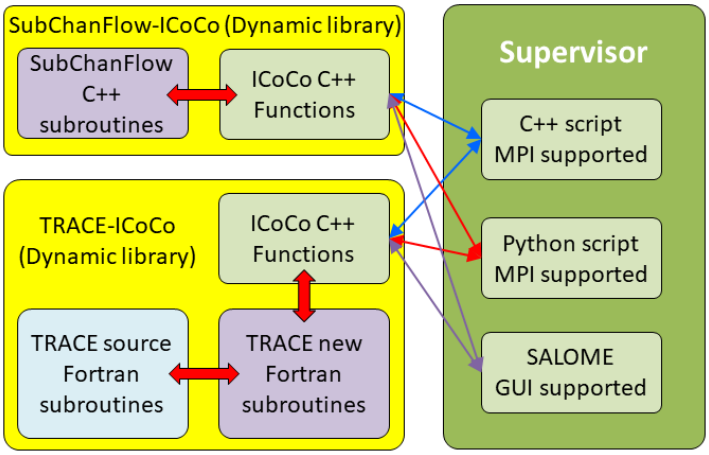


Figure 14: The coupled codes TRACE/SubChanFlow with ICoCo coordinated by the supervisor

In [42], the details of this coupling of TRACE with SubChanFlow inside the SALOME platform are given. Modifications of the ICoCo-interfaces developed before for both codes were necessary and are documented in [43]. Currently, the ICoCo-Interface fo SubChanFlow consits of following methods:

- setDataFile_SCF,
- initialize_SCF,
- terminate_SCF,
- presentTime_SCF,
- computeTimeStep_SCF,
- initTimeStep_SCF,solveTimeStep_SCF,
- isStationary_SCF,
- getInputFieldsNames_SCF,
- getOutputFieldsNames_SCF,setInputMEDField_SCF, and
- getInputMEDFieldTemplate_SCF, getOutputMEDField_SCF.

In addition, three additional methods were added to run the stand-alone SubChaFlow simulation (StandAlone_SCF), for the steady-state simulation (solveSS_SCF), and to get all data for the post-processing from the meshing (GetResults_SCF). On the other hand, the TRACE ICoCo-interface consists of the following methods:

- setDataFile_TRACE,
- initialize_TRACE,
- terminate_TRACE,
- presentTime_TRACE,
- computeTimeStep_TRACE,
- initTimeStep_TRACE,
- solveTimeStep_TRACE,
- isStationary_TRACE,
- getInputFieldsNames_TRACE,
- getOutputFieldsNames_TRACE,
- setInputMEDField_TRACE,

- getInputMEDFieldTemplate_TRACE, and
- getOutputMEDField_TRACE.

A computation route for the execution of coupled simulations of TRACE and SuChabFlow based on ICoCo was developed inside SALOME using the YACS-module and is shown in **Figure 15**.

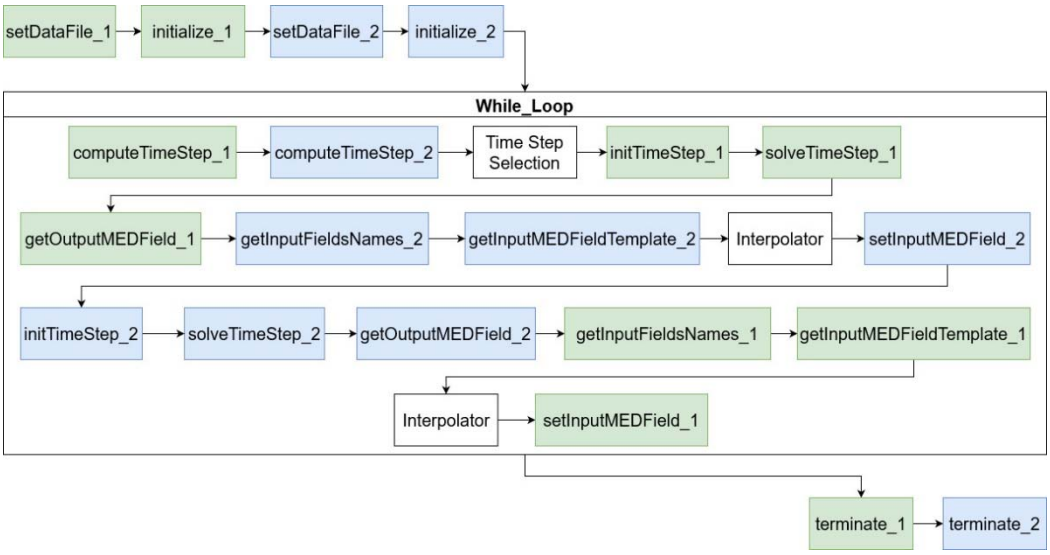


Figure 15: Generic computational route for a couple of simulation inside the SALOME-platform based on ICoCo

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

- 2D fields interpolation: Map two-dimensional fields.
- 3D edge fields interpolation: Map three-dimensional surface-based fields like the coolant velocity.
- 3D cell fields interpolation: Map three-dimensional cell-centered fields like the coolant temperature.

In **Figure 16** a screen capture of the YACS GUI of the SALOME platform is shown, where TRACE and SubChanFlow can be loaded as components for code coupling. Each code is characterized by the own meshing and it is split in 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 to mention, that key-data is stored in fields defined in meshes. Hence, by automatic mesh superposition, the MEDcoupling 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 of key-parameters can be monitored online.

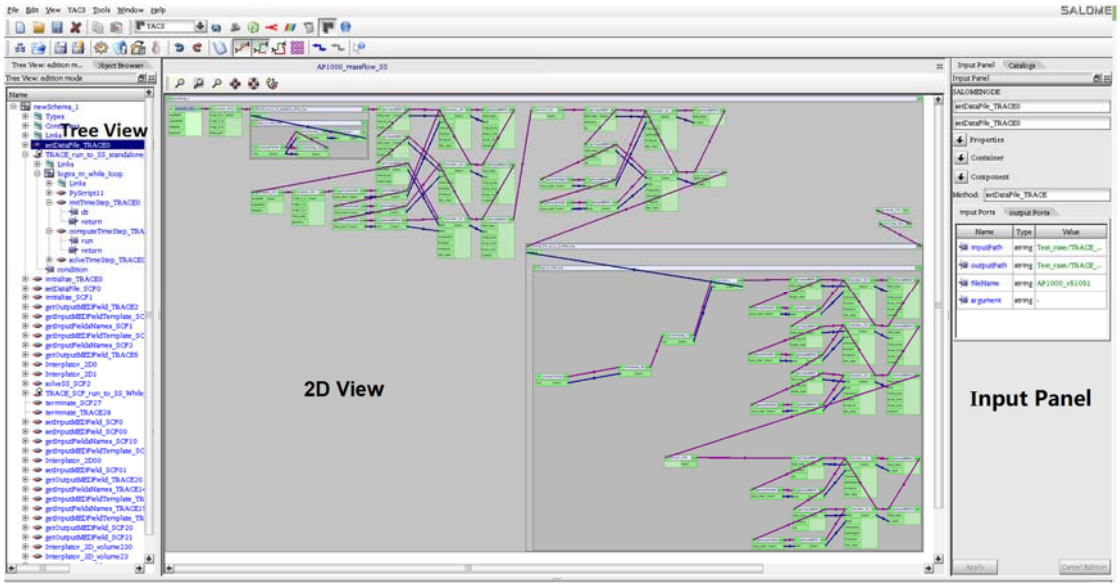
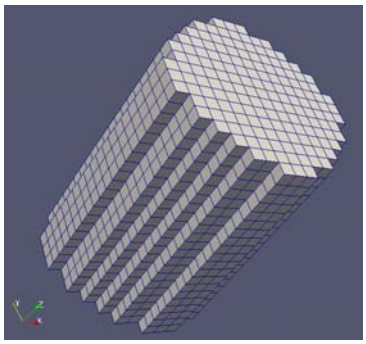


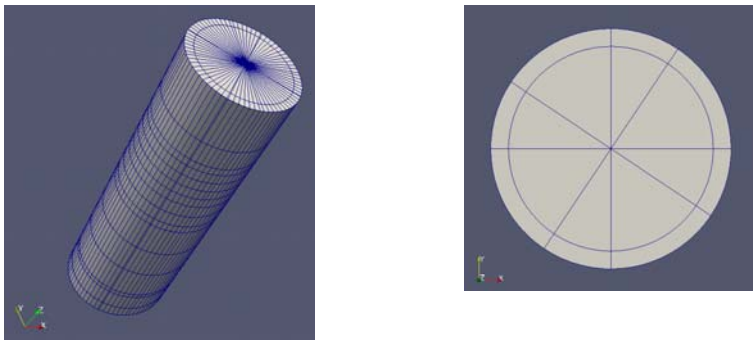
Figure 16: The SALOME YACS Graphical User Interface for the TRACE/SubCHanFlow simulations

5.2 First application of the coupled code TRACE/SubChanFlow

To demonstrate the prediction capability of the coupled code, the thermal-hydraulic behavior of the RPV of an AP-1000 reactor is evaluated when the coolant temperature of one loop is reduced within 10 s from 553.7 K to 503.7 K, the reactor being operated at nominal power. For this purpose, a TRACE model of the AP-1000 reactor developed in [44] was modified to evaluate only the RPV and core behavior. Besides, the fuel assembly based SubChanFlow model of the core was developed, where each fuel assembly is represented by one thermal-hydraulic channel. In **Figure 17** the meshes of the two thermal-hydraulic solvers are represented. Besides, TRACE also has a tetrahedron and an edge-face mesh.



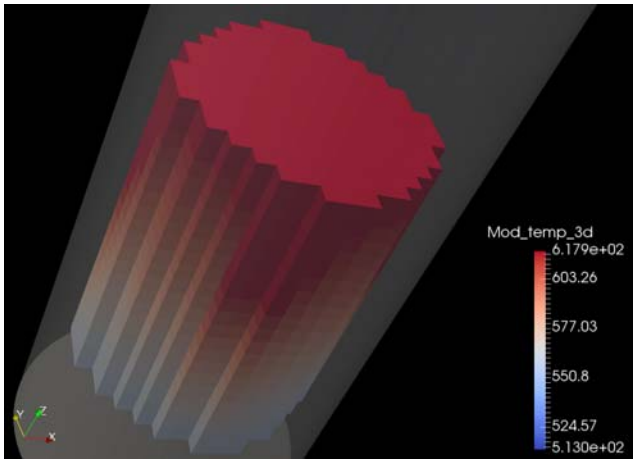
AP-1000: 3D SubChanFlow model



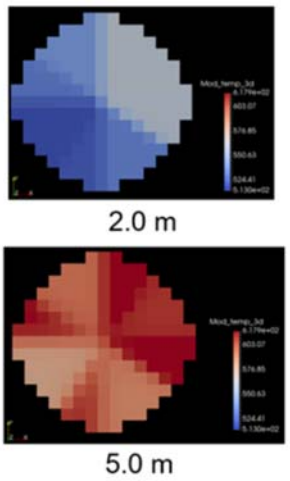
AP-1000 RPV: TRACE 3D polyhedron mesh (left) and TRACE 2D polyhedron mesh (right)

Figure 17: Meshing of the SubChanFlow and TRACE thermal-hydraulic codes to represent the core and the RPV

In **Figure 18**, the moderator temperature predicted with TRACE/SubChanFlow using the point kinetics models of SubChanflow for an coolant temperature transient is shown. The results seem to be consistent.



AP-1000 Core: Moderator temperature at steady-state conditions



AP-1000 core: Moderator temperature distribution after20 s at two different elevations of the core

Figure 18: AP-1000 Predicted moderator temperature at time 0 and 20 s

6. Summary and conclusions

In this paper, the current developments at KIT focusing on multi-scale thermal-hydraulics 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 safety parameters of reactor systems. After the implementation of the ECI and ICoCo coupling approaches, it can be stated that the ICoCo-concept is the most versatile and appropriate methodology that is independent of the involved solvers. 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 code and a coarse mesh solution of the system code. The inherent functionalities of the SALOME platform on which ICoCo relies on 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 an 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 as ParaView or inside SALOME.

It is worth to point out that for the validation of the multiscale coupled codes appropriate experiments are needed, which can be done either in integral test facilities uncluding 3D phenomena or in nuclear power plants. Since the new tools will be able to solve the computational domains e.g. core, downcomer, lower plennum, upper plenum with different degree of details (CFD, subchannels, system thermal hydraulics: meso, component and macro scale), well instrumented test facilities and/or test in nuclear power plants are required. Moreover, the information of 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 devices. 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.

7. Outlook

The exploration of the domain decomposition approach instead of the domain overlapping is one research directions of KIT for the near term which may offer more flexibility on the selection of different regions of an NPP to be treated with different solvers depending on the kind-of phenomena going on. Moreover, the validation of the coupling approaches has to be extended to consider safety-relevant cases. Applications of the multi-scale coupled codes for Small Modular Reactors (SMR) is under preparation.

Acknowledgment

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