FERMI: A MULTI-PHYSICS SIMULATION ENVIRONMENT FOR FUSION REACTOR BLANKET

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ABSTRACT

The Fusion Energy Reactor Models Integrator (FERMI) simulation framework aims to develop an integrated simulation environment for the coupled simulation of plasma, plasma-material interaction, first-wall and blanket. The FERMI goal is to significantly shorten the overall design cycle while guaranteeing unprecedented accuracy, thus integrating fusion design activities, advancing fusion technology, and supporting the US fusion industry by reducing the development risk in future designs. This will be achieved by coupling single-physics solvers in a multi-physics simulation environment using the open-source coupling library preCICE. In particular, the MCNP code is used for neutron and gamma transport, OpenFOAM for computational fluid dynamics and magnetohydrodynamics, including heat transfer of the first wall and blanket cooling, and Diablo for structural mechanics simulation of components. The features of FERMI are tested with the analysis of the blanket design of the ARC fusion reactor by Commonwealth Fusion Systems. In this paper, we show how MCNP simulations are used to calculate the tritium breeding ratio and estimate the heat deposited (neutronic and gamma) in the vacuum vessel and blanket, which feeds into OpenFoam thermal-hydraulic calculations of the FLiBe cooling flow in the blanket. Preliminary testing of OpenFOAM-Diablo couping through preCICE is also demonstrated on benchmark problems. To the author's knowledge, FERMI is the first attempt to simulate nuclear fusion first wall and blankets in a fully coupled multi-physics way. A critical technical problem, i.e. volumetric code coupling, integrated with the preCICE library, is also tackled here for the first time, and the first three-dimensional simulations of the ARC blanket are presented.

KEYWORDS
multi-physics, fusion reactors, digital twin, ARC

1. INTRODUCTION

The development of a reliable, low-cost, safe first wall and blanket system that provides self-sufficient tritium breeding and efficient conversion of the extracted fusion energy to electricity while meeting all material, design, and configuration limitations are critical fusion science and technology goals on the path to the Compact Pilot Plant (CPP) [1], DEMO, the Affordable Robust Compact (ARC) reactor [2], and to a commercial fusion power plant in the United States. In this context, it is desirable to construct a simulation tool that can predict and assess the performance of these fusion reactor concepts while accelerating and improving the design cycle for fusion reactors. Sophisticated, integrated computer simulation tools are essential to address the complexity of the physical processes and the highly interconnected nature of systems and components in fusion design. The structures immediately surrounding the fusion plasma that form a plasma chamber - the first wall, the blanket, and the divertor - serve a vital role in fusion energy systems, providing tritium fuel self-sufficiency, radiation shielding of the vacuum vessel, efficient power extraction, and plasma cleaning. The physical environment around the plasma is unique and complex. Modelling and simulating the extreme combination of physics involves neutron radiation, heat transfer, strong electromagnetic fields, unsteady fluid flow, production and transport of tritium, and structural deformation. Modelling and simulating all of these factors is fundamental to the development of robust first wall and liquid metals (LMs), the molten salt (MS) breeding blankets, and novel LMs—all of which are plasma-facing component concepts and designs. The potential to develop integrated simulations of the entire blanket system and integrated first-wall and plasma interactions is promising. Computational design optimization can deliver improved performance, safe operation, and reduced cost. It can streamline efforts with fewer, more targeted experiments to test the materials and the entire system or its components. Furthermore, the identification of optimal operations and maintenance regimes can also result. The need for integrated simulations has been recognized internationally, and research groups in Germany (PROCESS code, [3]), in the United Kingdom (BLUEPRINT and SYCOMORE codes [4]) and in China (CFETR code [5]) are developing integrated simulation environments for fusion reactors. Coleman et al. [4] state that with their integrated simulation environment BLUEPRINT, “the typical activities required to generate a DEMO design point can be sped up by four orders of magnitude—from months to minutes—paving the way for a rigorous and broad exploration of the design space.” However, the conceptual design phase, which extends the design point to the details of the components surrounding the plasma, can take up to three years, and they are challenging to speed up using the current technology and design system. In fact, as for the DEMO reactor, it is predicted that the iteration of multiple designs for the design baseline definition could take up to 9 years (Figure 1).

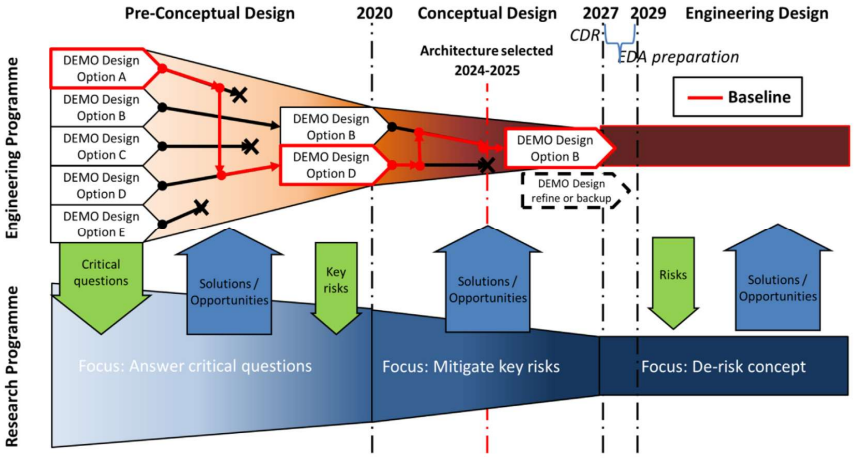

Figure 1: EU-DEMO design strategy leading up to the start of an engineering design phase in the late 2020s [6].

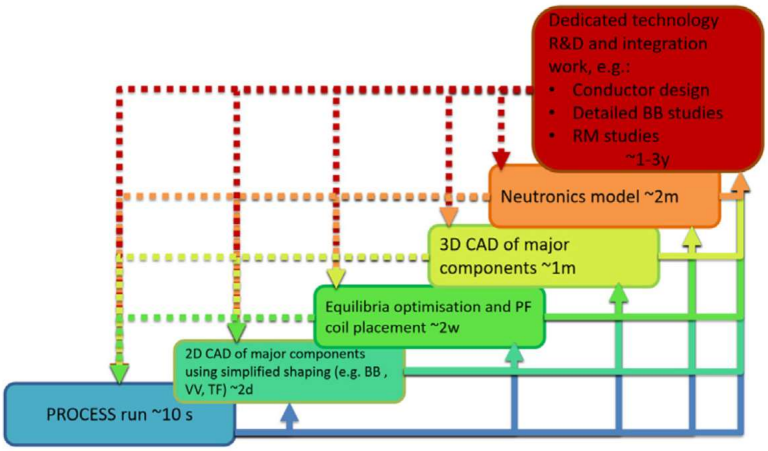

Figure 2: Schematic representation of the DEMO reactor design point definition and evaluation procedure in Europe [4].

The largest share of the iteration duration (3 years) is due to the complex multi-physics, multiscale analysis of different components, as detailed in the red box in Figure 2; particularly time-consuming is also the complex coordination of the work of large multidisciplinary groups of researchers/designers in different countries and specializing in specific reactor analyses. Most of the time required by such analyses is to establish the model accurately, especially if it is appropriately coupled with the models and results of other codes from other disciplines and other groups. At present, much of this work is performed manually, with the geometry and the results being ported across to whichever software the analysts of different volumes wish to use. The geometry, boundary conditions, and other data are often shared in an ad-hoc fashion (by email or through clouds) with no organized, shared repository and no configuration or lifecycle management. More robust management of fundamental system data and geometries is needed to avoid coordination errors across the different design / R&D groups and to reduce the typical large uncertainty and design margins that result from an independent and isolated simulation of problems that are intrinsically multi-physics and coupled. FERMI aims to increase the modelling and simulation speed that reduces design cycles from years to months, allowing the investigation of multiple design points to reach the optimal design to meet the design objectives - ultimately, a commercial fusion reactor. An efficient design cycle brings major benefits such as reduced costs, shorter schedules, avoidance of technical inconsistencies, and facilitating learning and innovation. The FERMI project started in March 2021, and it has assessed the individual simulation tools' performance that captures the relevant physics (neutronics-MCNP, thermal-hydraulics - OpenFoam, structural mechanics-Diablo) of nuclear fusion reactor blankets coupling them for the simulation of the multi-physics interactions. This work follows the precedent established by the Virtual Environment for Reactor Applications (VERA) for the simulation of Light Water Reactors (LWRs) through the Consortium of Advanced Simulation of LWRs (CASL) [7]. VERA is an effective tool for multi-physics coupling methods [8], and the expertise gained through developing VERA has been utilized to guide the development of FERMI.

1.1. Previous work and the FERMI features

Several commercial codes (ANSYS, StarCCM and others) and open-source codes (OpenFoam) are able to solve multi-physics simulations (fluid-dynamics, structural mechanics, heat transfer, MHD), yet they miss critical components necessary for the simulation of fusion reactor blankets, i.e. neutronics, plasma physics, plasma material interaction and two-way coupling. The simulation of all the physical phenomena involved is required to have a reliable analysis of fusion first wall and blankets, assess whether the fluid flow can

successfully remove the heat deposited by the plasma to maintain the structural components within their respective thermal constraints, breed enough tritium to sustain the fusion reaction, prevent plasma disruptions. The FERMI simulation environment has been built with single-physics codes coupled together. From a computational point of view, coupling single-physics codes may introduce limitations on stability, accuracy, and robustness with higher severity than each single-physics simulation [9]. This is because the single-physics codes for the multi-physics simulation were not initially developed to run in unison. Hence, particular code coupling strategies should be taken to perform such simulations so that the results make numerical and physical sense. The alternative to coupling single-physics codes is to construct one computer code (of course comprising multiple modules, sub-programs, and functions) which would solve all the relevant single-physics together in one shot. This is the philosophy behind "monolithic" coupling, which is guaranteed to resolve all relevant inter-dependencies of the single-physics. From a numerical methods point of view, a monolithic approach refers to constructing a single Jacobian to solve for all unknowns and resolving all inter-dependencies of every single-physics, and it is known as a tightly coupled approach. An example of tightly coupled technology is MOOSE (Multiphysics Object-Oriented Simulation Environment) [10] which harnesses modern HPC (high-performance computing) resources to achieve complex multi-physics simulations, and it has found widespread application in a wide range of engineering problems, including porous media, light water reactors (LWRs), coupled reactor physics simulations, nuclear fuels etc. Besides using a monolithic framework in some cases, MOOSE also uses multiscale modeling approaches to ensure tight coupling. However, its turbulence and MHD models are not suitable for fusion blankets [11]. Whereas a monolithic-type approach may be best from a physics standpoint, it is challenging to implement numerically. Considerable effort must be spent to develop strategies to construct a single Jacobian for all the single-physics, the resolution of which might vary in spatial and temporal scales adding further ill-conditioning of the numerical system [9]. Also, some of the single-physics may not have significant inter-dependency with another, thereby rendering such a tightly coupled numerical method not necessary. Such couplings are referred to weakly coupled systems and mathematically translate to negligible off-diagonal Jacobian entries compared to their diagonal counterparts. Due to these limitations of monolithic coupling, partitioned multi-physics simulations have become attractive over the years [12]. Partitioned multi-physics simulations created a new paradigm of coupling multiple individual scientific applications, each targeting their particular physics and characteristic length and time scales. This is also attractive since single-physics validated software for numerical simulations already exists and is developed and maintained by their respective developer's community. Many partitioned multi-physics simulations rely on the operator-splitting approach. Such approaches ignore strong couplings between single-physics codes and it may give unreliable numerical results [9]. The identification of these drawbacks has led to further developments in the field of partitioned multi-physics simulations to improve operator-splitting methods [13]. These include higher-order treatment of non-linearities, resolving truncation errors and using staggered time grids. Such techniques improve the accuracy of data transfer between single-physics simulations while reducing the numerical uncertainties involved. Alternatives to operator-splitting methods include Jacobian-free Newton-Krylov (JFNK) methods and approximate block Newton (ABN) methods [13]. JFNK methods use a linear decomposition of PDEs on a Krylov vector base to iteratively solve multiple Newton steps applied to a residual of the equations. Although most such methods are Jacobian free, they often require preconditioning for numerical stability and speedup. ABN methods offer the advantage to readily inherit from the development of existing solvers to seek modularity in the coupling. MOOSE uses the JFNK method to achieve monolithic coupling, while other coupling strategies such as SUNDIALS [14] and Trilinos [15] use methods similar to ABN. These offer extensive capabilities for a wide range of solvers and algorithms for coupled simulations. However, keeping with the recent push towards fully partitioned multi-physics simulations [12], the chosen software for FERMI is preCICE (precise Code Interaction Coupling Environment) [16] which is an open-source coupling library that follows a peer-to-peer approach. It allows for the high flexibility needed to keep an efficient time-to-solution for complex multi-physics scenarios and has proven scalability on 10,000s of MPI ranks [16]. The peer-to-peer approach allows existing software for single-physics simulations to be coupled through this library with minimal modification of each software. The additional requirement is an adapter, a code to

communicate data from the single-physics solver with preCICE, which development depends on the knowledge of the solver and the appropriate library calls. The resulting software framework simulates each physical aspect (plasma, neutronics, flow and solids) together with the respective codes exchanging information through preCICE during run-time: MCNP (Monte Carlo N-Particle) code [17] for neutronics simulations, OpenFOAM [18] for thermal-hydraulic simulations and the Diablo code developed at Lawrence Livermore National Laboratory (LLNL) for solid mechanics [19]. While preCICE already includes high-order non-linearity treatment and resolution of truncation errors, time-interpolation implementations are underway [20] to allow the use of staggered temporal grids. A new volumetric coupling capability for preCICE was developed and it is shown next.

The workflow for FERMI is shown in Figure 3a. The required grids for the computational solution are generated by Cubit (for neutronics and structural mechanics) and Ansys' ICEM-CFD (for thermal-hydraulics). The neutronics and shielding calculations are performed by MCNP to calculate tritium breeding and the energy deposition (due to neutrons and gamma rays). This energy deposition is mapped onto the grid for thermal-hydraulics and structural mechanics respectively through preCICE. Coupled simulations are performed between OpenFOAM and Diablo through preCICE to resolve fluid-structure interactions (FSI) and conjugate heat transfer (CHT) between the fluid parts (molten salt cooling channel and blanket) and the solid parts (first wall, vacuum vessel etc.). At the end of the simulation, tools such as Paraview and others (Tecplot, Cubit, Visit, etc.) are used to visualize the results. The capabilities of FERMI are tested for the ARC (affordable, robust, compact) reactor [2], which is described next

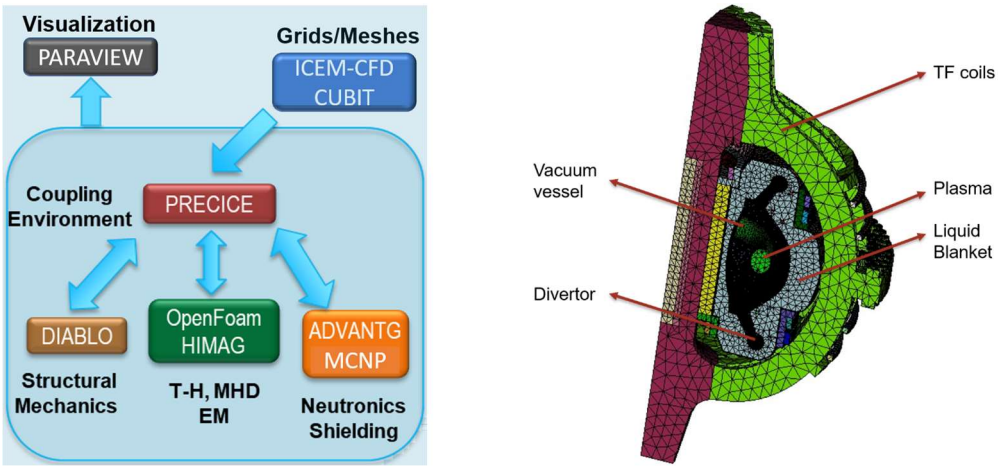

Figure 3. (a) Envisioned FERMI workflow (b) CAD Model of the ARC reactor with tetrahedral mesh for testing of FERMI workflow

1.2. The ARC reactor and its simulation

The FERMI multi-physics environment is tested with the simulation of the fusion reactor ARC first wall and blanket [2]. ARC is a 200-250 MWe tokamak reactor with a major radius of 3.3 m, high-temperature rare Earth Barium Copper Oxide (REBCO) superconducting toroidal field (TF) coils with an on-axis magnetic field of 9.2 T. The main innovation of ARC is that it contains a single, replaceable vacuum vessel and a fully liquid immersion blanket (LIB) of slowly flowing Fluorine Lithium Beryllium (FLiBe) molten salt. Further details of this reactor can be found in [2] and [21]. Figure 3b shows a sectional view (90 degrees) of the ARC reactor with its various components. The plasma, contained by the TF coils, is surrounded by the vacuum vessel with the first material layer facing the plasma, the first wall, made of

Tungsten (W). The structural component of the vacuum vessel is made of Inconel-718 and cooled by a channel (about 2 cm thickness) of FLiBe. The vacuum vessel is "immersed" in the "Liquid Immersion Blanket" which has a cooling and tritium breeding capacity. The divertors are positioned at the bottom and top of the vacuum vessel. The over-arching goal of FERMI is to simulate these individual components to assess the feasibility of the ARC design and guide future design iterations. Section 2 discusses the simulation results of the ARC reactor using the single-physics codes described above. One-way coupling is performed between the neutronics-gamma rays heat deposition and the thermal-hydraulic calculations of FLiBe as a coolant. In Section 3, the approach to multi-physics coupling is discussed using the preCICE software. Current capabilities and advancements are discussed in detail. Section 4 discusses learnings from the activities presented here and the future work planned for FERMI.

2. SINGLE-PHYSICS SIMULATIONS OF THE ARC REACTOR

As the first step of building a multi-physics simulation environment, each single-physics code must be tested and assessed. First, neutronics simulations are performed to evaluate the heat deposited by the neutrons and gammas on the blanket. Next, thermal-hydraulic simulations are performed on the FLiBe flowing in the blanket as well as the cooling channel inside the vacuum vessel. The CAD model is obtained from the developers of the ARC reactor concept, and it is used to generate the meshes for the neutronics and the thermal hydraulics as described in the respective sections below. Figure 4 shows the current workflow adopted for FERMI, i.e., the coupling of neutronics and thermal-hydraulics in a 10-degree CAD model of the ARC reactor. The CAD model is used to compute the neutronics heat deposition, which is then transferred to the thermal-hydraulic OpenFoam solver. For the thermal-hydraulics simulations, only the FLiBe sections of the CAD model are used. Figure 4 shows a coarse CFD model (25000 cells) which was used for initial estimates, while Section 2.2 discusses refinements.

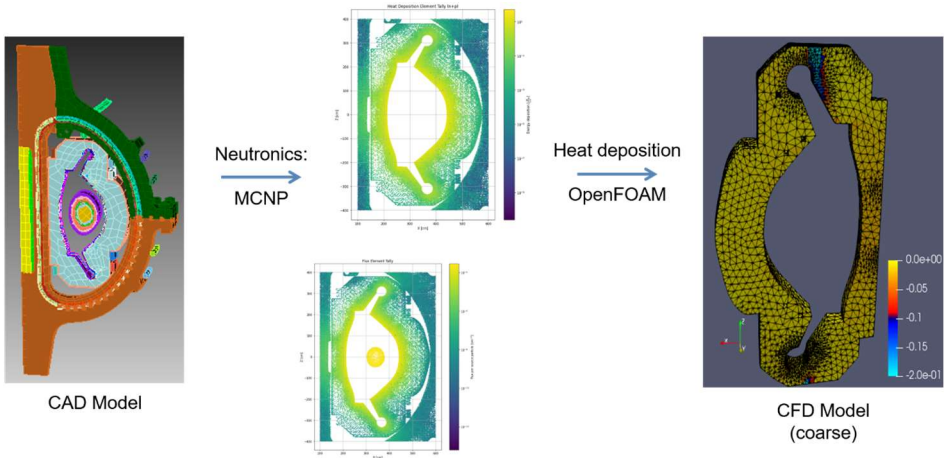

Figure 4. Workflow for First Coupled Physics Simulation: CAD model shows different materials of the ARC reactor in different colors. The MCNP output shows heat deposition (top, W/cm^3) and flux per source particle (bottom, cm^{-2}). The OpenFOAM model shows flow velocity (m/s).

2.1. Neutronics

The Deuterium-Tritium fusion reaction generates 14.06 MeV neutrons. Most of the reactor's energy output comes from the neutrons' interaction with the material, such as neutron and gamma heat loading. Therefore, accurate analysis of the neutronics of the fusion reactor is a crucial starting point for the fusion reactor

multi-physics analysis. There are four important neutronics metrics for the ARC fusion reactor: (1) tritium breeding ratio, (2) energy deposition, (3) high-energy neutron fluence, and (4) shutdown dose rate. For the interest of multi-physics coupling, only the energy deposition values are passed to the other codes. Detailed results and explanations of the other metrics will be published in future publications. For this work, a state-of-the-art code suite of Attila4MC [22] and MCNP is used to perform the high-resolution neutron transport calculation on the ARC fusion reactor geometry. The original Computer Aided Design (CAD) model of the ARC reactor is provided by CFS, which is then cleaned up by ANSYS SpaceClaim (https://www.ansys.com/products/3d-design/ansys-spaceclaim) and exported to a Parasolid file. The Parasolid file is imported by Attila4MC to generate an unstructured tetrahedral mesh (UM) and exported as an Abaqus file. The resulting Abaqus file is used in the MCNP 6.2 UM transport calculations. The MCNP 6.2 UM transport calculation outputs not only cell-averaged tallies but also tetrahedral mesh tallies. For metrics that do not require a fine spatial resolution, such as tritium breeding ratio and structural material fluence, cell tallies are used. For the energy depositions, tetrahedral mesh tallies are used for coupling with OpenFOAM. A coupled neutron-photon transport case is run, where the 14.06 MeV neutron source is placed as a uniform, isotropic volumetric source to where the plasma would be. There are different ways to model the neutron source, and future work is planned to perform a sensitivity analysis of fusion neutron source modeling. The Evaluated Nuclear Data File (ENDF)-B/VII.1 data libraries [23] are used for the calculation. The tetrahedral energy deposition mesh tallies (`F6 tallies') are in units of MeV/g. The value for each mesh is then multiplied by the density of the material and then multiplied by the number of neutrons emitted per second for the ARC reactor power level of 525 MW. The resulting value is energy deposition per volume per second or W/cm^3-s. A 2d-cutaway of the derived power deposition is shown in Figure 5. This processed result is collected to a machine-readable format and sent to OpenFOAM as input. The energy deposition per volume per second are similar to the values reported in other ARC reactor simulation reports [24].

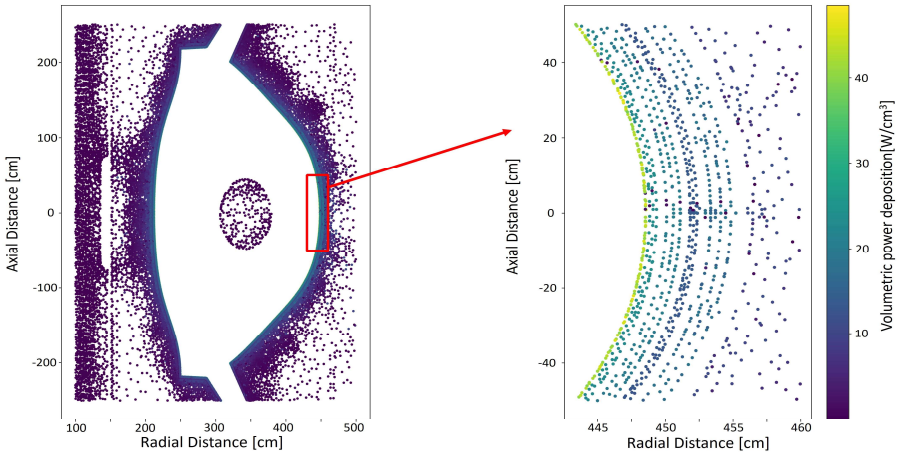

Figure 5. 2D cutaway of the derived ARC reactor power deposition. x=0 and z=0 is the center of the reactor. The image on the right is the zoomed in image of the left images' red box. The dots denote the centroid location of the tetrahedral mesh.

2.2. Thermal Hydraulics

Thermal-Hydraulics simulations of the LIB and first wall cooling channel is performed using the open-source CFD software OpenFOAM which is based on finite-volume discretization of the Navier Stokes equations with robust capabilities for simulating engineering flows, including effects of MHD and heat transfer in blankets of nuclear reactors [25]. For the simulations of the incompressible flow of the molten

salt FLiBe, the *buoyantPimpleFoam* solver is used, which accounts for heat transfer and uses a simple PISO (Pressure Implicit with Splitting of Operators) scheme. Currently, constant density simulations are performed with variable density (invoking the Boussinesq approximation) and MHD effects reserved for later. The discretization schemes used are the *limitedLinear* and *Euler* schemes for spatial and temporal discretization, respectively. The former is a second-order linear scheme in most regions and approaches an upwind scheme in regions of rapidly changing gradient, while the latter is a first-order backward scheme. The standard k-epsilon RANS turbulent model is used for the simulation. This is the most basic and widely used RANS turbulent model which was used to assess its performance in simulation fusion reactor blankets. Other models will be tested as a part of future work. In the following paragraphs, the grid design, flow parameters and results are discussed for this first analysis of the LIB of the ARC reactor.

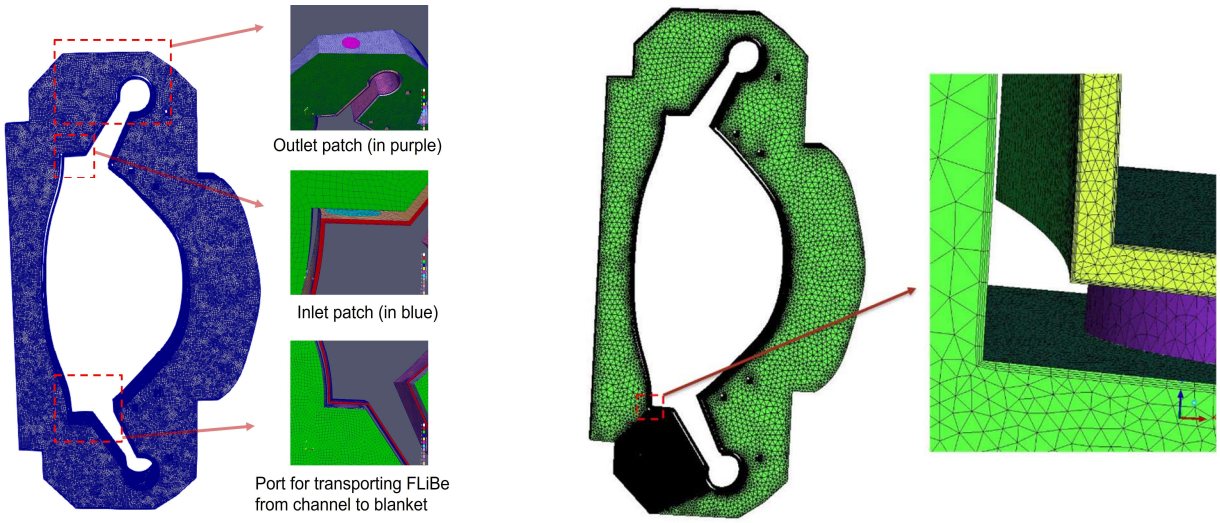

Figure 6. Fine grid CFD simulations of 10^{O} ARC reactor model: (a) 2.2 M cells (b) 3.4 M cells

The CAD model described in Section 2.1 is cleaned up using Cubit to remove the volumes of the model not required for CFD simulations. The coarse CFD mesh (25000 cells) of the LIB shown in Figure 4 is taken from the blanket part of the mesh used for neutronic simulations (by MCNP). As a first step, CFD simulations are performed on this coarse mesh by defining an inlet (at the top face) and an outlet (at the bottom face) for the flow of FLiBe. After initial testing and discussions with the designers (from MIT and CFS) of the ARC reactor, a better CFD model was developed, as shown in Figure 6a. A much finer grid of 2.2 million hexahedral cells was constructed using ANSYS ICEM-CFD for the blanket and the cooling channel of the vacuum vessel. Additional patches were added for inlet (to the cooling channel) and outlet (top of the blanket) and a port to transfer flow from the channel to the bulk blanket. Thus, the flow in the channel enters through the inlet patch and bifurcates into two streams, one moving down the channel to the port and the other initially moving up along the top divertor and then moving down to complete the loop and exit the channel through the port. The flow in the blanket is primarily upward towards the outlet. Initial simulations showed that the flow through the channel was quite turbulent, and a jet-type flow was formed downstream of the port in the blanket while the upward flow in the blanket was only mildly turbulent (see Figure 7a). These led to a better design of the mesh (Figure 6b) comprising 3.4 million cells. Although the mesh is made coarser in the bulk blanket, the total mesh count increased primarily because of the grid refinement near the port and the additional boundary layer cells at all walls. Other segments of FLiBe flow for divertor cooling [21] are not implemented yet, and they are reserved for future simulations.

Table I. Properties and Inlet Conditions of FLiBe

Physical Quantity	Symbol	Units	Value
Density	ρ	kg/m^3	1940
Specific heat capacity	c_p	kJ/kg-K	2.4
Thermal conductivity	k	W/m-K	1.0
Viscosity	μ	mPa-s	6.0
Inlet area	A_{in}	m^2	0.07
Inlet velocity	V_{in}	m/s	2.0
Inlet temperature	T_{in}	K	800.0

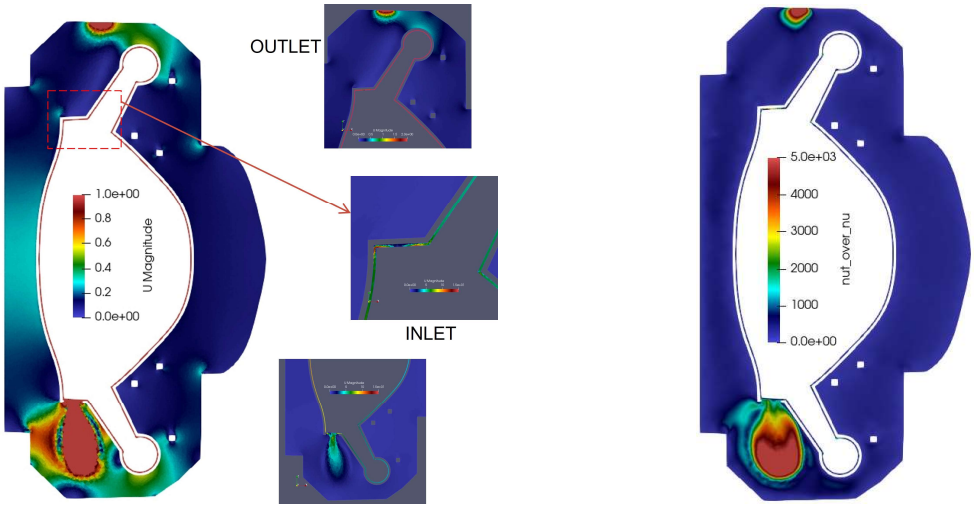

Figure 7. (a) Velocity Magnitude in different parts and (b) turbulent viscosity normalized by fluid kinematic viscosity from CFD simulations of the ARC reactor blanket and cooling channel

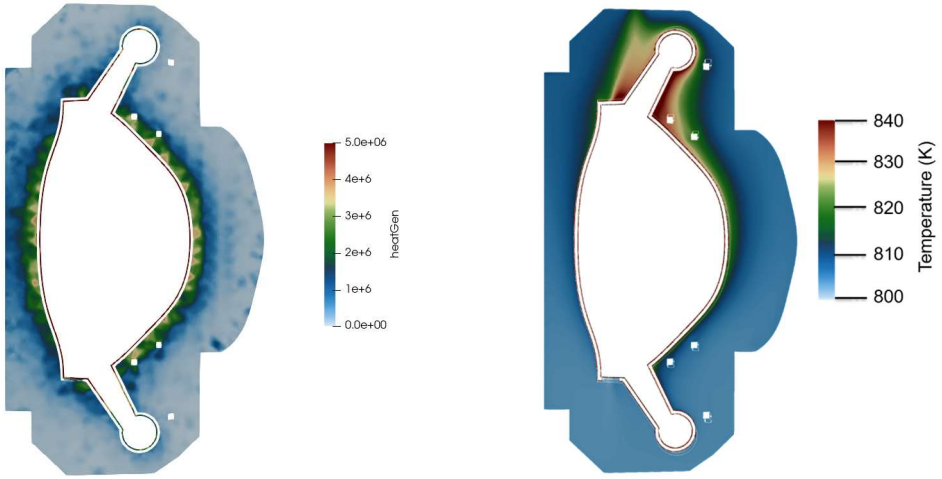

Figure 8. (a) Heat deposition (W/m^3) and (b) temperature (K) of FLiBe from CFD simulations of the ARC reactor blanket and cooling channel.

Once the grid is generated, the heat deposition from the neutronics needs to be input to the CFD model to perform the simulations. This heat deposition is added as a heat source term in the energy equation of the solver as a one way coupling. Interpolations need to be performed since different meshes are used for the neutronics and the CFD. This is done using the *mapFields* feature of OpenFOAM, which maps the volumetric heat generated data from the grid used for neutronics to the mesh generated for CFD. Next, the inlet conditions of the FLiBe, the boundary conditions at the walls and the thermophysical properties of FLiBe are specified before performing CFD simulations. Table I shows the thermophysical properties of FLiBe obtained from [26] and the inlet conditions from [24]. At the wall, no-slip boundary conditions are set with constant wall temperatures at the cooling channel wall (850 K), inner vacuum vessel (900 K) and outer vacuum vessel (1000 K). Cyclic boundary conditions are used at the two faces of the 10-degree mesh, i.e., flow leaving/entering one face enters/leaves through the other one to maintain conservation of mass, momentum, and energy.

Figure 7a shows the flow of FLiBe through the cooling channel and into the blanket. The cooling channel is significantly smaller in dimension as compared to the blanket; hence, the flow velocities are higher (reaches a maximum of 20 m/s). This causes the flow to be significantly turbulent, thereby causing effective heat removal from the first wall and inner vacuum vessel components. The flow in the blanket is very mildly turbulent except downstream of the port and near the outlet. The normalized turbulent viscosity (Figure 7b) shows a lack of turbulence in the blanket, which reduces the heat transfer, as noticed by the high temperatures near the upper divertor in Figure 8b. These are regions of potential design improvement to be investigated later in the project. Figure 8a shows the heat deposited (in W/m^3) in the FLiBe from the neutronics simulation and interpolated onto the CFD mesh. The temperature field of FLiBe shows significant heating up in the channel and near the upper divertor leg in the blanket. Since experiments for the validation of these simulations are not available, a global energy balance analysis was performed to assess the correctness of the CFD results. The total mass flux specified at the inlet was $\dot{m} = \rho A_{in} V_{in} = 1940 * 0.07 * 2 = 271.6\, kg/s$. The outlet mass flux was found to be within machine error (<0.01%) of this value. The total heat deposited from neutronics on the FLiBe was found to be $P_n = 7.98\, MW$. The CFD simulation was post-processed to calculate the total heat transfer at the walls due to the constant temperature boundary condition. This was found to be $P_{ht} = 1.56\, MW$. For perfect energy balance, this would mean a total temperature rise of FLiBe (from inlet to outlet) of $\Delta T_{peb} = (P_n + P_{ht})/(\dot{m} c_p) = 14.63\, K$. The rise in FLiBe temperature obtained from the CFD simulation was found to be $\Delta T_{cfd} = 14.49\, K$ (~ 0.96% error). For the other two meshes tested, the error percentages obtained were 3.1% for the coarse (25000 cells) mesh and 1.4% for the first fine mesh (2.2 million cells). This error is quite small, but it could be attributed to approximate wall heat transfer models (a constant turbulent Prandtl number 0.85 is used). Here only conductive and convective modes of heat transfer in FLiBe are modeled and studied. The high temperatures (maximum of about 1000 K) in FLiBe could lead to relevant radiative heat transfer; this is a topic of active research, and it is found that radiative heat transfer in molten salts such as FLiBe is more important for laminar flow than turbulent flow [27]. This fact combined with the finding that the total Nusselt number is within 10% for radiation and no-radiation simulations [28] in idealized conditions for FLiBe flow, suggests that radiation mode will be suppressed for the turbulent flow regions in the present case. Further, there are uncertainties in the turbulence-radiation interaction phenomenon for molten salts, especially in how it affects the absorption spectra. These studies are reserved for future investigation.

3. MULTI-PHYSICS COUPLED SIMULATIONS

This project uses and develops preCICE for all multi-physics inter-code coupling. Hence, a brief introduction to the preCICE open-source coupling library is provided here. The coupling library preCICE is written in C++ with additional bindings for C, Fortran, Python and Matlab. Figure 9 shows a schematic of the coupling interface of preCICE. The green box in the middle represents the coupling library with

included features such as coupling schemes (explicit and implicit coupling with sub-cycling as well as serial and parallel), data mapping schemes (nearest neighbor, nearest projection, and radial basis functions) and communications (consistent and conservative). To couple a solver through the preCICE libraries, a few function calls need to be made to the library using a piece of code called "adapter". The adapter is written in the same language as the code being coupled and depends mainly on the characteristics of the code coupled rather than with preCICE. This makes preCICE a largely non-intrusive coupling platform, ideal for partitioned multi-physics simulations. Adapters for some open-source codes (OpenFOAM, CalculiX etc.) are already available through preCICE, while those for in-house solvers or other commercial solvers can be written. In this section, two new enhancements of the preCICE software are presented – volumetric coupling and Diablo – OpenFOAM coupling.

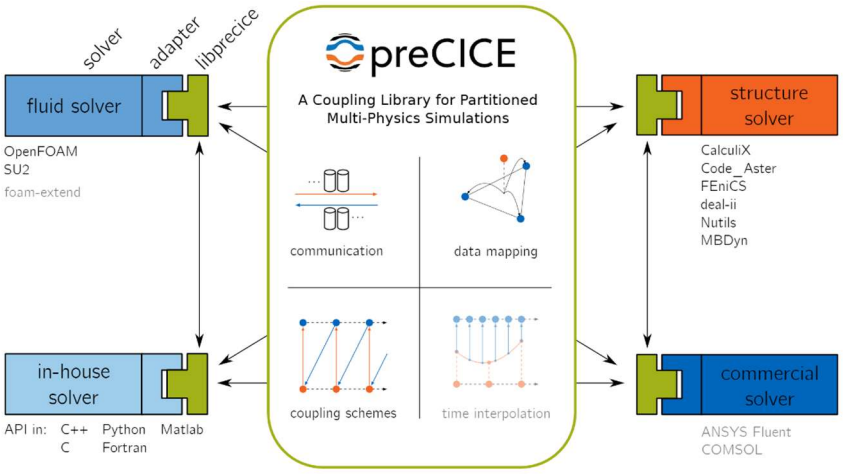

Figure 9. preCICE coupling library (reproduced from [15])

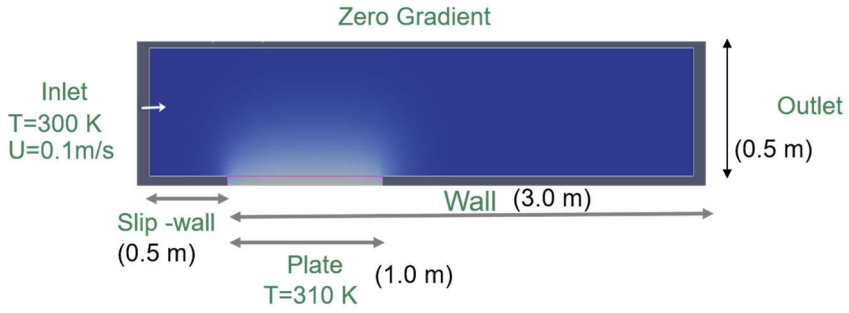

Figure 10. Test case for volumetric coupling: flow over a heated plate

3.1. Volumetric coupling

The preCICE library was developed for surface coupling of multiple solvers. For the purposes of FERMI, the volumetric coupling has been added to the OpenFOAM adapter and tested on sample problems. The sample problem selected for testing the volumetric coupling is the flow over a heated plate test problem from the preCICE tutorial cases, shown in Figure 10. The flow inlet and outlet are perpendicular to the plate, a part of which is at a temperature higher than the incoming flow. The dimensions of the plate are

shown in black in brackets with flow and boundary conditions in green. The flow is laminar and requires solving the Navier Stokes equations and the energy equation to simulate the flow field and temperature field of the channel. This problem can be solved using the *buoyantPimpleFoam* in-built solver (transient and incompressible) in OpenFOAM, which solves the above equations using the PISO scheme discussed previously. The fluid properties used are - kinematic viscosity $\mu = 0.0002\, kg/ms$, density $\rho = 1\, kg/m^3$, specific-heat capacity $c_p = 5000\, kJ/kgK$ and Prandtl number $Pr = 0.01$.

To demonstrate the new volumetric coupling capability for the OpenFOAM preCICE adapter, the *buoyantPimpleFoam* solver is split in *flowSolveFoam* and *energySolveFoam,* which solve the Navier Stokes equations and the energy equations separately (and respectively). After the solvers are split up (details provided in the next paragraph), the preCICE adapter with volumetric coupling is used to transfer information between the two solvers to simulate the flow and temperature field. These fields from the separate solvers coupled through preCICE are compared with the single in-built OpenFOAM solver (*buoyantPimpleFoam*) to ascertain the effectiveness of preCICE's volumetric coupling capabilities. This capability is tested for both one-way coupling and two-way coupling. The coupling approaches are dictated by the relevant physics, which needs to be resolved. For example, for the flow criterion discussed above, i.e., with constant density, the hydrodynamics and thermodynamics are loosely coupled and solved sequentially. However, if temperature-dependent density is used, the hydrodynamics and thermodynamics are tightly coupled, and a two-way coupling approach needs to be used when using separate solvers for the two. For the two-way case, a Boussinesq approximation for the variation of density is used, given by, $\rho(T) = \rho_0[1 - \beta(T - T_0)]$, where the reference density $\rho_0 = 1.0\, kg/m^3$, reference temperature $T_0 = 300\, K$ and the thermal expansion coefficient is $\beta = 0.001\ kg/m^3\, K$.

The splitting of the solver is shown in Figure 11, where the no coupling solver shows the monolithic OpenFOAM in-built solver and the steps within to simulate the flow and energy fields. The next two schematics show the one-way coupling and two-way coupling approaches, respectively. The solvers *flowSolve* and *energySolve* are created by splitting up the Navier Stokes solver part and energy equation solver part of the monolithic solver *buoyantPimpleFoam*. For the one-way coupling, at every time step, the hydrodynamics solver is executed first, and the preCICE coupling libraries are used to transfer the velocity field to the thermodynamics solver, which uses the velocity field to solve for the transport equation for energy and outputs the temperature field. During two-way coupling, the two solvers iterate between themselves by sharing the velocity field from the hydrodynamics solver to the thermodynamics solver, evaluating the energy equation to solve for temperature and update the density based on the Boussinesq approximation. This updated density is then communicated back to the hydrodynamics solver using the preCICE libraries. The iteration continues a few times in each time step before convergence is reached between the values communicated between the solvers. This allows comparison of results from the one-way coupled solvers' predictions with the solver with no coupling for the constant density case and the two-way coupled solvers' predictions are compared with no coupling for the case with Boussinesq density.

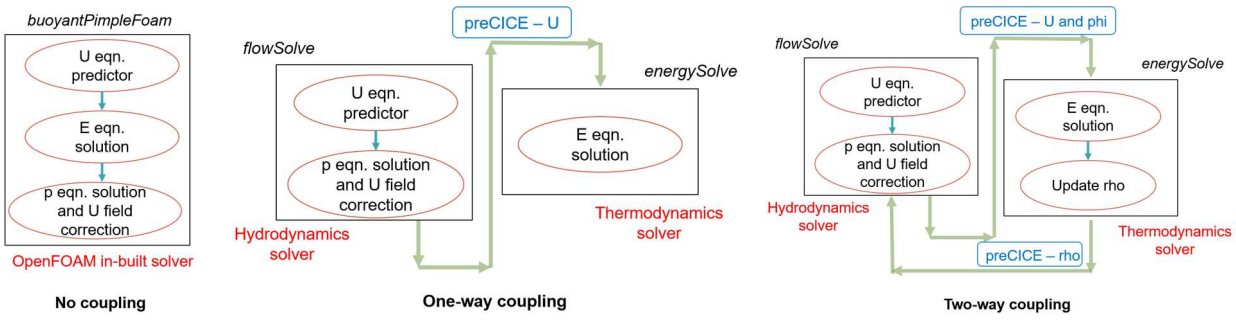

Figure 11. Splitting of OpenFOAM solver for coupling with preCICE

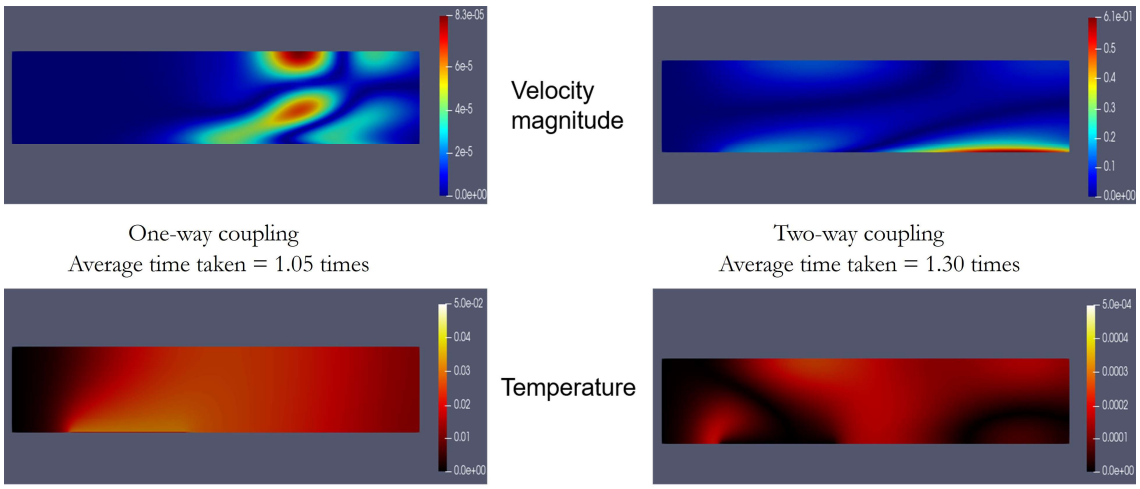

Figure 12. Differences (L1 norm) in velocity (top) and temperature (bottom) for one-way (left) and two-way (right) coupled simulations calculated against their respective no-coupling simulations, i.e., constant density for one-way coupling and Boussinesq density for two-way coupling.

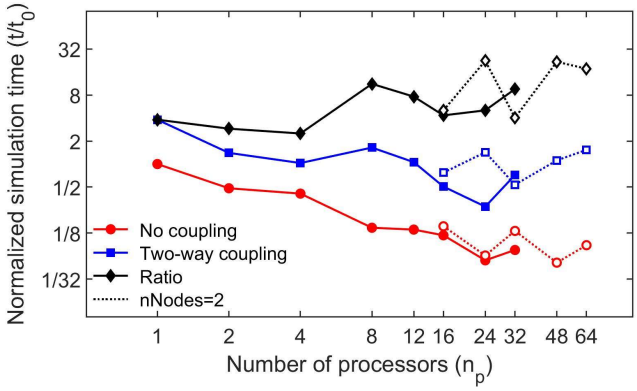

Figure 13. Simulation time (normalized by serial simulation time of no-coupling case) vs number of processors for two-way coupled turbulent flow case simulated with 313,803 cells.

The results for the simulations with and without preCICE are shown in Figure 12. These simulations were performed on ORNL clusters that use Intel(R) Xeon(R) Silver 4100 CPUs at 2.10 GHz. There are 32 processors per node with processor MHz varying between 800-2100 and a cache size of 12MB. The differences in results are small, with less than 0.05% error for all cases except for the velocity magnitude of the two-way coupled case, which shows regions of error up to 0.6%. The time for one-way coupling is 5% higher than the no-coupling case and 30% higher for the two-way coupling case. Presently, on-node performance was tested, and the preCICE coupling scaled exceptionally well up to 32 processors with the execution time staying between 24 - 32 % higher (for the two-way coupling case) than the corresponding no coupling simulation on the same number of processors. This is because, for two-way coupling, there needs to be a few iterations between the solvers per time-step. After the simulations of laminar flow and heat transfer, turbulent simulations were performed for the same case by increasing the inlet flow velocity to 10 m/s. The grid size was increased (from 12k cells for the laminar flow to about 300k cells for turbulent flow) to accommodate the requirement for higher resolutions with the simple k-ϵ turbulence model. The simulation times are shown in Figure 13 and they show that while the computational time increases significantly for the coupled simulations using preCICE, a good scaling with the number of processors is

observed. The additional parameter in the two-way preCICE coupling data transfer was the turbulent thermal conductivity which is calculated on the hydrodynamics solution side and passed to the thermodynamics solution side to resolve the increased heat transfer due to turbulence. Initially, a tightly coupled scheme with data transfer at every time step showed coupled simulation time increased almost 30 times on a single node with multiple processors (up to 32). This was reduced to about 5-10 times (as shown in Figure 13) by exchanging information every 10 time-steps and performing iterations (on average, two were required for convergence). The increase in computational time on multiple nodes (two in this case) will be studied in detail later, and the effect of different coupling schemes, under-relaxation strategies and partitioning schemes offered by preCICE are being tested to improve this.

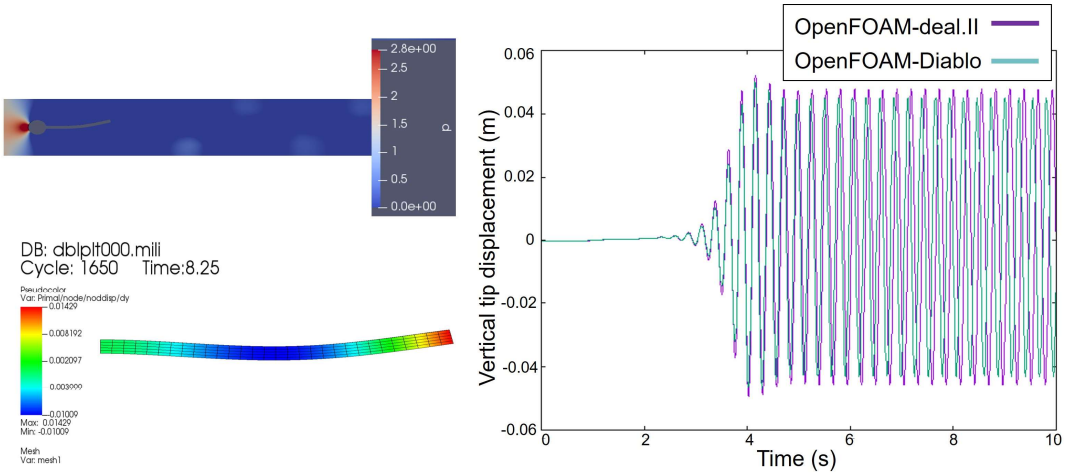

Figure 14: OpenFOAM-preCICE-Diablo coupling for simulation of Turek FSI problem: (top-left) pressure field from OpenFOAM (bottom-left) vertical displacements from Diablo (right) comparison of tip displacement time-history from OpenFOAM/Diablo and OpenFOAM/deal.II simulations using preCICE surface coupling

3.2. OpenFOAM-preCICE-Diablo surface coupling demonstration

As a first demonstration step for the coupling capabilities of preCICE, OpenFOAM and Diablo have been coupled through surface coupling. While the OpenFOAM adapter is maintained by preCICE developers, the Diablo adapter for preCICE was developed to demonstrate parallel coupling via surface exchange of surface displacements and pressures, using an OpenFOAM adapter modified to communicate via surface pressures. The resulting code was validated on the well-known Turek benchmark [29] and compared against the OpenFOAM-preCICE-deal.II results [30]. Figure 14 shows the results from the coupled simulation. The pressure from the OpenFOAM simulation is passed to Diablo via preCICE libraries, and the point displacements calculated from Diablo are passed back to OpenFOAM to update the OpenFOAM mesh. This communication is performed at every time step of the solvers to achieve a tight coupling. This results in the prediction of the tip displacements, also shown in Figure 14, which shows good agreement with the OpenFOAM-deal.II coupling results. This shows that surface coupling between OpenFOAM and Diablo is complete using preCICE. Currently, it is being extended to coupling of heat transport parameters such as temperature and heat flux to enable performance of conjugate heat transfer simulations (CHT). In addition, the volumetric coupling developed via preCICE (as discussed in Section 3.1) for OpenFOAM will be extended to Diablo to enable solid mechanics calculations which include volumetric effects from neutron and gammas (for both neutron heating as well as radiation-induced creep and damage) and forces from MHD effects.

4. CONCLUSIONS AND FUTURE WORK

This paper introduces the FERMI project and its current status. FERMI is a muti-physics simulation environment under development for three-dimensional simulation of fusion reactor blankets. The goals of FERMI are to provide efficient and accurate first wall and blanket simulations to speed up fusion reactor design cycles and to increase reactor performance. Neutronics coupled with CFD and thermal simulations of the conceptual ARC reactor are presented on different meshes, appropriate for the respective physical resolution; in particular, neutronics heat deposition evaluated using MCNP has been transferred to OpenFOAM for thermal-hydraulic simulation of the FLiBe in the cooling channel and blanket of ARC. It is found that this one-way coupled simulation can provide important information about the flow of FLiBe, hot spots in the blanket and the effectiveness of the liquid immersion blanket concept. These learnings will be used for further parametric analysis (variable inlet dimension, inlet velocity, inlet temperature, turbulence models, etc.) to assess optimum engineering design conditions. One of the significant limitations identified for performing simulations of fusion blankets is the lack of experimental validation data. In order to circumvent this issue, until new experimental facilities are constructed, large-scale scale-resolving simulations such as large-eddy simulations (LES) with higher-order discretization schemes in space and time may be sought. This would yield reliable data and allow better analysis of flow configurations. The preCICE coupling library has been tested and further developed, proving its capability of performing partitioned multi-physics simulations. The OpenFOAM-Diablo coupling through preCICE has been demonstrated and will be further exploited. The additional capability of volumetric coupling has been included in the OpenFOAM adapter and demonstrated to show good accuracy and good scaling for parallel simulations. Current and on-going tasks of the FERMI project include:

1. CFD simulations with Boussinesq approximation for more realistic physics of FLiBe with temperature-dependent thermophysical properties [31].
2. Parametric simulations and optimization of the ARC design using reduced-order models
3. Incorporation of MHD effects and MHD turbulence models (such as [32])
4. Further testing and scalability studies of preCICE's volumetric coupling capabilities
5. Two-way coupling (surface and volumetric) of Diablo, MCNP and OpenFOAM using the preCICE libraries

Initial FERMI simulations already show the contributions it can make in informing design choices. It is expected that the FERMI code simulation suite will expedite the design cycle of fusion reactors. FERMI addresses a present and future need in the fusion community in light of the ongoing CPP and ARC activities, and it can lead directly into product development in collaboration with members from the manufacturing sector. FERMI will deliver an innovative integrated first wall and blanket fusion reactor simulation environment with high-resolution representation on current and future computational platforms, creating distinct technological innovation and paving the way for a nuclear fusion power industrial revolution. The goals of FERMI leverage recent rapid advancements in computational hardware and software engineering.

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