

FAST REACTOR MULTI-SCALE AND MULTI-PHYSICS MODELLING AT NRG

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Abstract

With the increase in computational power and capacity, and the advancements being made in numerical modeling, it has become possible to model the various physical phenomena that take place in nuclear reactors with more and more detail and accuracy. This includes phenomena related to structural mechanics, fluid dynamics and reactor physics amongst others. Additionally, there has been an increased interest to simulate these combined, interacting phenomena simultaneously by coupling various numerical tools. This coupling of different codes is currently a topic high on the research and development agenda of the international nuclear community. It is also a focus point within the research done at NRG in the national PIONEER research program funded by the Dutch ministry of economic affairs.

This focus has resulted in two branches of research at NRG: multi-scale modeling of the complete primary system of a nuclear reactor by coupling a 3D Computational Fluid Dynamics (CFD) code with a 1D System Thermal Hydraulics (STH) code, and multi-physics modelling through the coupling of dedicated and advanced thermal-dynamics, structural mechanics and reactor physics solvers. The paper presents simulation results of both branches applied to fast reactors. As both fields of research require the coupling of codes, it has led to the creation of an independent, external, Fortran-based coupling tool named myMUSCLE (MultiPhYsics MUltiscale Simulation CoupLing Environment) that arranges the efficient and robust coupling of the different codes. The paper presents the proof-of-principle and first validation of the myMUSCLE tool under development. Additionally, results obtained with MUSCLE-Foam will be presented, which is a new multi-physics code being developed at NRG that includes several reactor physics as well as structural mechanics solvers.

1. INTRODUCTION

In order to enhance the safety standards and culture of Nuclear Power Plants (NPPs), it is important to provide the system designers with accurate information and data. However, especially for Gen-IV Liquid Metal Fast Reactors (LMFRs), experimental data relating to the operation of this type of reactors in both nominal conditions and, in particular, accident scenarios, such as loss of flow (pump breaking down) or loss of heat sink (heat exchanger malfunction), is very scarce. Therefore, numerical tools are often used as design support to help predicting, amongst others, coolant flow and thermal behaviour and reactivity feedbacks in such scenarios.

Historically, the primary computational tool to study an NPP's behaviour are System Thermal-Hydraulic (STH) codes. These were initially designed and validated to be used for Light Water Reactors (LWRs) but have recently been adapted for application of liquid metals as coolant in LMFRs. The advantage of using STH codes is that they require relatively low computational efforts as they are often 1D and/or use a relatively coarse nodalization in 3D. The drawback though is that no details of the flow and temperature fields are resolved and that rather simple neutronics and thermal-mechanics solvers are used.

With the increase in computational power and capacity, and the advancements being made in numerical modeling, it has become possible to model the various physical phenomena that take place in nuclear reactors with more and more detail and accuracy. This includes phenomena related to structural mechanics, fluid dynamics and reactor physics amongst others. Additionally, there has been an increased interest to simulate these combined, interacting phenomena simultaneously by coupling various numerical tools. This coupling of different codes is currently a topic high on the research and development agenda of the international nuclear community, see e.g. the Strategic Research and Innovation Agenda (SRIA) of the Sustainable Nuclear Energy Technology Platform in Europe (SNETP) [1]. It is also a focus point within the research done at NRG in the national PIONEER research program funded by the Dutch ministry of economic affairs.

This focus has resulted in two branches of research at NRG: multi-scale modelling of the complete primary system of a nuclear reactor by coupling a 3D Computational Fluid Dynamics (CFD) code with a 1D System Thermal Hydraulics (STH) code, and multi-physics modelling through the coupling of dedicated and advanced thermal-hydraulics (CFD), structural mechanics (Computational Structural Mechanics (CSM)) and neutronics (neutron diffusion and/or transport) solvers. Multi-scale modelling combines the best of both worlds; it uses CFD where detailed solutions are desired and STH codes where 1D solution gives accurate enough results, allowing the simulation time to remain manageable. Multi-physics modelling on the other hand allows to solve multiple physical phenomena in detail simultaneously for cases in which these phenomena are strongly coupled and hence have a direct impact on each other's evolution. The relation between these two fields lies in the efficient and correct coupling of data between the codes, a crucial aspect in order to get a converged and accurate solution.

This paper presents simulation results of both branches applied to fast reactors. First, in Chapter 2, multi-scale simulations of the primary system of various fast reactors are presented, both in steady-state and transient conditions. Secondly, in Chapter 3, multi-physics modelling work done at NRG is presented. These have been focussed so far mainly on Fluid-Structure Interaction (FSI), i.e., the coupling of fluid dynamics and structural mechanics. Hence, the focus of that chapter will be on FSI. As both fields of research require the coupling of codes, it has led to the creation of an independent, external, Fortran-based coupling tool named myMUSCLE (Multi-physics MULTiscale Simulation CoupLing Environment) that arranges the efficient and robust coupling of the different codes. Chapter 4 presents the proof-of-principle and first validation of the myMUSCLE tool under development. NRG also started the development of a multi-physics code MUSCLE-Foam (MULTi-physics Simulation CoupLed Environment based on OpenFOAM) based on the open source OpenFOAM CFD code. MUSCLE-Foam will include several reactor physics solvers as well as computational structural mechanics solvers. Chapter 5 will present the basic principles of MUSCLE-Foam and an overview on the ongoing verification and validation activities. Finally, conclusions and future work is presented in Chapter 6.

2. MULTI-SCALE MODELLING

NRG has been working since several years on performing multi-scale simulations of fast reactors. In first instance, the in-house developed STH code SPECTRA [2] was coupled to the commercial CFD software ANSYS CFX [3]. This chapter gives a short description of the general methodology of this coupling, as well as results obtained by applying this coupling to two different cases.

2.1. Multi-scale modelling approach

The coupling approach used for the CFX-SPECTRA coupled calculations is explicit in time and based on a domain-overlapping two-way approach. This means the full domain is present in the SPECTRA model of the case at interest, while CFX only contains those parts of the domain where 3D effects play an important role. For fast reactors, these parts generally are the cold and hot pools, in which strong mixing and circulation takes places. At the inlets and outlets of the CFX domain, data is exchanged between CFX and SPECTRA, with data being exchanged in both directions. The data that is exchanged depends on the specifics of the case. The data is exchanged at the end of each time-step of CFX via external data exchange routines, written in FORTRAN. These routines check if the correct number of parameters are exchanged, if the time of exchange between both simulation is equal and ensures the codes wait in case either code has not reached the point of data exchange yet. This latter is important, as generally a CFD code takes longer to come to a converged solution within a time step, hence it is important SPECTRA waits for CFD to be ready for data exchange. It should be noted here that the time step used in the SPECTRA simulation can be smaller than the data exchange time step, as SPECTRA uses an adaptive time step size.

2.2. CIRCE

CIRCE (CIRColazione Eutettico) is an integral effect pool type facility designed and realized at the ENEA Brasimone Research Centre consisting of a cylindrical vessel filled with about 70 tons of molten Lead-Bismuth Eutectic (LBE). It includes argon as cover gas and a recirculation system for LBE heating and cooling. The CIRCE facility is depicted in the left of FIG. 1 . It consists of an inner loop and a main pool. The LBE enters the inner

loop through a feeding conduit, after which it flows through a flow meter before entering the Fuel Pin Simulator (FPS). The FPS is a mechanical structure representing the heat source of the system. After exiting the FPS, the LBE passes through the fitting volume and flows inside the riser. Inside the riser there is a nozzle installed to allow argon injection, which forces the flow. The LBE subsequently enters the separator. It is open from the top and allows for the separation of the argon, which flows into the cover gas through the free surface, while the LBE flows downward into the heat exchanger. Here it gets cooled and eventually re-enters the main pool. More information on CIRCE can be found in [4]-[6].

A multi-scale model of the CIRCE facility was created in order to simulate a Protected Loss Of Heat sink and Loss Of Flow (PLOH + LOF) transient, an accident scenario that was performed with the experimental test facility as part of the European Horizon 2020 project SESAME (thermal hydraulics Simulations and Experiments for the Safety Assessment of METal cooled reactors) [7]. In such a transient, the facility transitions from full power forced convection into natural convection decay power operation, with the pump and heat exchanger inactive and the total mass flow rate being about 5-10% of the nominal level. More information on the precise conditions of this transient can be found in [8].

For the multi-scale model, the CFD code ANSYS CFX is used to model the main pool and vessel of the CIRCE facility. The CAD used in the CFD simulations is shown on the left of FIG. 1. The internal elements indicated by the arrows are removed from the CAD, so that only the region between the external vessel wall and the structure walls remains, i.e., the main pool. The CFD geometry only extends up till the free surface to avoid multi-phase flow calculations. The SPECTRA model of the facility includes the full primary side of the facility, including the pool and structural walls, as well as the secondary side of the heat exchanger. The nodalization used in the SPECTRA model can be seen in the right of FIG. 1. It should be noted that even though SPECTRA's model includes the pool, the pool's temperatures are overwritten by those coming from CFX and hence not used in the coupled simulation.

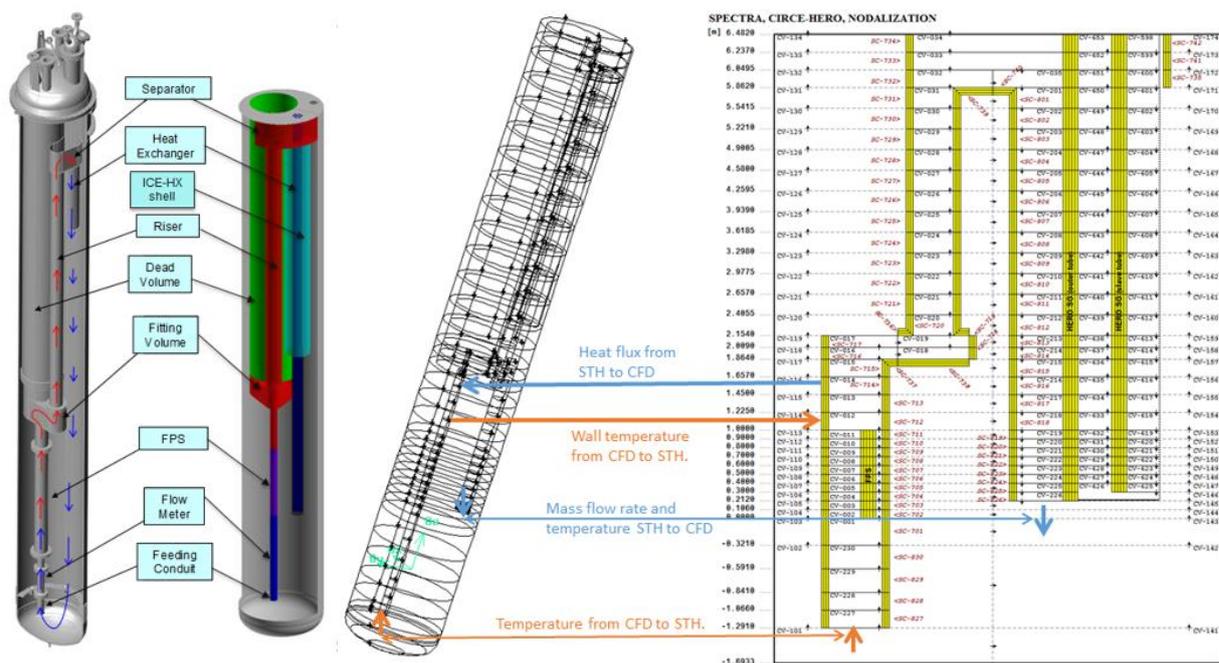


FIG. 1. CIRCE-HERO primary loop (left), with the CFD CAD (middle) and SPECTRA nodalization (right) used for the simulation [9].

The coupling used in the multi-scale simulations is schematically depicted in the middle of FIG. 1. Temperature of the LBE is exchanged between the two codes on the inlet and outlet of the CFD domain, i.e., SPECTRA provides CFX with a temperature at the outlet of HERO (inlet of CFX), while CFX in return couples the temperature of LBE at the FPS inlet (CFX outlet) back to SPECTRA. SPECTRA also provides the LBE mass flow rate at HERO's outlet to CFX. As the inner loop has only one inlet and outlet, this mass flow rate is also used at the FPS inlet as boundary condition for the CFD code. Additionally, in order to get a proper stratification inside the main pool, SPECTRA feeds a thermal heat flux over the inner loop's wall to CFX, with CFX providing

a wall temperature back to SPECTRA. Hereto, it was ensured that the CFD and STH domains use equal sized volumes throughout their respective domains, shown in the middle of FIG. 1.

In the left of FIG. 2 the experimental and numerical mass flow rate through the inner loop as function of time is plot. As can be seen, the initial value is quite a bit lower in the simulation (~ 28 kg/s) when compared with the experiment (~ 34 kg/s). This is a result of the coupling not having started from an actual coupled steady-state but a more forced steady-state, as it takes very long to reach a converged, mutual steady-state in multi-scale simulations. The trend afterwards is well predicted, with the final value of the simulation matching that of the experiment well.

Pool stratification plots are shown for various instances of time in the right of FIG. 2. These line plots are obtained by measuring the temperatures at various location across a vertical line through the main pool and give an indication of how well the coupling works with regards to data exchange across the structural walls. In general, a good match is found with the experimental data; the temperatures in the top, the location of the strong stratification and the temperature difference between the upper part of the pool and bottom part are recovered well. Only at the end of the simulation, at $t = 15$ minutes, the temperature in the bottom of the pool is quite a bit lower in the model than in the experiment. This is a result of the heat exchanger outlet temperature being underpredicted in the simulations (not shown). More results, and comparison with experimental data, of the multi-scale simulation can be found in [9].

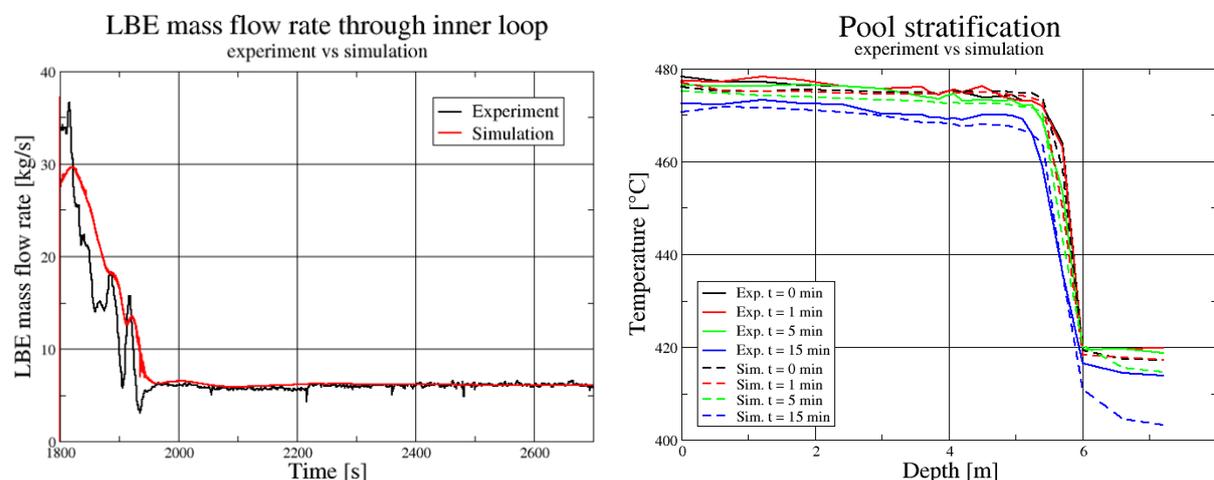


FIG. 2. Comparison between results obtained with the multi-scale model and experimental data for the mass flow rate (left) and pool stratification at various instants of time (right) [9].

2.3. Phénix

Phénix is a sodium-cooled fast reactor that was operated by CEA in France from 1973 till 2009. The experimental reactor was equipped with extra instrumentation in order to produce data during normal operation and transients that were performed at the end of the reactor's operational period. Phénix had a nominal power level of 340 MWth, 3 primary pumps (PP) and 4 intermediate heat exchangers (IHX), with 2 IHXs per primary pump for PP1 and PP3. The IHXs of the second PP were replaced by the so-called DOTEs (fake IHXs). More on the Phénix reactor can be found in [10].

Within the same H2020 SESAME project as where the described CIRCE experiment was analysed, a dissymmetric transient is analysed as benchmark for STH codes and for multiscale simulations. In this transient, one of the secondary pumps, belonging to one of the sets of two IHXs, is tripped at $t = 0$ s, leading to an automatic reactor shutdown after 5 s, in which the turbine is tripped as well as the secondary pump of the other set of intermediate heat exchangers. Subsequently a reactor scram is induced at 48 s. The benchmark consists of a blind phase, with only boundary conditions of the transient being provided to the modellers, followed by an open phase, in which the full data of the dissymmetric transient is shared.

The multiscale model is again a coupling between ANSYS CFX and SPECTRA with an explicit coupling at the end of each time-step. The SPECTRA model covers the complete reactor system and the CFX model consists of the cold pool, the hot pool and the primary side of the IHXs (in the open phase). The core outlet and the vessel cooling bypass system are the inlets of the CFD domain. From there, the sodium flows into the hot pool,

into the IHXs and leaves the domain through the PPs. The CFX geometry and the SPECTRA nodalization are provided in FIG. 3. Heat losses, mass flow rates, power removed by the IHXs and internal heat exchanges through structures are exchanged between CFX and SPECTRA. The temperature field just after the reactor scram is provided in FIG. 4, showing the temperature in the CFX part overlaid with velocity vectors. The temperatures in the SPECTRA IHX and the different fuel assembly types of the core are provided as inlays on the right and bottom of the figure respectively.

The first 400 s of the transient, being the most interesting and dynamic part, were predicted quite well with the multiscale model. After the blind phase of the benchmark it became evident that it is important to include the IHX in the CFD model to have a proper temperature and velocity distribution at the IHX outlets. In the blind phase, the IHXs were not included in the CFD model; thus the IHX inlets were outlets of the CFD hot pool and the IHX outlets were inlets to the CFD cold pool. The mean temperature and mean velocity of the IHX outlet in SPECTRA were provided to CFX. However, as is clear from FIG. 4, neither the temperature nor the velocity is uniform at the IHX outlet (IHX is shown at the right side of the left figure).

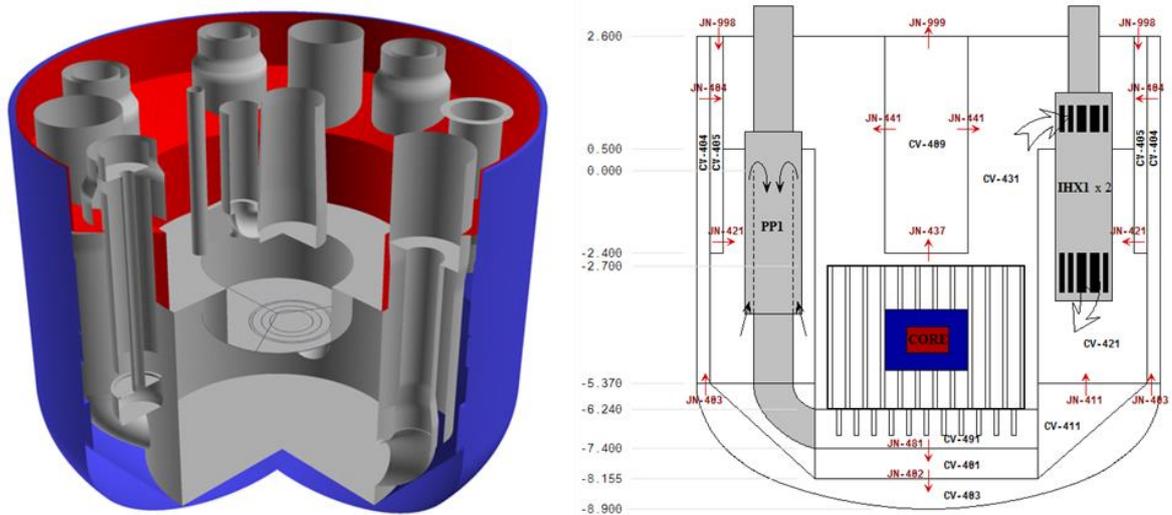


FIG. 3. Multiscale model of the Phénix reactor with CFX geometry on the left and SPECTRA nodalization at the right [11].

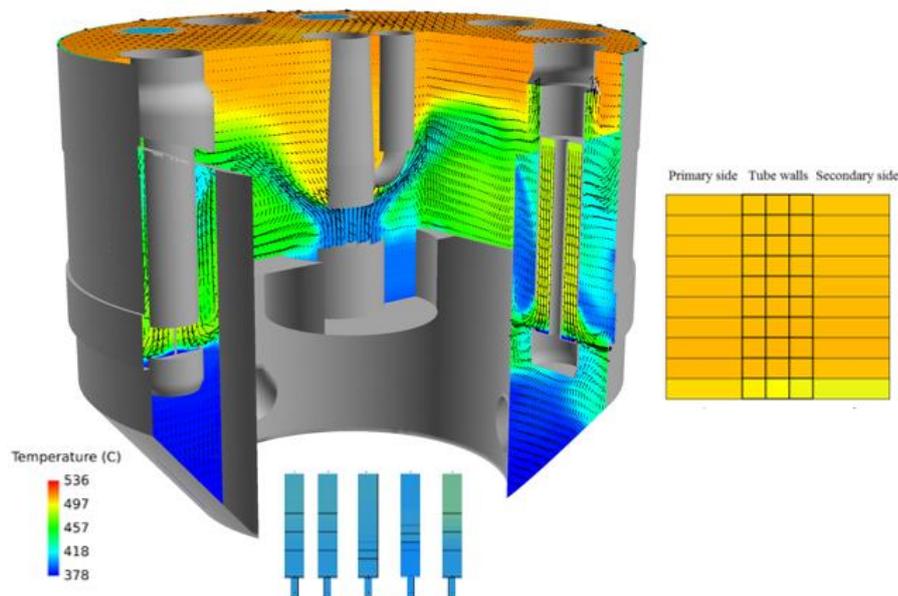


FIG. 4. Flow- and temperature field just after the reactor scram.

In order to include the IHXs in CFX, additional information had to be exchanged. The inlet temperature of each IHX and the mass flow rates through the IHXs were now provided from CFX to SPECTRA. The power that is removed in the IHX is then provided by SPECTRA to CFX, since the secondary side is included in the SPECTRA model. The IHXs are divided in several horizontal sections, similar to CIRCE in FIG. 1, to allow for different values for the heat sink along the height of the IHXs. The non-uniform flow through the IHXs combined with the different heat sinks leads to a more accurate flow and temperature distribution inside and at the outlet of the IHXs. These non-uniform distributions at the IHX outlets lead to a completely different flow and temperature distribution in the cold pool, especially when the transient enters the (transition to) natural convection and buoyancy becomes dominant for the temperature and flow distribution. This also leads to different temperatures of the sodium that leaves the cold pool via the PPs. The mean inlet temperature of one of the IHXs is provided in FIG. 5 for the blind and open phase, compared to the experimental data, confirming the improvement of the predicted temperature in the open phase. More on the multiscale model and more computational results and comparisons to the measurements of the dissymmetric test is described in [11].

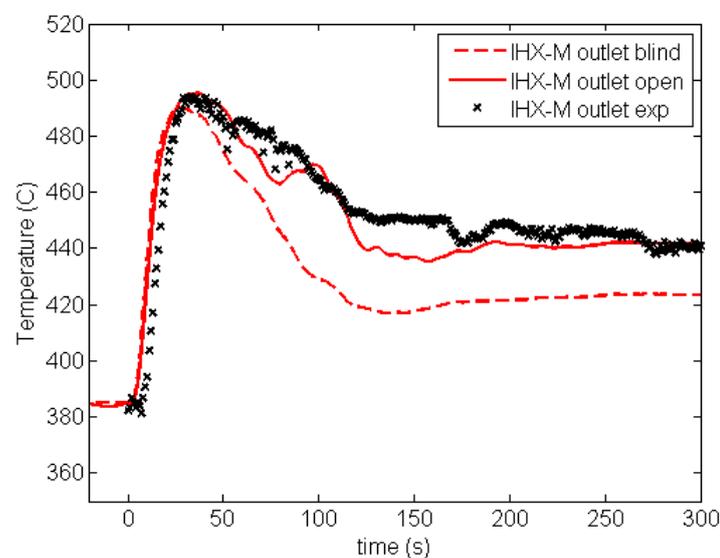


FIG. 5. Mean outlet temperature of one of the IHXs for the blind phase and the open phase of the benchmark, compared to the experimental data.

3. MULTI-PHYSICS MODELLING

Multi-physics simulations have so far mainly been performed at NRG in the framework of Fluid Structure Interaction (FSI), in which fluid dynamics codes are coupled with structural mechanics solvers. The main interest in FSI simulations is to get information on the vibration frequency and amplitudes of the structural elements induced by the coolant flow. Knowledge hereof is of particular importance, as it can lead to increased wear and tear and/or material fatigue, thereby contributing significantly to key components' failures. The two main components of concern with respect to FSI in a NPP are fuel rods and steam generator tubes.

The highly turbulent coolant flow in fuel assemblies during operation results in an asymmetric and fluctuating pressure on the fuel rods' surfaces, leading to flow-induced vibrations (FIV) of the fuel rods. As the rods are generally kept in place by spacer grids, it causes dynamic grid-to-rod contacts and frictions, resulting in material wear in the contact region between the rod and its support. Grid-to-rod-fretting wear (GTRFW), resulting from such vibrations, is the cause of 58% of fuel failures in PWRs worldwide and one of the major causes of fuel failure in boiling water reactors (BWRs) [12]-[13].

In steam generators, vibrations of the tubes as a result of FIV may lead to SG tube rupture (SGTR). The repeated vibrating of the tubes due to the highly fluctuating velocity and force field induced by the coolant, gives rise to extensive wear and material fatigue of the tubes, which may eventually lead to rupturing of the tubes. SGTR as a result of FIV has been observed in many reactors in the past [14]-[16].

For heavy liquid-metal fast reactors, very limited operational experience is available on the possible impact of FSI induced by a much denser fluid on the rods and tubes present in the reactor. Therefore, this is generally assessed using numerical tools. At NRG, two different frameworks are using: one using the intrinsic FSI solver of STAR-CCM+ and the other based on the coupling of the CFD code OpenFOAM to the structural solver Deal.II. Work done using these two platforms is described separately in the following two sections.

3.1. FSI simulations using STAR-CCM+

The intrinsic FSI solver of STAR-CCM+ couples its finite volume URANS solver, with a wide range of turbulence models available, to its finite element structural mechanics solver, which allows for both linear and nonlinear geometry applications. For the coupling, a block Gauss-Seidel scheme is employed with coupling taking place in each iteration of a time step. An Arbitrary Lagrangian-Eulerian (ALE) frame of reference is used, with mesh morphing done based on either Radial-Basis Functions (RBF) or the B-Spline method. More detailed information on all the options and methods available in the FSI solver of STAR-CCM+ can be found in its manual.

The main focus at NRG when using STAR-CCM+ for FSI simulations has been on assessing the difference in structural behaviour when using a heavy liquid metal instead of the conventionally used water as coolant in a nuclear reactor, and in particular of that of a fuel rod. Hereto, FSI simulations have been performed of a single fuel rod submerged in axial flow, with the used fluid being either water or Lead Bismuth Eutectic (LBE). The domain used for such simulations is depicted in FIG. 6. As can be seen, fluid enters from the left and exits from the right, with the outer fluid domain have a fixed, no-slip, wall. The wall of the rod is floating, thereby allowing for structural vibrations. Simulations are performed for both a bar rod and a wire-wrapped rod.

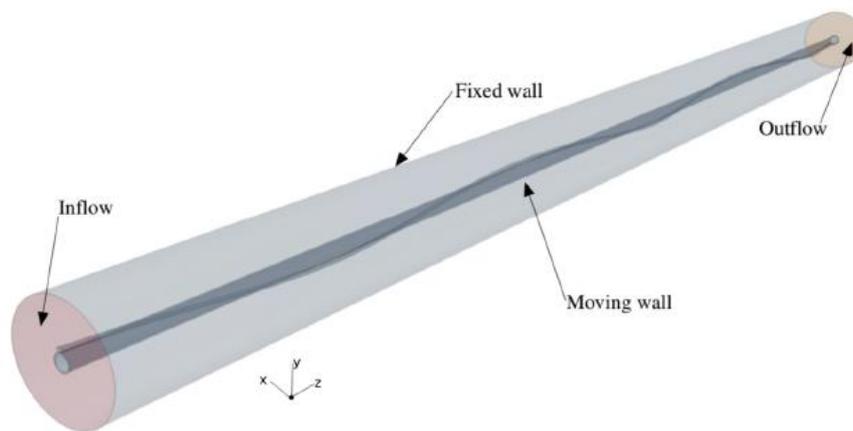


FIG. 6. Sketch of the fluid domain for FSI simulations [17].

Results obtained for simulations of a bar rod in both water and LBE are shown in FIG. 7, with the left figuring showing the vibration frequencies of the first three modes and the right figure depicting the damping ratios. Clearly, the vibration frequencies of a bare rod in LBE are much lower than that in water. This is due to the added mass effect of the surrounding fluid, which adds inertia to the system as the rod needs to deflect some fluid as it moves through it. It can be shown that the vibration frequency, ω , of such a system is inversely proportional to the square root of the sum of the mass of the rod, M , and the mass of the displaced fluid, m_f , i.e., $\omega \sim 1/\sqrt{M + m_f}$. Hence, a heavier liquid will result in a lower vibration frequency.

The damping ratio, on the other hand, is clearly increased when using LBE instead of water as working fluid. This effect is related to the higher viscosity of LBE, although added mass effects might play a role in a higher level of the damping ratio.

A more detailed analysis on the impact of the working fluid, and in particular its density and viscosity, on the frequency and damping ratio of a fuel rod can be found in [17] and [18]. The latter paper also gives correlations between the vibration frequency and density of the fluid, as well as that between the damping ratio and that of the fluid's density and viscosity.

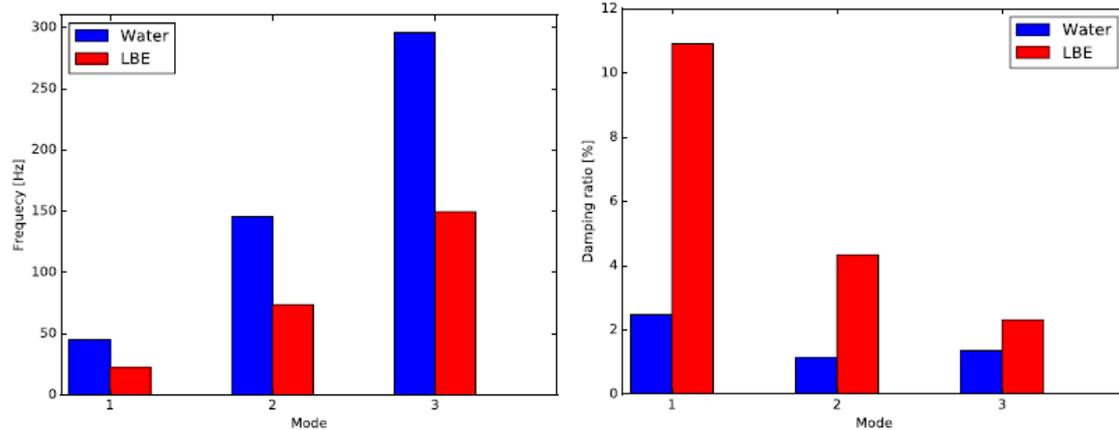


FIG. 7. Vibration frequencies (left) and damping ratios (right) of first three modes for of a bare rod in water and LBE flows [17].

3.2. FSI simulations using OpenFOAM

In general, flow-induced vibrations relevant for NPPs can be classified in two flow categories: axial flow, typically found in fuel assemblies, and cross flow, which mostly occurs in steam generators. In the latter category, the vibrations are induced by periodic wave shedding, and are more commonly known as Vortex-Induced Vibrations (VIV). As for axial flow problems, such as the one presented in the previous section, the vibrations are a result of the local turbulent flow field, and hence are named Turbulence-Induced Vibrations (TIV). They are not only phenomenally very distinct, the methodology used to numerically simulate them is also very distinct. While VIV can reasonably be resolved by using a URANS approach for the velocity field, higher-resolution methods are needed in order to reproduce TIV, as information of the fluctuating pressure field driving the structural vibrations is needed. And as URANS only resolves the average velocity and pressure field, it means either hybrid solutions or Large-Eddy Simulations (LES) are generally required to perform FSI simulations involving TIV. For the case described in the previous section, this was overcome by prescribing an initial displacement to the solid structure. However, when using URANS, the vibration will decay over time and hence no real TIV study can be performed.

To address this problem, NRG has been working for quite some time on a Pressure Fluctuation Model (PFM). In order to include the chaotic effect of the turbulence in this model, the velocity field is synthesized by means of a stochastic method. In this approach, a random velocity field is generated as a finite sum of Fourier modes. The turbulent field is assumed to be locally homogeneous isotropic within each grid cell, but anisotropy between neighbouring cells is allowed. The energy per mode is distributed according to a prescribed modified Kolmogorov energy spectrum, whose total energy is equal to the local turbulent kinetic energy, obtained from the URANS solution. The pressure fluctuations are subsequently obtained by solving for a Poisson equation for these pressure fluctuations. This equation results from the Navier-Stokes equations after splitting the velocity and pressure into its mean and fluctuating parts. More details on this approach can be found in [19] and [20].

As the PFM requires close interaction with the URANS solution, it is impossible to implement such a model in a commercial code in which no access to the solution structure is readily available. Hence, the PFM has been implemented in the open source CFD framework of OpenFOAM. The drawback of OpenFOAM though is that it is a dedicated fluid dynamics solver, lacking a structural mechanics solver needed for FSI simulations. Some structural modules have been written by external contributors, though these are very limited in applicability and hence not adequate for detailed FSI analyses [21]. Hence, at NRG, the NRG-FSIFOAM framework was created. In this framework, the finite volume CFD solver of OpenFOAM is coupled to the finite element CSM solver of Deal.II [22]. The fluid and solid solvers are coupled through the preCICE library [23] for solving FSI problems. For the coupling, an IQN-ILS scheme is employed with coupling taking place in each iteration of a time step. More information on the implementation of this coupling and NRG-FSIFOAM itself can be found in [19] and [20].

To demonstrate that NRG-FSIFOAM, which includes the PFM, can indeed resolve turbulence-induced vibrations, it has been applied to an experimental test case involving a flexible brass beam in turbulent water. The experiment was performed to study the effects of a turbulent flow of water along on a cylindrical brass beam in a

rigid container and consists of a flexible brass rod, enclosed inside of a rigid steel cylinder. The axis of the outer cylinder is aligned with that of the inner brass rod, and both are suspended vertically to avoid gravitational effects. The beam is clamped (fixed) on both the ends (at the inlet and the outlet of the fluid domain). More information on this experiment can be found in [24].

The displacement of the flexible brass beam resulting of a simulation using PFM in NRG-FSIFOAM as function of time is shown in FIG. 8. It should be noted here that for this simulation, the beam was not given an initial displacement as was done for the simulations in the previous section. As can be seen, vibrations of the brass beam are sustained throughout the simulation. The modal frequency was found to be 26.0 Hz, which is quite close to the experimental one of 27.9 Hz. More results can be found in [19].

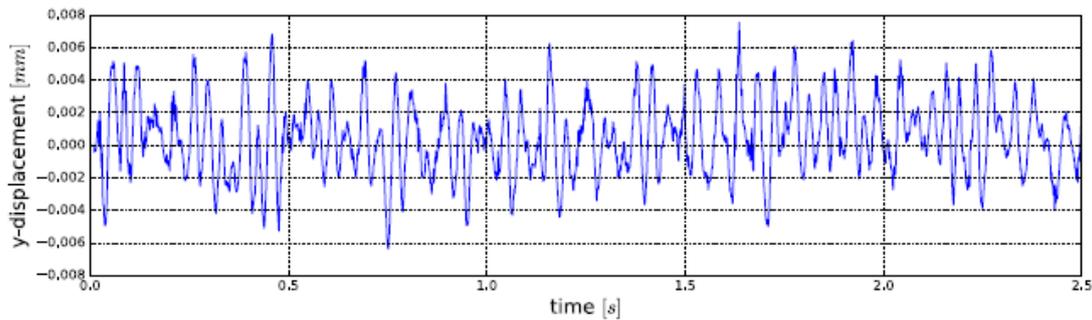


FIG. 8. Displacement vs time signal of the beam center obtained from applying the PFM to FSI solver [19].

Having demonstrated that PFM is reproducing TIV quite adequately, currently more development and validation of the model is going on to improve the results obtained with the model further. Results hereof will be presented in future publications.

4. MULTIPHYSICS MULTISCALE COUPLING TOOL MYMUSCLE

Following the relatively successful participation to the two multi-scale benchmarks described in Chapter 2 based on the coupling between SPECTRA and ANSYS CFX using a domain-overlap approach, it became clear that having to set up a new coupling strategy for each new case is quite labour intensive and prone to errors. Additionally, when studying other possible test cases, it was also evident some may need other approaches than explicit, domain-overlap coupling, and that for some cases other STH or CFD tools would be better suited. Based on among others these considerations, NRG has been working recently on the development of a user-friendly and flexible code coupling tool called myMuscle: Multiphysics MULTiscale Simulation CoupLing Environment.

MyMuscle is an independent, external, code which arranges the correct communication between different codes, allows selection of various coupling algorithms and performs coupling specific tasks. The coupling tool under development aims at being flexible with respect to the number of coupling interfaces, the parameters to be coupled, and the codes being coupled, i.e. commercial and open source codes. The current code-couplings available in myMuscle and the foreseen expansions are graphically shown in FIG. 9. As can be seen, a total of 4 different CFD codes has been coupled so far to SPECTRA through the myMuscle tool.

Setting up a coupling for a multi-scale, or in future multi-physics, simulation in one central place makes it easier to extend the tool to other couplings and to implement additional algorithms and methods. And it also avoids potential mistakes and complications that frequently occur when applying a case specific setup to a different case. Additionally, a single coupling tool should enhance quality assurance and should eventually facilitate approval by safety authorities.

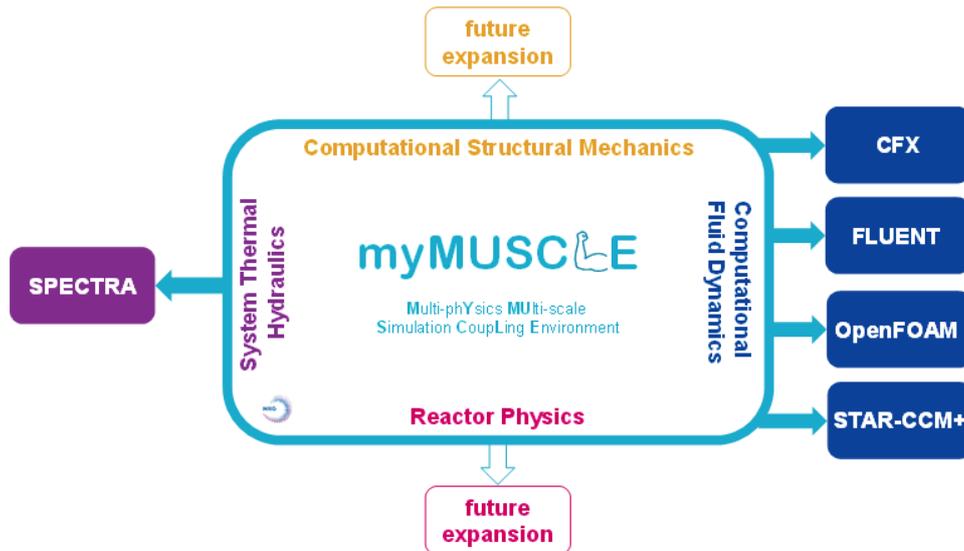


FIG. 9. Graphical representation of the myMuscle coupling tool (status spring 2021) indicating available and tested coupling possibilities and future expansions [26].

A first test-case used to validate myMUSCLE and check the correct coupling between SPECTRA and the various CFD tools is that of a 8.5m pipe split in two. This two pipe test-case is inspired by the PhD thesis of Toti [25] and is used for testing the implementation of the coupling procedure at one (thermal)hydraulic coupling interface. The diameter of the pipe is 0.1 m. The first 4 m of the pipe is modelled in SPECTRA and the second part, being 4.5 m, is modelled in a CFD code, see FIG. 10. There is thus one coupling interface, where the velocity or mass flow rate is provided from SPECTRA to CFD and the mean inlet pressure is provided from CFD to SPECTRA.

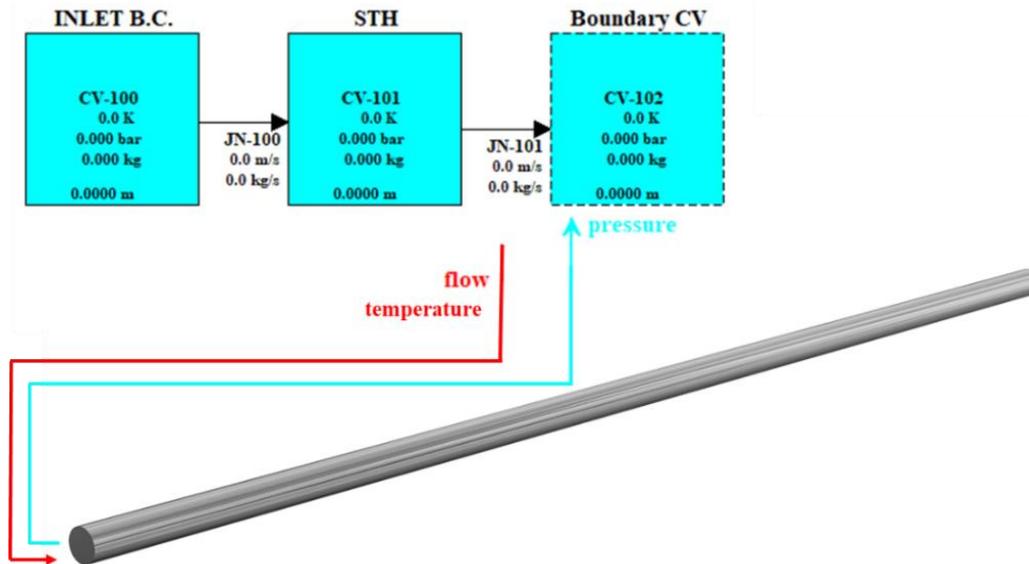


FIG. 10. Two-pipe case with a representation of the SPECTRA part (top) and the CFD part (bottom) [26].

At the start, the fluid is at rest and has a uniform temperature. At $t = 0$, a sudden pressure of 20 kPa is imposed at the inlet of the pipe, setting the water into motion. Furthermore, the inlet temperature is linearly increased by 20 °C between 1 and 2 s. More details on the test case and the setup of the various multi-scale simulations can be found in [26].

FIG. 11 shows the time evolution of the temperature at the coupling interface (left) and pipe outlet (right) resulting from the various multi-scale simulations, where SPECTRA is coupled to four different CFD codes. As can be seen, the timing of the temperature increase at the coupling interface shows a very good agreement between all codes, just as the temperature at the outlet. A similar agreement was also found for the mass flow rate, with

the final mass flow rate being in close agreement with the expected mass flow rate based on the Colebrook-White correlation [27] for the friction factor.

Further results obtained for the two-pipe test case, as well as myMUSCLE applied to a more complex test case of a thermal mixing chamber placed inside a loop, with sodium as the working fluid, are reported in [26]. For further validation, and in particular to being able to apply myMUSCLE to LMFBRs, currently multi-scale simulations are being performed of TALL-3D [28]. TALL-3D is an experiment with the aim to support the design of LMFBR by producing reference data for modelling natural and forced convection in a pool. It is an LBE facility equipped for validation of simulations using system codes, CFD codes and coupled codes. The coupling of the SPECTRA model and the STAR-CCM+ model, is currently being tested. The steady state of the stand-alone simulations is depicted in FIG. 12. Results of this validation phase will be reported in the near future.

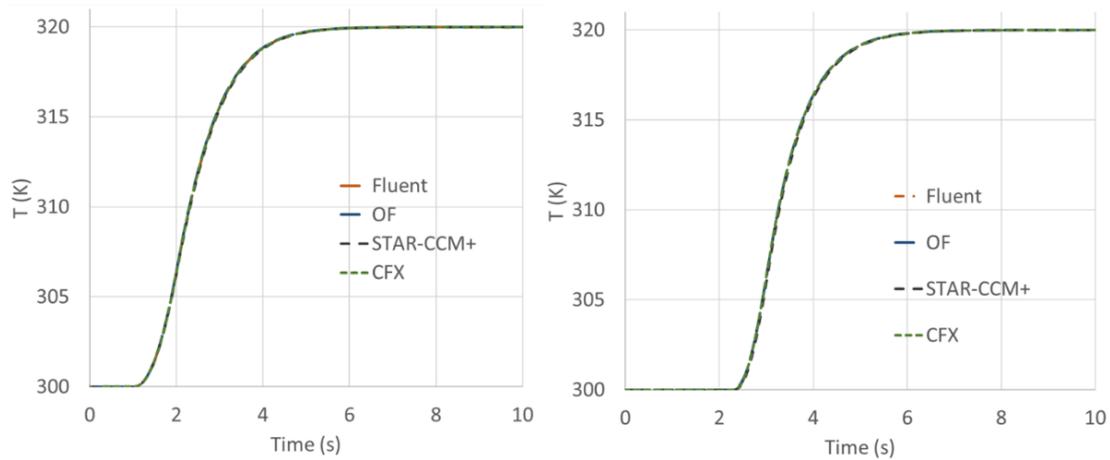


FIG. 11. Mean temperature at the coupling interface (left) and at the outlet (right) for the various multi-scale simulations, with OF being OpenFOAM [26].

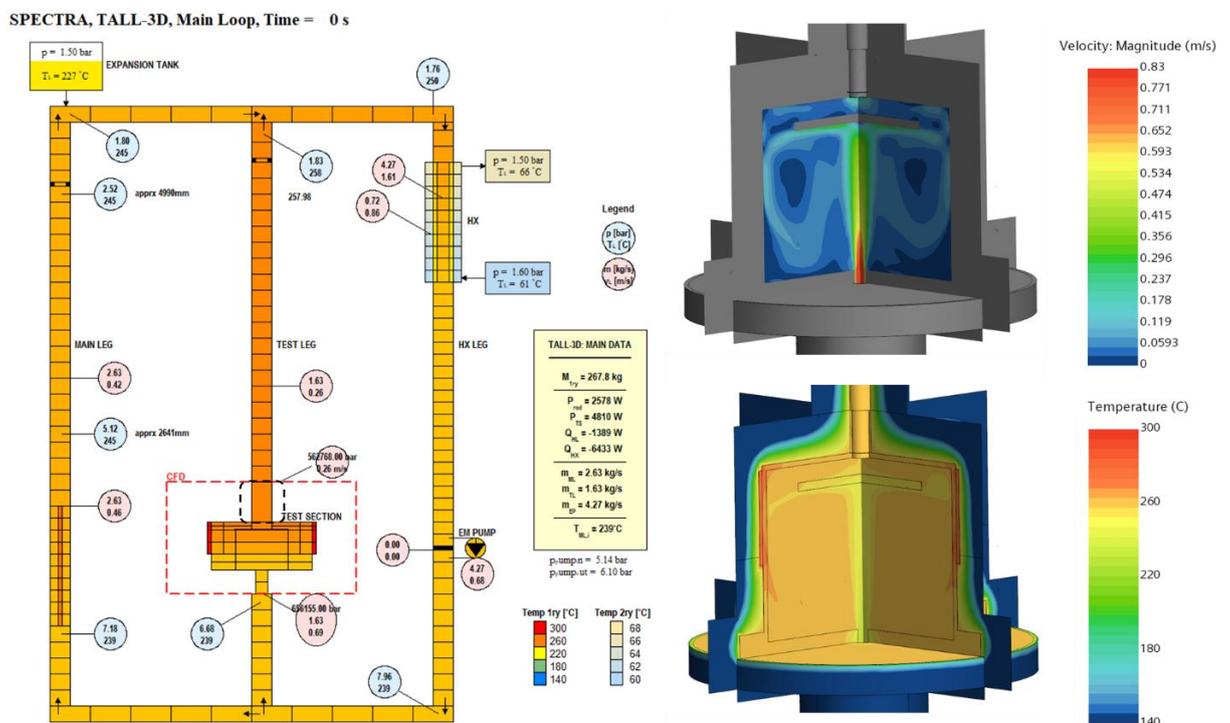


FIG. 12. Initial steady state of stand-alone simulations of the SPECTRA model (left) and the STAR-CCM+ model showing velocity (top right) and temperature (bottom right).

5. OPEN SOURCE MULTIPHYSICS CODE PLATFORM: MUSCLE-FOAM

Multi-physics simulations have always been important within the nuclear field. Traditionally, so-called system thermal hydraulic codes mostly contain multi-physics modules to couple the thermal hydraulics solvers to a reactor physics solver (mostly point kinetics) and sometimes to 0D or 1D models for thermal mechanics. With increasing computer power, the coupling of different physics at a higher resolution becomes feasible leading to the increased interest in multi-physics simulation tools. A quick scan of the available options in literature shows that a combination of neutron transport models, multi-phase and compressible thermal hydraulics, and thermal mechanics allowing large deformations is currently not available in a single (open-source) simulation environment. To fill this gap, the initiative was taken to develop an open-source based multi-physics platform within NRG which has the following innovative features:

- Multi-material formulation
The simultaneous presence of solid, liquid and gaseous materials, characterized by different equations of state can be simulated in the same mesh with just one set of mass, momentum and energy balance equations, without requiring matching boundaries at material interfaces and the specification of interface conditions.
- Arbitrary Lagrangian-Eulerian (ALE) mesh option
The new platform includes an ALE moving mesh algorithm to preserve the mesh quality in case of large deformations, while an accurate Lagrangian mesh is maintained in regions where deformations are small. This meshing technique is especially implemented for fluid-structure interaction simulations in which solids can be treated with a Lagrangian technique while an Eulerian or ALE technique is required for liquid regions.
- Pressure-velocity coupling
A hybrid pressure- and density-based formulation, suitable for all flow velocities, has been implemented. This feature is of value for simulations including a high rate-of-strain such as some accidental scenarios involving rapid deformations or hydrogen explosions.

To achieve this, NRG selected the existing open-source CFD code OpenFOAM as a basis, and is developing and validating a new multi-physics code platform including reactor physics and thermal mechanics solvers. This development builds upon existing OpenFOAM multi-physics code coupling developments by [29], [30], [31] and [32] in which a variety of neutron physics solvers and a thermal mechanics solver are coupled to the multi-material OpenFOAM CFD code. The existing neutron physics solvers include a multi-group neutron diffusion solver, a multi-group SP3 approximation of the neutron transport equation code, and a multi-group discrete ordinate neutron transport code. Recently, also a development to include a point kinetics solver in the code platform has been initiated. The thermal mechanics solver is an OpenFOAM based solver which allows application of an Arbitrary Lagrangian-Eulerian model to deal with computational mesh deformations. The new open-source code platform is being called MUSCLE-Foam (MULTi-physics Simulation CoupLed Environment based on OpenFOAM). An overview of the various solvers and the physics covered within MUSCLE-Foam is provided in TABLE 1.

TABLE 1 MUSCLE-FOAM SOLVERS

Solver	Physics covered
OpenFOAM	3D thermal hydraulics & mechanics
Point Kinetics	0D reactor physics
Neutron Diffusion	3D reactor physics
SP3	3D reactor physics
Discrete ordinate neutron transport	3D reactor physics
Arbitrary Lagrangian Eulerian	Mesh remapping

Within MUSCLE-Foam, the reactor physics code package is setup in a flexible way which will facilitate coupling to any OpenFOAM CFD or thermal mechanics solver. For the thermal mechanics solver, it is important to note that the solver in MUSCLE-Foam is limited to the lower-Mach equation of states and does not adopt the hypersonic models presented in [32] which are not required for nuclear reactor applications.

With the full integration of MUSCLE-Foam in the OpenFOAM environment, it is foreseen that coupling the various MUSCLE-Foam solvers to other codes, e.g. the system thermal hydraulics code SPECTRA and/or other CFD codes, can be achieved through the myMUSCLE coupling tool.

Any simulation code requires validation which is part of the development. This also holds for MUSCLE-Foam. The validation of the 3D CFD solver is primarily considered to be covered by the international developments on this well-known and widely used open-source code. Nevertheless, certain applications in the nuclear field still require validation. TABLE 2 provides an overview of the validation and verification currently being carried out and in preparation for the MUSCLE-Foam code platform. Obviously, one of the main applications for MUSCLE-Foam will be for liquid fuel molten salt reactors. Therefore, some specific cases are included covering such applications, i.e. the DYNASTY molten salt experimental loop, the liquid fuel lid driven cavity benchmark, and the simulation of the Molten Salt Reactor Experiment (MSRE). The validation efforts will be published in dedicated articles in the (near) future. Apart from that, future developments will focus on further verification and validation of the MUSCLE-Foam platform and on the proof-of-principle of coupling MUSCLE-Foam through myMUSCLE to the SPECTRA system thermal hydraulics code or commercial CFD codes.

TABLE 2 VALIDATION & VERIFICATION (V&V) CASES

V&V case	Physics covered	Status	Reference
Tank critical assembly	neutronics	almost completed	[33]
DYNASTY experimental loop	thermal hydraulics	in preparation	--
Liquid fuel lid driven cavity	thermal hydraulics + neutronics	completed	[34]
Godiva super-prompt-critical burst	neutronics + thermal mechanics	completed	[35]
Flexible beam	thermal hydraulics + mechanics	in progress	[36]
TRIGA reactor	thermal hydraulics + neutronics	in preparation	--
Molten Salt Reactor Experiment	thermal hydraulics + neutronics	in preparation	--

6. SUMMARY AND OUTLOOK

An overview of the multi-scale and multi-physics simulation activities at NRG applied to fast reactors has been provided. Initially, the work done was focussed on the two separate branches, and the modelling approach used was very case specific. Examples hereof are participation to the CIRCE and Phénix benchmarks using separate multi-scale models based on the coupling of the CFD code ANSYS CFX with the STH code SPECTRA, and the study on the impact of a heavier liquid on the vibration frequencies and damping ratios of rods as a result of flow-induced vibrations.

With a growing interest in such multi-scale and multi-physics simulations, and with their applicability growing due to an increase in computational power and capacity, it became apparent that there is a need for a more universal platform to perform such multi-scale and multi-physics simulations. This has led at NRG to the development of two different, but strongly-related, tools: myMUSCLE and MUSCLE-Foam. The former focusses on the efficient and case-independent coupling of two or more codes, while the latter is an OpenFOAM based platform to perform multi-physics simulations involving reactor physics and thermal mechanics. Both tools are presented in the paper, giving an overview of the capabilities and current status of development.

Future work will be aimed at further developing and validating the myMUSCLE and MUSCLE-Foam tools, and by further expanding their applicability. Additionally, the plan is to merge the tools together in the future, to allow a wider range of multi-scale and multi-physics problems to be tackled with these tools. The desire is to be able to perform in the end simulations of a full LMFR with detailed analysis of the thermal-hydraulics, reactor physics and structural mechanics where necessary.

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REFERENCES

- [1] SNETP, SNETP Strategic Research and Innovation Agenda. SNETP, Brussels, Belgium (2021).
- [2] M.M. STEMPNIEWICZ, SPECTRA Computer Code Manuals”, Version 3.61, , Volume 1 – Program Description, Volume 2 – User’s Guide, Volume 3 – Verification and Validation, <https://dyfuzjastudio.com/marekstempniewicz/files/Spectra-Vol1.pdf>
- [3] <https://www.ansys.com/products/fluids/ansys-cfx>
- [4] G. BANDINI et al., CIRCE experimental set-up design and test matrix definition, ENEA UTIS-TIC Technical Report, IT-F-S-001. February 2011.
- [5] M. TARANTINO et al., Mixed convection and stratification phenomena in a heavy liquid metal pool, NED, **286**, 261 (2015).
- [6] D. ROZZIA, A. DEL NEVO AND M. TARANTINO, Experimental Investigation of Double Wall Bayonet Tubes Performance in Pool Type Integral Test Facility, 16th International Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-16), Chicago, US, August 30-September 4, American Nuclear Society (2016).
- [7] F. ROELOFS et al., The SESAME Project: State of the Art Liquid Metal Thermal Hydraulics and Beyond, ATW, vol. 61, Issue 8/9, p.p. 531-537, (2017).
- [8] P. LARUSSO et al., Total loss of flow benchmark in CIRCE-HERO integral test facility, NED, **376** (2021)
- [9] K. ZWIJSEN et al., Multi-Scale Modelling Of The Circe-Hero Facility, NED, **355** (2019)
- [10] J. GUIDEZ, Phénix: the experience feedback. EDP Sciences (2013).
- [11] H.J. UITSLAG-DOOLAARD, F. ALCARO, F. ROELOFS, X. WANG, A. KRAUS, A. BRUNETT, J. THOMAS, C. GEFFRAY, A. GERSCHENFELD, Multiscale modelling of the Phénix dissymmetric test benchmark, Nuclear Engineering and Design, **356**, 110375 (2020).
- [12] IAEA, Review of Fuel Failures in Water Cooled Reactors, IAEA No NF-T-2.1, NE1445, Vienna, Austria (2010)
- [13] IAEA, Review of Fuel Failures in Water Cooled Reactors (2006-2015), IAEA No NFT-2.5, NE1864, Vienna, Austria (2019)
- [14] MACDONALD, P.E., SHAH, V.N., WARD, L.W., AND ELLISON, P.G., Steam generator tube failures, NUREG/CR-6365 INEL-95/0383 (1996).
- [15] PAÏDOUSSIS M., Real-life Experiences with Flow-induced Vibration, Journal of Fluids and Structures, vol. 22, p.p. 741-755 (2006)
- [16] NRC, <https://www.nrc.gov/docs/ML1501/ML15015A419.pdf> (2015)
- [17] D. DE SANTIS, A. SHAMS, Analysis of flow induced vibrations and static deformations of fuel rods considering the effects of wire spacers and working fluids, J. of Fl. and Struc., **84** (2019) 440-465
- [18] D. DE SANTIS, A. SHAMS, “Scaling of added mass and added damping of cylindrical rods by means of FSI simulations”, JFS, **88** (2019) 241-256
- [19] S. KOTTAPALLI ET AL., “Numerical investigation of an advanced U-RANS based pressure fluctuation model to simulate non-linear vibrations of nuclear fuel rods due to turbulent parallel-flow.”, ANE, **128** (2019) 115-126
- [20] D. DE SANTIS, A. SHAMS, “An advanced numerical framework for the simulation of flow induced vibration for nuclear applications.”, ANE, **130** (2019) 218-231
- [21] E. TER HOFSTEDDE ET AL., “Numerical prediction of flow induced vibrations in nuclear reactor applications.”, NED, **319** (2017) 81-90
- [22] ALZETTA, G. ET AL., “The deal.II library”, version 9.0. J. Numer. Math. (2018)
- [23] H.-J. BUNGARTZ ET AL., “preCICE – a fully parallel library for multi-physics surface coupling.” Comput. Fluids **141** (2016) 250–258
- [24] S.S. CHEN., M.W. WAMBSGANN, “Parallel flow induced vibration of fuel rods”, NED, **18** (1972) 253–278

- [25] A. TOTI, Development and Validation of a System Thermal-Hydraulic/CFD Codes Coupling Methodology for Multi-Scale Transient Simulations of Pool-Type Reactors, section 3.2.6, University of Gent, Gent, Belgium
- [26] UITSLAG-DOOLAARD, H., ZWIJSEN, K., ROELOFS, F., STEMPNIEWICZ, M., myMUSCLE, a new: Multiphysics Multiscale Simulation Coupling Environment, NURETH19, Brussels, Belgium (2022)
- [27] F. COLEBROOK, “Turbulent flow in pipes with particular reference to the transition region between the smooth and rough pipe laws”, *J. Inst. Civ. Eng.*, **4** (1939) 14-25
- [28] P. KUDINOV, “Experimental activities report on TALL-3D”, Deliverable D5.2.04 of the THINS project (grant agreement 249337), March 2, 2015
- [29] CERVI, E., LORENZI, S., CAMMI, A., LUZZI, L., Development of a multiphysics model for the study of fuel compressibility effects in the Molten Salt Fast Reactor, *Chemical Engineering Science* **193** (2019) 379-393
- [30] CERVI, E., LORENZI, S., CAMMI, A., LUZZI, L., Development of an SP3 neutron transport solver for the analysis of the Molten Salt Fast Reactor, *Nuclear Engineering and Design* **346** (2019) 209-291
- [31] CERVI, E., LORENZI, S., LUZZI, L., CAMMI, A., Multiphysics analysis of the MSFR helium bubbling system: A comparison between neutron diffusion, SP3 neutron transport and Monte Carlo approaches, *Annals of Nuclear Energy* **132** (2020) 227-235
- [32] CERVI, E., LORENZI, S., LUZZI, L., CAMMI, A., An Arbitrary Lagrangian-Eulerian, coupled neutronics-shock physics model for the analysis of shockwave implosion of solid fissile materials, *Annals of Nuclear Energy* **141**, 107322 (2020).
- [33] KITAMURA, Y., SUZAKI, T., HAIFENG, Y., OKAJIMA, S., NAKAJIMA, K., Temperature effects on reactivity in light water moderated uo2 core with soluble poisons at TCA. *International Handbook of Evaluated Reactor Physics Benchmark Experiments 2014 Edition* (2014).
- [34] TIBERGA, M., OLIVEIRA, R.G.G. DE, CERVI, E., BLANCO, J.A., LORENZI, S., AUFIERO, M., LATHOUWERS, D., RUBIOLO, P., Results from a multi-physics numerical benchmark for codes dedicated to molten salt fast reactors, *Annals of Nuclear Energy* **142**, Article 107428 (2020).
- [35] WIMETT, T.F., Time behavior of Godiva through prompt critical, LA-2029, Los Alamos National Laboratory (1956).
- [36] TUREK, S., HRON, J., Proposal for Numerical Benchmarking of Fluid Structure Interaction between an Elastic Object and Laminar Incompressible Flow, *Fluid-Structure Interaction*, (2006) 371– 385