# Multi-Scale Coupling of TRACE and TrioCFD Based on ICoCo

K. L. Zhang<sup>1,\*</sup>, X. L. Zhang<sup>1,2</sup>, V. H. Sanchez-Espinoza<sup>1</sup>, R. Stieglitz<sup>1</sup>

1. Karlsruhe Institute of Technology (KIT) Hermann-von-Helmholtz-Platz 1 76344 Eggenstein-Leopoldshafen, Germany

2. University of Science and Technology of China (USTC) No.96, JinZhai Road Baohe District Hefei,Anhui, 230026,P.R.China

kanglong.zhang@kit.edu; xilin.zhang@kit.edu; victor.sanchez@kit.edu; robert.stieglitz@kit.edu

## ABSTRACT

The paper describes the implementation of the multi-scale coupling of an advanced, best-estimate reactor system code – TRACE and an open-source CFD code – TrioCFD, in order to better simulate the 3D thermal-hydraulic in the Reactor Pressure Vessel (RPV). The coupling of a system and a CFD code was implemented based on the Interface for Code Coupling (ICoCo), which relies on key-functionalities of the European open-source SALOME platform and it defines a standardized specification for code coupling. Implementation of the coupling was divided into two parts: spatial and temporal coupling. The spatial coupling could be further subdivided into computational domain coupling and physical field mapping. The domain-overlapping strategy was selected for the domain coupling and the SALOME mesh/field-processing library - MED and MEDCoupling- were used to handle the data mapping between different meshes of TRACE and TrioCFD. The temporal coupling is implemented for both Steady State (SS) and Transient simulations. An Operator Splitting (OS) approach was adopted for the temporal coupling in order to ensure the codes' synchronization during the time advancing. An OpenMPI-based C++ parallel supervisor was developed to coordinate the operation and data exchange of the two codes. This multi-scale coupled code system was verified with a special mass flow distribution problem and the results indicate that the implementation was physical sound.

KEYWORDS: MULTI-SCALE COUPLING, TRACE, TrioCFD, ICOCO, SALOME

## **1. INTRODUCTION**

Thermal-hydraulic simulation tools are playing increasing roles in the present-day nuclear industry and research. The spatial scales of the thermal-hydraulic phenomena occurring in the NPP mainly involve system scale, component scale, mesoscale and microscale [1]. Furthermore, with the help of more powerful tools and technologies, nanoscale could also be involved [2]. The corresponding characteristic length of those spatial scales could vary from meters down to nanometer. Many thermal-hydraulic (TH) simulation tools have been developed worldwide over the past decades. System codes e.g. RELAP, TRACE, ATHLET are extensively used to simulate various scenarios on system scale e.g. Large Break Loss of Coolant Accidents (LBLOCA). Sub-channel codes e.g. COBRA-TF, FLICA, SUBCHANFLOW are used to estimate safety parameters in the core on component scale e.g. Critical Heat Flux (CHF). In order to catch TH-details and phenomena taking place in mesoscale e.g. turbulence, CFD codes e.g. FLUENT, STAR-CCM, OpenFOAM and TrioCFD are also applied by the nuclear communities, increasingly. Investigations are also underway to improve the two-phase models of CFD codes and to

enhance the numerical stability, physical models, treatment of the different flow and heat transfer modes which may exist within a reactor core or during accidental situations such as the multi-phase Critical Heat Flux (CHF) [3].

Few investigations are also devoted to simulating a complete nuclear power plant using CFD-codes [4], [5] [6] [7]. In practice, the primary and secondary sides are relatively well resolved in space and others such as the core are represented by means of the porous-media approach. Otherwise, the computational problem could be too big to fit in the memory of current computers. Another shortcoming is that the description of each fuel rod and each subchannel within the core as part of an integral CFD-plant model may result in an unmanageable input deck. Consequently, the combination of the simulation capabilities of different thermal-hydraulic codes by developing multi-scale thermal-hydraulic coupling approaches seems to be a promising area of research in order to increase the prediction accuracy of safety-relevant phenomena of nuclear power plants with acceptable computing resource consumption. Examples of such developments are coupled code systems such as MARS [8], RELAP-3D/COBRA-TF [9], TRACE/FLUENT [10], ATHLET-CFX [11].

At the Karlsruhe Institute of Technology (KIT), the multi-scale investigations are devoted to the coupling of system codes with sub-channel and CFD codes. This paper is dedicated to the coupling of the system thermal-hydraulic code TRACE with the open source CFD code TrioCFD using a new modularized and standardized Interface for Code Coupling (ICoCo) [12]. Several explicit meshes in MED-format were created for the TRACE post-processing, field mapping and interpolation between the involved computational domains of the different TH-solvers. Furthermore, TRACE was split into several functional components as a prerequisite for the coupling. The time advancement and data exchange of the coupled codes are managed by a newly developed parallel C++ supervisor. A brief description of the selected codes and tools will be presented in chapter 2. The coupling approaches are presented in chapter 3. The code testing is discussed in chapter 4. The summary and outlook complete this paper.

# 2. SELECTED TOOLS AND CODES FOR MULTI-SCALE COUPLING

### 2.1. The System Code TRACE

TRACE is the reference best-estimate thermal-hydraulic system code of the U.S. Nuclear Regulatory Commission (NRC) for Light Water Reactors (LWR). A system of six balance equations in the two-fluid formulation plus additional equations to describe the transport of boron dissolve in the liquid phase and of non-condensable in the gas phase is solved for one-dimensional and three-dimensional components used to represent a nuclear power plant. TRACE takes a component-based approach to model a reactor system. The complete nuclear power plant can be represented by the use of TRACE-components such as PIPE, PUMP, VALVE, POWER, VESSEL, etc. The VESSEL-component is the special 3D component which can model the Reactor Pressure Vessel (RPV) and other components in which 3D phenomena take place. State equations for water and steam as well as for other coolants e.g. Sodium, CO2, Lead, Lead-Bismuth are also included. Dedicated models are available for the description of critical flow, thermal stratification, counter-current flow, etc. Both stationary and time-dependent thermal hydraulic problems can be solved by TRACE. Moreover, neutronic kinetics is also implemented in TRACE using a point kinetics model. It is also coupled with a three-dimensional diffusion solver, named PARCS [13].

At KIT, substantial programming effort was made to integrate TRACE into the SALOME platform and to develop the ICoCo-module for TRACE [14], [15]. As a result, TRACE has its own explicit meshes (based on MED, which is a module in SALOME) and functional components (based on YACS which is also a module in SALOME). This paves the way for the coupling of TRACE with other solvers within the

SALOME-platform using ICoCo. In total four mesh types were developed for TRACE for different purposes as follows:

- Polyhedron-cell-mesh: for cell-data e.g. temperature, pressure post-processing,
- Tetrahedron-cell-mesh: for cell-data e.g. temperature, pressure interpolation,
- 3D-edge-mesh: for spatial edge-data e.g. velocity, pressure-drop post-processing and interpolation, and
- 2D-edge-mesh: for plane edge-data post-processing and interpolation.

#### 2.2. The open source code TrioCFD

TrioCFD is an open source CFD code based on the TRUST platform (TRio\_U Software for Thermohydraulics) being developed by the Thermo-hydraulics Service and Fluid Mechanics (STMF) of the Department of Nuclear Energy at the CEA. TrioCFD includes many physical models and it applies advanced numerical methods with the help of massive parallelism allowing the simulation of various problems varying from local two-phase flows to turbulent flows on industrial facilities such as portions of nuclear reactors. Two main models in TrioCFD are the Reynolds-Averaged Navier-Stokes (RANS) and the Large Eddy Simulation (LES). The Direct Numerical Simulation (DNS) is also available but mostly for academic purposes. The governing equations are solved with a staggered finite-volume approach. TrioCFD is able to generate robust meshes or import meshes from other software. The code supports full parallelepiped or full tetrahedral meshes, which could be structured or unstructured. The spatial discretization methods corresponding to the different types of mesh elements are called finite volume differences (V.D.F.) for parallelepipeds and finite volume elements (V.E.F.) for the tetrahedron. The V&V is now a major process providing an evaluation of the reliability level of the computed solutions, as well as the correct implementation of the desired models [16].

ICoCo is an inherent module in TrioCFD developed to couple TrioCFD with the system code CATHARE [17]. The explicit meshes always exist for both TrioCFD-standalone and coupled code applications. Nevertheless, compulsive modifications and re-compilation of the source code are required in order to transform the stand-alone TrioCFD to the coupled codes despite ICoCo is already part of the TrioCFD source code.

### 2.3. The Interface for Code Coupling (ICoCo) and the Supervisor

Each involved code in the coupled system is referred to as the "Problem" notion, which could be treated as an object computing a time-dependent simulation. ICoCo specifies several methods that the problem has to provide as well as the descriptions of what they are supposed to do. ICoCo doesn't contain any real functional codes but it just poses a framework and standard. Developers have to fill in the frame and to establish the connections between ICoCo and the target codes [12]. Table 1 lists the ICoCo methods and the corresponding functions.

		ð	
setDataFile	initTimeStep	iterateTimeStep	getInputMEDFieldTemplate
setMPIComm	solveTimeStep	save	setInputMEDField
initialize	validataTimeStep	restore	getOutputFieldsNames
presentTime	abortTimeStep	foget	getOutputMEDField
computeTimeStep	isStationary	getInputFieldsNames	ternimate

Table 1 – Methods defined by ICoCo

ICoCo supplies the methods to insert various input ports and output ports to the coupled-codes making the inter-code interaction quite flexible and convenient. Those methods are coordinated by a supervisor,

which completes the coupling system. The general form of the system is shown in Figure 1. There, the following key features are listed:

- 1) ICoCo is a cross-language interface. Within this coupling system, TRACE is in Fortran and TrioCFD is in C++.
- 2) Two essential prerequisites are called: a) each code should first be equipped with explicit meshes which are used for post-processing and field mapping and interpolation with other codes; b) the codes must be split into several functional components for the sake of flexible coupling. The two prerequisites are exactly the ICoCo key functions. Normally, once the ICoCo was well developed, the two requisites should be already implemented.
- 3) Three options are available for the supervisor: C++, Python and SALOME. Since MPI is essential for TrioCFD, it plays a key role in the supervisor selection. Python supports MPI but this capability was not widely used. SALOME is the European open source platform which dedicates for pre- and post-processing of simulation data as well as for codes coupling. But MPI is not supported by SALOME for the time being. C++ not only supports MPI but the community also has rich experience in MPI usage. So, the supervisor was written in C++.
- 4) Another feature which is not illustrated in Figure 1 is that the supervisor could run in both serial and parallel mode. But codes structure of the two kinds of supervisors differs significantly. The parallel C++ supervisor was developed in this paper.



Figure 1 – Multi-Scale Coupling of TRACE and TrioCFD based on ICoCo

## **3. DESCRIPTION OF THE COUPLING**

Key-elements of the coupling of two different solvers are the spatial coupling and the temporal coupling.

### **3.1. Spatial Coupling**

The intended application of the coupled code TRACE/TrioCFD is to improve the description of the physical phenomena within a nuclear power plant, where e.g., TRACE simulates the whole system dynamic and TrioCFD simulates the downcomer and lower plenum. In this case, TrioCFD could describe the flow conditions e.g. during an MSLB or Boron dilution transient in a much precise manner leading to an improved core behavior by the 3D TRACE-simulation. In principle, the coupling approach and its corresponding spatial mapping are very flexible and it may allow the combination of different solution domains of the involved codes for example regarding the flow and heat transfer within an RPV.

The spatial coupling is composed of two parts. The first one is domain coupling which handles the domain division strategy. The other one is field mapping which manages the field data translation between different meshes of TRACE and TrioCFD. As to the domain coupling, two approaches are possible: domain-decomposition and domain-overlapping, Figure 2 (here the CFD part only includes downcomer for consistency with the testing case in chapter 4). There, for example, TrioCFD simulates the downcomer for both modes. TRACE only simulates the rest of the vessel (do not include the downcomer) under the former mode while it simulates the whole vessel (including the downcomer) under the latter mode. The domain-decomposition method can be easily and straightforward implementated since only 2D-plane fields need to be passed over between the codes as boundary conditions. However, it may crash under some special conditions. The domain overlapping method is more difficult to implement compared to the domain decomposition since part of the transferred data is in 3D. But it is more robust than the

domain-decomposition method. Thanks to the powerful mesh processing capability of SALOME-MED [18] and a newly-developed closure-on-demand approach [19] [20], the domain-overlapping method was selected for the sake of robustness in this investigation.



In the coupled code system, the 2D-plane pressure field at the TRACE downcomer outlet is transferred to the downcomer outlet of TrioCFD as the new pressure outlet boundary condition. The inlet boundary condition of TrioCFD is predefined to strictly follow the TRACE-inlet conditions. Once TrioCFD gets the new field data after one-time step calculation, it will pass the 3D spatial velocity and 3D spatial pressure fields to TRACE correcting the flow friction coefficients in the overlapped downcomer region. The correlation was done by implementing a so-called closure-on-demand approach, which uses 3D TrioCFD fields to correct the TRACE-resolution on the fly and finally forces TRACE to produce CFD-like velocity profile, pressure profile and pressure-drop [21] [22]. At the moment, only velocity and pressure correlations were implemented. Other correlation e.g. the temperature will be done in the near future. This approach will be further explained in next section.

A new overlapped-cell-auto-recognition algorithm was developed enabling TRACE to recognize the overlapped cells whose parameters should be corrected while keeping other cells untouched. This is a fully automated process which indicates that no additional modifications have to be done to the original TRACE model. The already existing TRACE-models for a standalone execution could be directly used for the coupling calculation. This is a remarkable improvement compared to the domain-decomposition method where abundant modifications have to be done to the original TRACE-model.

As it was stated before, the MED-module of the SALOME-platform was used to manage the field mapping and mesh interpolation between different meshes of the codes. The MED-module can mainly handle three kinds of mesh interpolation: 1) cell-to-cell; 2) cell-to-edge; 3) edge-to-edge. The intersections are based on an "overlapped volume or area weighted fraction" algorithm which could map source field on all source mesh cells, which joint one single target mesh cell and calculate the target field by different weighted fractions or contribution ratio. Figure 3 presents a simple intersection case of two typical unstructured cells. Moreover, both point-based fields and cell-based fields can be processed by the MED-module. In the current coupled system, TrioCFD runs an unstructured cell-based mesh, which contains only tetrahedron cells. A new TRACE tetrahedron cell-based mesh has four natures: 1) IntensiveConservation; 2) ExtensiveConservation; 3) IntensiveMaximum; 4) ExtensiveMaximum [18]. Selections of these functionalities are essential for the interpolation between TRACE and TrioCFD since the codes' meshes differ significantly.



Figure 3 – The Mesh Intersection Could be Handled by MED

#### 3.2 Principles of the Correlations to TRACE for Domain-Overlapping Coupling

The momentum equation of TRACE is carefully studied in order to successfully implement the coolant velocity and pressure correlations. Take the 1D components in TRACE for instances, the governing motion equation is Equation 1, whose items could be characterized to four types of pressure drop as shown in Equation 2. Similar items could also be derived for TrioCFD, Equation 3. From left to right, they are:

- $\Delta P_{acc}$  The acceleration pressure drop or inertial pressure drop which comes from the variation of coolant velocity along the problem time.
- $\Delta P_{con}$  The convective pressure drop which comes from the mass and momentum transfer along the flow path.
- $-\Delta P_{tot}$  The total static pressure drop which is also known as the manometer pressure drop. The minus sign stands for its negative correlations with the other three pressure drops.
- $\Delta P_{fric}$  The friction pressure drop which is caused by the friction between the fluid and the solid structures. It could also include form losses.

$$\frac{V_{j+\frac{1}{2}}^{n+1} - V_{j+\frac{1}{2}}^{n}}{\Delta t} + V_{j+\frac{1}{2}}^{n} \cdot \frac{\partial \tilde{V}^{n+1}}{\partial x} \bigg|_{j+\frac{1}{2}} + \frac{1}{\langle \rho \rangle_{j+\frac{1}{2}}^{n}} \cdot \frac{\tilde{P}_{j+1}^{n+1} - \tilde{P}_{j}^{n+1}}{\Delta x} + K_{j+\frac{1}{2}}^{n} \cdot \left(2V_{j+\frac{1}{2}}^{n+1} - V_{j+\frac{1}{2}}^{n}\right) \cdot \bigg| V_{j+\frac{1}{2}}^{n} \bigg| = 0 \qquad \text{Equation 1}$$

$$\Delta P_{acc}^{TRACE} + \Delta P_{con}^{TRACE} + (-\Delta P_{tot}^{TRACE}) + \Delta P_{fric}^{TRACE} = 0 \quad \text{Equation } 2$$

 $\Delta P_{acc}^{TrioCFD} + \Delta P_{con}^{TrioCFD} + \left(-\Delta P_{tot}^{TrioCFD}\right) + \Delta P_{fric}^{TrioCFD} = 0 \qquad \text{Equation 3}$ 

Since the convective and friction pressure drops predicted by other TH codes are more accurate than TRACE, the two corresponding terms in Equation 2 are replaced with that from the fine results, as Equation 4 shows. The reason why the acceleration pressure drop can't be erased is because of the ineradicable time term which explicitly binds two adjacent time layers. In order to counteract  $\Delta P_{acc}^{TRACE}$ , the corresponding acceleration pressure drop  $\Delta P_{acc}^{TrioCFD}$  was dropt from the total static pressure drop  $\Delta P_{tot}^{TRACE}$  of sub-channel or CFD codes. The new added two pressure drops could be further integrated into one fake friction pressure drop  $\Delta P_{fric,fake}^{TRACE} = \Delta P_{con}^{TrioCFD} + \Delta P_{fric}^{TrioCFD} = \Delta P_{tot}^{TrioCFD} - \Delta P_{acc}^{TrioCFD}$  by imposing a fresh friction factor  $C_{j+\frac{1}{2},fake}^{n}$  which equals  $\Delta x \cdot \rho \cdot K_{j+\frac{1}{2},fake}^{n}$ . Now the TRACE motion governing equation becomes Equation 5.

$$\Delta P_{tot}^{TRACE} = \Delta P_{acc}^{TRACE} + \Delta P_{con}^{TioCFD} + \Delta P_{fric}^{TrioCFD} = \Delta P_{acc}^{TRACE} + \left(\Delta P_{tot}^{TrioCFD} - \Delta P_{acc}^{TrioCFD}\right)$$
Equation 4

$$\frac{V_{j+\frac{1}{2}}^{n+1} - V_{j+\frac{1}{2}}^{n}}{\Delta t} + \frac{1}{\langle \rho \rangle_{j+\frac{1}{2}}^{n}} \cdot \frac{\tilde{P}_{j+1}^{n+1} - \tilde{P}_{j}^{n+1}}{\Delta x} + \frac{C_{j+\frac{1}{2}fake}^{n}}{\Delta x \cdot \langle \rho \rangle_{j+\frac{1}{2}}^{n}} \cdot \left(2V_{j+\frac{1}{2}}^{n+1} - V_{j+\frac{1}{2}}^{n}\right) \cdot \left|V_{j+\frac{1}{2}}^{n}\right| = 0$$
 Equation 5

The fake friction pressure drop  $\Delta P_{fric,fake}^{TRACE}$  in Equation 5 is proportional to the product of  $C_{j+\frac{1}{2},fake}^{n}$  and the square of velocity. Thus, the fresh fake coefficient could be calculated by Equation 6.

$$C_{j+\frac{1}{2},fake}^{n} = \frac{\Delta P_{fric,fake}^{TRACE}}{V^{TrioCFD^{2}}} = \frac{\Delta P_{tot}^{TrioCFD} - \Delta P_{acc}^{TrioCFD}}{V^{TrioCFD^{2}}}$$
Equation 6

The general data flow between TRACE and TrioCFD within the coupling system is illustrated in Figure 4. Here please note that the boundary data from TRACE to TrioCFD includes both of the inlet and outlet boundary conditions, which is slightly different from the demonstrated spatial coupling in section 3.1. Nevertheless, this diagram is displayed from a general perspective so that each possible boundary condition exchange is considered.



Figure 4 – The temporal workflow of the coupling code TRACE/TrioCFD

#### 3.3. Temporal Coupling

The Operator Splitting (OS) method [23] was implemented for temporal coupling of TRACE and TrioCFD. It is more or less an explicit coupling approach since field mapping and data exchange performs only one time for one time step. The coupling workflow during the time advancement is illustrated in Figure 5.



Figure 5 – The temporal workflow of the coupling code TRACE/TrioCFD

The program chart illustrates the ICoCo-based execution procedures of the coupled codes under the management of a parallel supervisor. Moreover, TrioCFD may also run in parallel within the coupling framework. The workflow is described in detail hereafter:

- 1) The supervisor launches and opens the TRACE-ICoCo and TrioCFD-ICoCo libraries.
- 2) The two codes read in their input files, set their output path to put the output files and do the initialization. TrioCFD will additionally set its MPI environment.
- 3) The two codes enter the time loop and calculate the current time step size first.
- 4) The supervisor collects the two time step size, select one as the public time step size and send it to the two codes.
- 5) The codes reset their time step size based on the public one.
- 6) The codes propose the names of their desired fields from the other code and check them.
- 7) The supervisor collects the names of the desired fields from one code and passes them to the other code.
- 8) Depending on the names of the desired fields from the code itself, the codes generate a target field template to receive the target field from the other code.
- 9) Depending on the names of the desired fields from the other code, the codes derive the source fields to be sent to the other code.
- 10) The supervisor maps the field from the source field from one code to the target template of the other code, produces the target field and sends it to the target code.
- 11) The codes write the fields they got from the supervisor into the memory to update the new parameters for the current time step.

12) Check whether the codes terminate or not. If yes, the calculation ends. Otherwise, go ahead to a new time step.

## 4. TESTING OF THE ICoCo BASED COUPLING CODES TRACE/TrioCFD

To test the new capabilities of the coupled code, an academic problem is analyzed with TRACE/TrioCFD. This problem describes a single-phase flow within an RPV of a four loop PWR. The TRACE model of the RPV consists of a 3D VESSEL (includes 4 azimuthal sectors, 2 radial sectors and 15 axial levels), four inlet boundary conditions (mass flow rate/velocity and temperature) and four outlet boundary conditions (pressure), Figure 6. The TrioCFD-model represents the four RPV-inlet volumes and the downcomer.



Figure 6 – Cross-section Sketch of the Vessel and Four Primary Loops of the Testing Case

In this test problem, a steady state solution of a flow distribution within the RPV is analyzed with the coupled code TRACE/TrioCFD. The boundary conditions for the test problem are given in Table 2. There it can be seen that the inlet mass flow rate of three loops (#2, #3 and #4) amounts 5 m/s while the first loop is 7 m/s. All other boundary conditions such as pressure and inlet temperature of all four loops have the same value. The power of the core is zero.

	Loop #1	Loop #2	Loop #3	Loop #4		
Inlet Velocity	7 m/s	5 m/s				
Temperature	400 K					
Outlet Pressure	15.55 MPa					

 Table 2 – Boundary Conditions of the Testing Case

The TRACE model is presented in Figure 7, where the flow paths were illustrated from the cold leg to the downcomer, enter the lower plenum, go up through the core and finally go to the hot legs.



#### Figure 7 – TRACE model in SNAP

The TRACE and TrioCFD computational domains with their different meshes (MED format) are displayed in Figure 8. The tetrahedron mesh for TRACE is shown in Figure 8a, while the edge mesh for TRACE is presented in Figure 8b. There, one can clearly see how the two computation domain overlaps to each other. In this exercise, two types of interpolation are realized: cell-to-cell (Figure 8a) and cell-to-edge (Figure 8b) interpolation.



a) cell-to-cell b) cell-to-edge Figure 8 – TRACE and TrioCFD Meshes for the Coupling Codes and the Two Overlapped Interpolation Types Between TRACE and TrioCFD

The goal of this test problem is to check if TRACE in the coupled system is able to predict the similar velocity distribution and pressure drop within and along the downcomer region as TrioCFD fields which are believed to be more precise. Since now the TRACE-meshes are explicitly defined and several ICoCo functions e.g. getOutputMEDField can be conveniently called during the calculation to derive various data sets from TRACE-memory to the meshes on the fly. The post-processing module PARAVIS in SALOME supplies powerful, intuitionistic and visual inspection capabilities for the TRACE-data. In Figure 9, the velocity distribution predicted by TRACE and TrioCFD is exhibited by SALOME-PARAVIS, where it can be observed that TRACE in the coupled system now is able to generate a TrioCFD-like velocity profile.



Figure 9 – Axial Velocity Distribution of TRACE and TrioCFD Indicating TRACE Could Generate CFDlike Velocity Profile

It is worth to note that the TRACE-cells overlapped with TrioCFD-mesh could be automatically identified in the coupling approach so that only the fields in those overlapped TRACE cells are corrected

while others remain untouched. In Figure 9, only the overlapped cells of TRACE are assigned with corrected data (colourful) while others kept the original TRACE fields (dark). Significant improvements were obtained when comparing the velocity predicted by the coupled code and TRACE-standalone, see Figure 10 and Table 3.



Figure 10 – Correlations of the Velocity Distribution in the Four Loops by TRACE Before and After Coupled with TrioCFD

1  able  3 - velo	city Errors of	I RACE Before	and After the	Jouphing	Compared	to Irlour	D Solution

	TRACE Before	TRACE After	TrioCFD	Error 1	Error 2
Outlet #1	-2.79 m/s	-1.87 m/s	-1.92 m/s	45.3%	2.6%
Outlet #2	-2.62 m/s	-2.91 m/s	-3.02 m/s	13.2%	3.6%
Outlet #3	-2.61 m/s	-2.89 m/s	-2.95 m/s	11.5%	2.0%
Outlet #4	-2.62 m/s	-2.97 m/s	-3.03 m/s	13.5%	1.9%

Within the coupled codes TRACE/TrioCFD, TRACE and TrioCFD first run isolated until they both reach steady state (in this case, the isolated computation lasted around 120 seconds). Subsequently, the coupled code TRACE/TrioCFD is initiated and data exchange begins. The errors are calculated by the relation: E= ABS [( $V_{TRACE} - V_{TrioCFD}$ ) /  $V_{TrioCFD}$ ]. It is obvious that the error of the velocity distribution predicted by TRACE after the coupling point is dramatically reduced in order of magnitude compared to that before the coupling point. The other key parameter to be examined is the pressure drop along the downcomer. In Figure 11, the pressure evolutions of the loop-1 predicted by TRACE before and after the coupling with TrioCFD are shown. In Table 4, the pressure drop errors are calculated by the relation: error = ABS [( $P_{drop_TRACE} - P_{drop_TrioCFD}$ ) /  $P_{drop_TrioCFD}$ ]. It was found out that the error of the pressure drop along downcomer predicted by TRACE after the coupling point is dramatically reduced also in order of magnitude compared to that before the coupling point the coupling point is dramatically reduced also in order of magnitude compared to that before the coupling point indicating that the pressure drop in the downcomer region is greatly improved.



Figure 11 – Correlations of the Pressure Drop in the Four Loops by TRACE Before and After Coupled with TrioCFD in Downcomer Sector #1

 Table 4 – Pressure Drop Errors of TRACE Before and After the Coupling Compared to TrioCFD Solution

	TRACE Before	TRACE After	TrioCFD	Error 1	Error 2
Sector #1	12604 Pa	51661 Pa	54092 Pa	76.7%	4.5%
Sector #2	11435 Pa	49321 Pa	53606 Pa	78.7%	7.9%
Sector #3	11503 Pa	49651 Pa	53249 Pa	78.4%	6.7%
Sector #4	11445 Pa	49309 Pa	52433 Pa	78.2%	5.9%

At last, it is worth to note that the correlations is not just directly using TrioCFD pressure and velocity fields to force TRACE produce totally the same hydraulic fine fields. Instead, the applied approach in this paper use the TrioCFD pressure and velocity fields correct the TRACE momentum loss coefficients on each edge and "guide" the system produce the desired fields, naturally. This is also the reason why TRACE with this method could not hundred percent reproduce the TrioCFD results. Though not perfect, it is reasonable.

# **5. CONCLUSIONS**

A multi-scale coupling of TRACE and the open source CFD code TrioCFD was developed using the ICoCo-methodology and a parallel C++ supervisor. The domain-overlapping approach was implemented along with a closure-on-demand approach. The SALOME-MED-module was used for field mapping and interpolation between different meshes of TRACE and TrioCFD. The Operator Splitting method, which is an explicit coupling approach, was adopted for the temporal coupling. The coupling system was verified with an academic flow distribution problem. The results show that TRACE in the coupling system is able to reproduce TrioCFD-like velocity distribution and pressure drop. This test case demonstrates that the coupled system TRACE/TrioCFD is working correctly and that it improved the simulation of 3D-flow inside the RPV.

# 6. OUTLOOK

Despite the promising results of the first testing of the coupled code TRACE/TrioCFD, realistic cases for the application and the experimental data need to be identified for validation purposes and for the demonstration of the new prediction capabilities and flexibility of the coupled code under development. This work paves the way for interesting applications not only to LWR but also to liquid metal cooled reactor systems.

#### 7. REFERENCES

- A. Guelfi, D. Bestion, M. Boucker, P. Boudier, P. Fillion, M. Grandotto, J. Hérard, E. Hervieu and P. Péturaud, "NEPTUNE: A New Software Platform for Advanced Nuclear Thermal Hydraulics," *Nuclear Science and Engineering*, vol. 156, no. 3, pp. 281-324, 2007.
- [2] B. Niceno, Y. Sato, A. Badillo and M. Andreani, "Multi-scale Modeling and Analysis of Convective Boiling Towards the Prediction of CHF in Rod Bundles," *Nuclear Engineering and Technology*, vol. 42, no. 6, pp. 620-635, 2010.
- [3] A. Tentner, E. Merzari and P. Vegendla, "Computational Fluid Dynamics Modeling of Two-Phase Boiling Flow and Critical Heat Flux," in 22nd International Conference on Nuclear Engineering ICONE22, Prague, Czech Republic, 2014.
- [4] M. B"ottcher, "Detailed CFX-5 study of the coolant mixing within the reactor pressure vessel of a VVER-1000 reactor during a non-symmetrical heat-up test," *Nuclear Engineering and Design*, vol. 238, p. 445–452, 2008.
- [5] M. Böttcher and R. Krüßmann, "Primary loop study of a VVER-1000 reactor with special focus on coolant mixing," *Nuclear Engineering and Design*, vol. 240, p. 2244–2253, 2010.
- [6] J. P. Cheng, L. M. Yan and F. C. Li, "CFD simulation of a four-loop PWR at asymmetric operation conditions," *Nuclear Engineering and Design*, vol. 300, pp. 591-600, 2016.
- [7] W. Cheng, Y. Ferng, S. Chen and C. Chieng, "Development of CFD methodology for investigating thermal-hydraulic characteristics in a PWR dome," *Nuclear Engineering and Design*, vol. 284, pp. 284-292, 2015.
- [8] J.-J. Jeong, K. Ha, B. Chung and W. Lee, "Development of a multi-dimensional thermal-hydraulic system code, MARS1.3.1," *Annals of Nuclear Energy*, vol. 26, no. 18, pp. 1611-1642, 1999.
- [9] D. Auliller, E. Tomlinson and R. Bauer, "Incorporation of COBRA-TF in an integrated code system with RELAP5-3D using semi-implicit coupling," in 2002 RELAP5 International Users Seminar, Park City, Utah, 2002.
- [10] Y. Ku, Y. Tseng, J. H. Yang, S. Chen, J. Wang and C. Shin, "Developments and applications of TRACE/CFD model of Maanshan PWR pressure vessel," in 16th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-16), Chicago, U.S., 2015.
- [11] A. Papukchiev, M. Jeltsov, K. Kööp, P. Kudinovb and G. Lerchl, "Comparison of different coupling CFD–STH approaches for pre-test analysis of a TALL-3D experiment," *Nuclear Engineering and Design*, vol. 290, pp. 135-143, 2015.
- [12] E. Deville and F. Perdu, "Documentation of the Interface for Code Coupling: ICoCo," NURISP-NUclear Reactor Integrated Simulation Project, 2012.
- [13] "TRACE TRACE V5.1051 theory manual," U. S. Nuclear Regulatory Commission, Washington, DC, U.S..
- [14] K. L. Zhang, "Instructions\_Setting\_TRACE\_SCF\_SALOME\_Debian\_Mandriva\_Vitualbox\_V10," Karlsruhe Institute of Technology, Karlsruhe, 2019.
- [15] K. L. Zhang, V. H. Sanchez-Espinoza and R. Stieglitz, "Implementation of the System Thermal-Hydraulic code TRACE into SALOME Platform for Multi-Scale Coupling," 50th Annual Meeting

on Nuclear Technology AMNT 2019, Submitted, Berlin, 2019.

- [16] P. E. Angeli, U. Bieder and G. Fauchet, "Overview of the TrioCFD Code: Main Features. V&V Procedures and Typical Applications to Nuclear Engineering," in 16th International Topical Meeting on Nuclear Reactor Thermal Hydraulics NURETH-16, Chicago, U.S., 2015.
- [17] R. Bavière, N. Tauveron, F. Perdu, E. Garré and S. Li, "A first system/CFD coupled simulation of a complete nuclear reactor transient using CATHARE2 and TRIO U. Preliminary validation on thePhénix Reactor Natural Circulation Test," *Nuclear Engineering and Design*, vol. 277, pp. 124-137, 2014.
- [18] "MEDCoupling Developer's Guide," SALOME-platform, [Online]. Available: http://docs.salomeplatform.org/latest/dev/MEDCoupling/developer/index.html. [Accessed 04 02 2019].
- [19] F. Cadinu, T. Kozlowski and P. Kudinov, "A Closure-On-Demand Approach to the Coupling of CFD and System Thermal-Hydraulic Codes," in NUTHOS-7: The 7th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Operation and Safety, Seoul, Korea, 2008.
- [20] F. Cadinu and P. Kudinov, "Development of a "Coupling-by-Closure" Approach between CFD and System Thermal-Hydraulics Codes," in *The 13th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-13)*, Kanazawa City, Ishikawa Prefecture, Japan, 2009.
- [21] T. Grunloh and A. Manera, "A novel domain overlapping strategy for the multiscale coupling of CFD with 1D system codes with applications to transient flows," *Annals of Nuclear Energy*, vol. 90, pp. 422-432, 2016.
- [22] T. Grunloh and A. Manera, "A novel multi-scale domain overlapping CFD/STH coupling methodology for multi-dimensional flows relevant to nuclear applications," *Nuclear Engineering and Design*, vol. 318, pp. 85-108, 2017.
- [23] S. Hamilton, M. Berrill, K. Clarno, R. Pawlowski, A. Toth, C.T.Kelley, T. Evans and B. Philip, "An assessment of coupling algorithms for nuclear reactor core physics simulations," *Journal of Computational Physics*, vol. 311, p. 241–257, 2016.