Nuclear Engineering and Design 387 (2022) 111604

Contents lists available at ScienceDirect

Nuclear Engineering and Design

journal homepage: www.elsevier.com/locate/nucengdes

On the development of multi-physics tools for nuclear reactor analysis based on OpenFOAM®: state of the art, lessons learned and perspectives

Carlo Fiorina [a,*], Ivor Clifford [b], Stephan Kelm [c], Stefano Lorenzi [d]

[a] Laboratory for Reactor Physics and System Behaviour, École polytechnique fédérale de Lausanne - EPFL, Switzerland
[b] System Behaviour Group, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
[c] Nuclear Waste Management and Reactor Safety (IEK-6), Forschungszentrum Jülich, Germany
[d] Department of Energy, Politecnico di Milano, Italy

ARTICLE INFO

Keywords:
Multi-physics
OpenFOAM
Open-source

ABSTRACT

In the last two decades, the use of OpenFOAM as a multi-physics library for nuclear applications has grown from a sporadic use for exploratory studies to a widespread application for the analysis of innovative reactor concepts and highly complex problems. This review paper provides an overview of the past and current development efforts in the field and summarizes some of the lessons learned during 10 years of R&D activities participated by the authors. The objective is to provide readers with an understanding of the benefits and challenges of this approach, thus facilitating an informed decision about its potential adoption for future studies.

1. Introduction

Modelling and simulation (M&S) has been an irreplaceable means to support reactor design and licensing for decades, as well as an increasingly central tool for research activities. The role of M&S is strengthened today by the growing availability of computational resources and by the relentless progress in the field of computational science, to the point where design-by-simulation has become a dominant paradigm in engineering. In the nuclear field, this trend is also favored by the large cost and licensing problems associated with new experimental facilities. The recent flourishing of activities dedicated to the design of advanced nuclear reactors and fuels, as well as to the life extension of operating nuclear power plants, have further nurtured M&S with the need of novel, more flexible and more accurate simulation codes that can comply with new modelling requirements.

In this context, the nuclear community has worked intensively towards a modernization of the available toolset. Large efforts have been directed towards improving existing legacy codes, including the coupling between some of these codes for multi-physics simulations. This allows decades of code validation and calibration to be built upon, while benefitting from an already solid user community. On the other hand, relatively few of these codes have incorporated modern programming best practices in their development and their modernization from this viewpoint requires considerable resources and time, with uncertain results in terms of overall code quality and High Performance Computing (HPC) capabilities. For these reasons, some developers have opted for writing new codes based on available numerical libraries for scientific computing, instead of writing codes from scratch or adapting existing legacy codes. Many of these libraries make available almost all the tools required for modelling physical systems, ranging from pre-processing (e.g., geometry and mesh creation) to the discretization and the solution of partial or ordinary differential equations (PDEs, ODEs), and to the post-processing (results visualization and output handling). The code developer can then rely on a tested, well-maintained, proven toolkit and focus on model development, without necessarily having to deal with issues associated with numerics, data handling, post-processing, etc. An additional strength of these libraries is often their object-oriented programming approach, which allows one: to quickly develop new solvers and routines; to reduce maintenance efforts; and to streamline code sharing. The developed solvers can also benefit from state-of-the-art features in terms of methods and parallel scalability. This paradigm brings advantages not only to code developers but to the entire community represented by users and "non-professional" developers (e.g., MSc or PhD students in academia or casual developers), generating more inclusion in the code creation process, feedback in debugging and error reporting, and awareness. A well-known example of this kind of development strategy in the nuclear context is the MOOSE platform (Gaston et al., 2009), which has been

* Corresponding author.
E-mail address: carlo.fiorina@epfl.ch (C. Fiorina).

https://doi.org/10.1016/j.nucengdes.2021.111604
Received 12 March 2021; Received in revised form 26 November 2021; Accepted 28 November 2021
Available online 23 December 2021

developed based on the libMesh open-source finite element library (Kirk et al., 2006). Other non-nuclear examples of numerical libraries include e.g., FeniCS (FeniCS, 2021), Elmer FEM (Elmer FEM, 2021), GetFEM (GetFEM, 2021), and FreeFEM (FreeFEM, 2021).

In this context, OpenFOAM (Open Field Operation And Manipulation) (OpenFOAM Foundation, 2021; OpenFOAM, 2021) has started gaining attention for its multi-physics capabilities. This library was initially developed, and it is still distributed, as an open-source toolbox for Computational Fluid Dynamics (CFD) applications. However, the underlying code has been conceived as a general, quality-assured library for the finite-volume discretization and parallel solution of partial-differential equations. It follows that several advanced solvers are available for single- and two-phase CFD applications, but also that new solvers can be developed for nuclear-specific applications like neutron-transport and fuel behavior. In this sense, OpenFOAM incorporates many favorable features such as a sound numerics, a massive parallel scalability, an easy-to-use high-level application programming interface (API), and an intuitive discretization strategy such as the finite volume method. Thanks to its flexibility, OpenFOAM has been used in the nuclear community as a CFD software, as a multi-physics library for the study of conventional and non-conventional reactors, and as a tool for developing and quickly testing numerical methods and algorithms.

The objective of this paper is to provide an overview about some of the past and current activities on the use of OpenFOAM for nuclear reactor safety analysis; describe OpenFOAM main features; highlight some of the pros and cons of its utilization; and help providing some development directions. The focus is on the use of OpenFOAM for multi-physics applications in a nuclear context while a complete review on its applications and use as a CFD toolbox is beyond the scope of the work.

2. Historical overview

To the authors' knowledge, the first effort on the use of OpenFOAM as a multi-physics library in the nuclear field dates back to the PBMR project in South Africa in the early 2000s. At the time, OpenFOAM was envisaged as the underlying framework for a modern three-dimensional code system for the analysis of High Temperature Gas-cooled Reactors (HTGRs), VulaSHAKA, and the development efforts resulted in the first OpenFOAM-based neutron diffusion solver (Clifford and Jasak, 2009). This was later extended to the solution of the simplified P3 (SP3) equations (Clifford and Ivanov, 2010). Soon after, a multi-scale thermal-hydraulics solver was developed for the analysis of prismatic HTGRs (Clifford, 2013). Concurrently, significant research activities have been carried out on the use of OpenFOAM for the multi-physics analysis of fast-spectrum Molten Salt Reactors (MSRs) (Aufiero et al., 2014). These reactors feature a peculiar thermal-hydraulics, due to the internal heat generation, as well as a tight coupling between neutronics and thermal-hydraulics, due to the transport of the delayed neutron precursors in the liquid fuel. In this context, OpenFOAM provided state-of-the-art CFD solvers, and the possibility to easily include the equations for neutron diffusion and precursor transport along with the required modifications to consider the interactions among the different physics. It thus proved to be an ideal tool for the task and OpenFOAM-based solvers = became a choice of reference for the MSR community (Altahhan et al., 2020; Cervi et al., 2019a, b; Hu et al., 2017; Laureau et al., 2017; Wan et al., 2020; German et al., 2019). It was by building on the above-mentioned work described in (Clifford, 2013; Aufiero, 2014) that the GeN-Foam multi-physics solver was first developed for the analysis of both solid- and liquid-fueled reactors (Fiorina et al., 2015). The solver now includes sub-solvers for neutronics (diffusion, SP3, SN and point kinetics), thermal-hydraulics (single- and two-phase thermal-hydraulics, both porous and open medium), and core deformations.

By the time OpenFOAM solvers were being developed for MSR applications, first efforts had also been directed towards the development of solvers for neutron transport. In particular, solvers have been developed for discrete ordinates (Jareteg et al., 2014; Aufiero, 2014; Fiorina et al., 2014), simplified spherical harmonics (Fiorina et al., 2017; Clifford and Ivanov, 2010), and methods of characteristics (Cosgrove and Shwageraus, 2017). Thanks to the use of unstructured meshes, and to the moving-mesh features of OpenFOAM, these solvers turned out to be valuable assets for the investigation of non-traditional geometries (Introini et al., 2017) and advanced reactor systems (Laureau et al., 2018); as well as for evaluating expansion reactivity feedbacks in fast reactors (Fiorina et al., 2015; Fiorina and Mikityuk, 2015; Fiorina et al., 2019).

Significant efforts have also been dedicated to the development of solvers for reactor thermal hydraulics. In its standard distributions, OpenFOAM offers several solvers for detailed CFD, but only limited capabilities for coarse-mesh analyses (viz., porous medium and sub-channel approaches). To tailor OpenFOAM to the needs of nuclear reactor analysis, researchers have then started developing advanced porous-medium solvers. A first single-phase solver had been developed in (Clifford, 2013) for HTGRs, and subsequently extended for more general reactor applications (Fiorina et al., 2015). More recently, a two-phase porous-medium solver has been developed (Radman et al., 2021a, b; Radman et al., 2019). Work has also been performed to adapt standard CFD solvers to fluids with internal heat generation, as in the case of MSRs (Fiorina, 2019).

In Germany, a coordinated collaborative development has been initiated for an OpenFOAM-based simulation platform for Light Water Reactor (LWR) safety assessment in the framework of the Helmholtz Associations' NuSafe program, as well as of the German CFD-Alliance. Efforts have been primarily dedicated to thermal-hydraulics transients and two-phase flows in the reactor cooling system (Kliem et al., 2018), as well as to containment studies (Kelm et al., 2021) and combustion processes (Hasslberger et al., 2017), showcasing a potential use of OpenFOAM that goes beyond core design and safety analysis.

A recent activity has also been dedicated to the use of OpenFOAM for fuel behavior analysis. Born as an exploratory work on the use of finite volumes for the thermo-mechanical analysis of the nuclear fuel pin, the work has evolved towards a full-fledged fuel behavior solver including irradiation effects in multi-dimensional cases (Scolaro et al., 2020).

Besides the development of solvers for reactor analysis, OpenFOAM represents a formidable tool for the testing and development of new methodologies. The most evident examples are related to the application of projection-based Reduced Order Modelling to nuclear reactor analysis (Lorenzi et al., 2016; Lorenzi et al., 2017; German et al., 2019). In addition, activities have been carried out to couple OpenFOAM-based applications with other available codes. Well-known examples are the development of a multi-physics interface in the Serpent 2 Monte Carlo code (Leppänen, 2014), and the development of a coupling interface with the ATHLET system code (Herb and Chiriac, 2016).

The growing use of OpenFOAM in reactor applications goes hand in hand with a general trend towards an open-source collaborative development paradigm, which is increasingly perceived as an effective way to stimulate synergies, avoid duplication of work, involve a broader community, enhance verification, and, ultimately, accelerate innovation. In 2020, the 'Open-source Nuclear Codes for Reactor Analysis' (ONCORE) initiative was launched under the aegis of the IAEA aiming at the development and application of open-source multi-physics simulation tools in support of research, education, and training in nuclear science and technology (Fiorina et al., 2021; IAEA, 2021). In this initiative, OpenFOAM represents one of the main candidates to attain the long-term objective of a consistent open-source platform for the nuclear community.

3. Short summary of high-level features of OpenFOAM as a multi-physics library

3.1. Workflow

While several commercial products are available for managing and

streamlining the CFD simulation workflow of OpenFOAM, the code itself is not distributed with any graphical user interface. Cases are set up by modifying entries in specific input files (called dictionaries) and run via command line. In addition, both meshing and post-processing are performed with separate tools. It follows that pre-processing, running the code, and post-processing are configured as three distinct steps performed with different tools and with the overall process requiring a good familiarity with a Linux operating system. This results in a more transparent but significantly less streamlined workflow when compared to proprietary CFD and multi-physics tools that usually provide a comprehensive graphical interface that integrates the whole simulation workflow. In addition, while a professional tool like ParaView® is distributed with OpenFOAM for post-processing, mesh generation often calls for additional proprietary tools when complex geometries must be modelled. Documentation is also poorer than for proprietary tools and the underlying theory of many sections of the code is not always cleanly documented.

On the other hand, having access to an intuitive and well-encapsulated source code allows for a better understanding of solvers and it stimulates a workflow that tends to integrate software application and development. This provides users with a formidable tool for research and advanced applications. In addition, OpenFOAM users can benefit from a very large and supportive community, and from the extensive efforts that e.g. the ESI group has recently started dedicating to comprehensive documentation of the code.

3.2. Structure of the base library

OpenFOAM is a very complete library for the finite-volume discretization and solution of partial differential equations that also includes advanced algorithms e.g. for mesh-to-mesh projections, mesh deformation, mesh manipulation, etc. In addition, different from other libraries for continuum mechanics, it includes an extremely large set of broader functionalities, including for instance: methods for solving ordinary differential equations; Monte Carlo methods; octree-based mesh search; methods for reduced-order modelling; built-in and third-party code coupling schemes (e.g. (Bungartz et al., 2016)); etc. This makes it a powerful tool to develop multi-physics applications, as well as to develop and test new methodologies.

The library is written in C++ and takes full advantage of the programming language's object-oriented paradigm. In particular, a strong code encapsulation allows for local modifications of one functionality without affecting the others, which allows in turn for quick and error-proof developments. In addition, object-oriented programming has been used in OpenFOAM to create an API that allows users to operate at various levels of complexity, depending on their knowledge. At the highest level, users can set-up equations by using standard operators with an intuitive naming. For example, one may implement the following one-group neutron diffusion equation:

$$\frac{1}{v}\frac{\partial \varphi}{\partial t} = D\Delta\varphi + \left(\frac{\upsilon\Sigma_f{}^*(1.0-\beta_t)^*\chi_p}{k_{eff}} - \Sigma_r\right)\varphi + S_d\chi_d$$

as

```
fvMatrix<scalar>
(
fvm::ddt(inverseVelocity,flux)
=fvm::laplacian(D, flux)
+fvm::Sp(nuSigmaF/keff_*(1.0-betaTot)*chiPrompt -
sigmaRemoval,flux)
+delayedNeutronSource_*chiDelayed
);
```

where constants and variables can be created beforehand by using standardized constructors. At the same (solver) level, one can employ various other classes for instance to project fields between meshes. At a deeper level, one can modify and create *ad-hoc* boundary conditions, linear solvers, discretization schemes, etc. Further down in the code, one can even operate on the Message Passing Interface (MPI) parallelization. In all cases, encapsulation will make these modifications fully independent of the rest of the code.

3.3. Numerical aspects

The use of OpenFOAM for numerical simulations and as a base numerical library to develop new applications entails specific numerical choices, some of which carry significant impact on its use for nuclear engineering applications. Here below, we summarize some of the OpenFOAM features that mainly affect its modelling capabilities.

3.3.1. Finite volume discretization

OpenFOAM employs a finite-volume approach for the discretization of various operators, allowing for both explicit and implicit finite volume discretization of divergence, Laplacian, and source terms, as well as for an explicit discretization of gradients and curls. Finite volumes is a powerful discretization method and has the advantage of providing an intuitive understanding that facilitates use and developments from a large community. On the other hand, finite-volume methods are at most second-order, thus requiring relatively fine meshes. Besides, the optimal choice in terms of discretization methodology is strongly application-dependent, and finite volumes are not necessarily the optimal choice for all nuclear related applications.

3.3.2. Unstructured meshes

Use of unstructured meshes offers complete flexibility in terms of geometry, which in turns favors the use of OpenFOAM for the analysis of non-traditional reactor designs and complex geometries. On the other hand, it implies a significant computational footprint: in terms of memory requirements, since all topological information and intermediate quantities must be stored at all times; and in terms of computing time, since all this information must continuously be retrieved from the memory. Retrieval of information is often slowed down by the fact that information is stored in a relatively disordered manner, causing frequent cache misses that ultimately limit performances and call for expensive high-cache CPUs (Fiorina et al., 2018; Spisso et al., 2018). Another aspect that tends to make some OpenFOAM simulations computationally intensive is that OpenFOAM meshes are first order, with all cell faces that are flat. This requires a high mesh resolution to correctly capture curved surfaces.

3.3.3. Operator-splitting

For the moment, OpenFOAM only allows for a segregated approach for coupling different equations[1]. Operator-splitting has pros and cons with respect to matrix-coupled approaches. The main disadvantage is that achieving an implicitly coupled solution requires iterating the coupled terms, with potential instabilities and slow convergence rates. The advantages emerge instead in stiff multi-physics applications characterized by different time scales. With operator-splitting, it is normally much easier to precondition and solve single-equation matrices; it is possible to implement time sub-stepping to solve only for faster physics at certain time steps; and it is possible to selectively solve physics depending on their degree of convergence. This way, the developers have more flexibility in the strategic solving choices for complex multi-scale and multi-physics problems.

3.3.4. Parallelization

OpenFOAM parallelization is based on domain decomposition and the MPI message-passing standard:

[1] It is worth mentioning that the foam-extend project distributes a code version that includes block-coupled capabilities. Unfortunately, porting classes from this code version to OpenFOAM is not trivial.

- the computational domain is subdivided into several subdomains;
- each subdomain is solved for by an MPI process;
- information is passed between adjacent subdomains using dedicated "processor" boundary conditions.

This strategy was proven to optimally scale up to few thousands of CPU cores (Culpo, 2011), which allows one to tackle most typical problems in the field of nuclear engineering. According to (Culpo, 2011), the known bottlenecks for massively parallel calculations are: 1) the limit in the parallelism paradigm itself; 2) the sub-optimal sparse matrices storage format (LDU) that does not enable any cache-blocking mechanism (SIMD, vectorization); 3) the I/O data storage system. The OpenFOAM HPC Technical Committee is currently working on the limitations of the linear algebra solver, which in turn will affect the second and third bottlenecks mentioned above. In particular, efforts are ongoing to create an interface to external linear algebra libraries for solving sparse linear system such as PETSc/Hypre. In general, OpenFOAM algorithms were not designed to make an efficient use of vectorization and can only exploit the potential of vector processing units and GPUs in a limited way (Fiorina et al., 2018). Several efforts are currently spent in this direction, including the mentioned interface with PETSc/Hypre, and recent work from NVIDIA (Martineau et al., 2020).

3.3.5. Multi-zone and multi-region treatment

It is often necessary to assign different models or physical properties to different components, or different parts of a component. OpenFOAM offers two main tools in this direction. The first one is the possibility to subdivide a mesh into so called "cellZones". This is equivalent to assigning a label to all cells that belong to a predefined region of a mesh. This possibility can be used to assign different physical properties to these zones. However, one should pay attention to the possible impact that a discontinuous property field can have on the solution (see discussion about multi-material properties in Section 4.4).

A second tool offered by OpenFOAM is the so-called multi-region approach. An unlimited number of different meshes can be used in the same simulation. This is useful for multi-physics applications to assign different meshes to different physics. To complement this, OpenFOAM provides mesh-to-mesh projection algorithms to facilitate coupling between the different meshes (and the different physics).

There is also the possibility of employing coupled boundaries and baffles. Coupled boundaries can be used to couple different boundaries belonging to the same mesh or to different meshes. Coupled baffles can be used to apply a specific condition on an internal face by splitting this face into two overlapping boundaries and assigning a coupled condition to the two.

3.3.6. Computational requirements

Computational requirements for OpenFOAM simulations varies considerably depending on the size of the problem, the physics being solved and whether the simulation is steady-state or transient. In terms of parallel scalability, the general rule of thumb for OpenFOAM simulations is to use around 30′000 mesh cells per CPU core. For instance, in the case of CFD, given that a typical 2D simulation using RANS turbulence modelling would require several hundred thousand cells, while large 3D CFD simulations (e.g., of the flow in a PWR fuel assembly at nominal conditions) would require several hundred millions cells, the optimal number of CPU cores can vary between 10 and ~5000. Thus, smaller problems can readily be run on a workstation with one or two HPC oriented CPUs, while larger problems are typically run on HPC clusters. As another example, in the case of coarse-mesh thermal-hydraulics and neutron diffusion, full-core models typically require few hundred thousand to few million cells, allowing to tackle the multi-physics analysis of nuclear reactors with standard workstations or even with modern laptops.

Considering computational runtime, steady-state simulations on the optimal number of CPU cores can take anywhere between several minutes and several hours, while long-running time-dependent problems may take up to a week to complete. In some specific applications, such as detailed containment simulations (see Section 6.3), simulation times up to a month are not uncommon.

Memory requirements can also vary wildly depending on the physics being solved. A 3D discrete ordinates neutron transport solution typically requires the storage of several thousand solution fields, while a basic single-phase RANS CFD simulation requires in the order of 10 fields. This equates to roughly 200 GB of memory per million mesh cells versus approximately 1 GB, respectively. Smaller problems can therefore be readily run on desktop PCs, while larger problems must be run on high memory machines.

3.4. License

OpenFOAM is distributed under the GNU GPLv3 license. This is a copyleft type license, which has the feature of automatically affecting all software that is produced based on OpenFOAM. This favors a collaborative development with minimal work duplication, with the drawback of: limiting investments from commercial players; and forbidding cross-compilation with software featuring non-compatible licenses.

4. Main modelling capabilities associated with nuclear reactor analysis

As described in Section 2, OpenFOAM has been used to address a variety of modelling challenges for various reactor types and issues at different scales. This allows drawing some conclusions on its pros and cons for the investigation of some of the most relevant phenomena in the field of nuclear reactor safety analysis.

4.1. Core thermal hydraulics

OpenFOAM was developed and is mainly distributed as a CFD library. As such, it offers several state-of-the-art solvers for standard CFD calculations. Limited possibilities are instead offered in terms of coarse-mesh applications (viz., porous medium and subchannel approaches). In particular, the only porous medium functionality that is available in the standard OpenFOAM distributions is in the form of a momentum sink based on a Darcy Forchheimer model. Fortunately, porous-medium (or sub-channel) solvers can be easily implemented using the available operators for Laplacian, divergence and gradient, and adopting a standard merged PISO-SIMPLE (PIMPLE) loop for pressure–velocity coupling. In addition, turbulent quantities can be modelled by tailoring one of the eddy viscosity (viz., k-ε and k-ω models) that are already available in OpenFOAM. Examples of single-phase porous medium solvers can be found in (Clifford, 2013; Fiorina et al., 2015; Aufiero and Fratoni, 2016).

Development of two-phase porous medium models in OpenFOAM is a more difficult task that was recently accomplished in the frame of a PhD thesis at the EPFL (Radman et al., 2021a, b), showing that it is possible to obtain an efficient and stable solution even for the numerically challenging case of sodium boiling.

Both for the one-phase and the two-phase porous medium implementations, the possibility exists to turn them into sub-channel codes by employing a regular mesh, with different porous-medium properties for different groups of cells (cellZones). The main drawback with respect to traditional sub-channel codes is that the solution algorithm was developed for unstructured meshes and cannot take advantage of the regularity of the mesh, which in turns negatively impacts computational performance. On the other hand, one can show that porous medium equations revert back to standard Reynolds Averaged Navier Stokes (RANS) equations in clear-fluid (i.e., without solid structures) regions, which allows for a very flexible geometry set-up with implicit coupling of sub-channel, porous and clear-fluid regions.

In addition to a sub-channel approach, one may also restrain the one-

and two-phase porous medium equation to one dimension and obtain the same set of governing equations that is normally used in system codes[2]. However, one should notice that it is impossible for OpenFOAM to simulate in 1-D sudden changes of direction. One can see this by imagining two 1-D channels in x and y directions connected by a single "corner" cell. In the corner cell, both the x-momentum and the y-momentum equations can only result in a non-physical, complete conversion of kinetic energy into pressure and vice versa. To overcome this problem, and to use OpenFOAM in a system-code-like manner, one may use coupled boundaries between the outlet of a component and the inlet of the next one.

Coupled boundaries and baffles can also be used to simulate the heat transfer across a thin wall. For instance, in case of shrouded fuel subassemblies, one may couple the temperature field inside the subassemblies with that in the subassembly gap or in other subassemblies by using a baffle that simulates the heat transfer resistance across the boundary layers and the metallic wrapper (Radman et al., 2019).

A main drawback that has been observed about the use of OpenFOAM for thermo-hydraulics is the purely segregated approach, which can slow down convergence for problems with a very strong coupling between pressure and velocity, or in multi-phase applications.

4.2. Containment analysis

Containment analysis primarily addresses the containment pressurization, the combustible gas mixing, and possible combustion loads during a severe accident. On this basis, a full-scale containment model can only be representative of an accident sequence if it covers all relevant phenomena and technical systems, as well as their strong interactions in a primarily buoyancy driven flow. In contrast to this requirement, OpenFOAM is shipped with a set of rather specialized solvers and loosely interlinked model libraries. Nevertheless, its object-orientation enabled utilizing the comprehensive set of existing classes and methods as building blocks to construct an integrated analysis package as it was demonstrated e.g. by fireFOAM (Le et al., 2018) or containmentFOAM (Kelm et al., 2021).

While fundamental models for the underlying physics (e.g., turbulent mixing and condensation heat transfer) are available in OpenFOAM, a challenge that researchers had to face is related to extending their application range to account for the prevailing flow conditions in containment studies (viz., free and mixed convection flows). Furthermore, accuracy is limited by the coarsest modeling assumption and the level of detail of the physical models must be well balanced to enable an efficient use of computational resources. For instance, multi-phase phenomena, such as condensation, must typically be reduced to a single phase or treated via a mixture model. In this context, it often proved necessary to perform significant tailoring work on the available OpenFOAM models (Kampili et al., 2019; Liu et al., 2019; Vijaya Kumar et al., 2021).

As a multi-purpose CFD toolbox, OpenFOAM does not provide models to represent technical systems in a containment. However, their implementation can build upon e.g., porous media models or coupling with other codes.

From a more applicative perspective, containment analyses involve a complex multi-compartmented 3D geometry. Even though the automatic mesh generator snappyHexMesh, distributed with OpenFOAM, has some practical limitations, e.g. sufficient refinement of the wall boundary layers can be problematic, its coupling with the adaptive mesh refinement algorithm in OpenFOAM offers a reasonable solution for efficiently capturing the strong and fast flow variations.

4.3. Neutronics and fuel burnup

Implementation of solvers for multi-group diffusion, SP3 and discrete ordinates can be obtained in OpenFOAM based on the availability of the Laplacian and divergence operators. Examples of these implementations can be found in (Fiorina et al., 2016, 2017; Aufiero, 2014; Clifford and Ivanov, 2010; Clifford and Jasak, 2009) while practical examples of implementation and input files can be found in (GeN-Foam Neutronics, 2021) and (GeN-Foam Tutorials, 2021), respectively. Isotropic discontinuity factors can be easily implemented, as shown in (Fiorina et al., 2016). More general discontinuity factors could instead be implemented by using baffles or modified cyclic boundary conditions. The authors are unaware of any implementation of this kind to-date but interested readers may refer to (Clifford, 2013) for an analogous treatment developed for heat transfer.

Solvers obtained by the simple application of the available OpenFOAM operators are easy to implement and offer the advantage of a complete geometrical flexibility thanks to the use of unstructured meshes. This geometrical flexibility was used to develop solvers for fast spectrum MSRs (Cervi et al., 2019a, b; Hu et al., 2017; Laureau et al., 2017; Wan et al., 2020; Aufiero, 2014), whose non-traditional core shape does not allow employing legacy nodal codes based on structured meshes. Once again, this geometrical flexibility comes with the drawback of a much higher computational footprint. This is particularly the case for non-orthogonal and skewed meshes, where reaching mesh convergence tends to require much finer meshes with respect to nodal codes. As shown in (Fiorina et al., 2016), a calculation that could be performed in a few seconds and several MB of RAM with the PARCS nodal code, required a few GB of RAM and several minutes with OpenFOAM. With specific regard to discrete ordinates, one may notice that the purely advective equations of this method allows to avoid full-matrix solutions and opt for directional sweeping. This sweeping could in principle be performed in OpenFOAM via a proper ordering of the cells. However, the use of domain decomposition makes the implementation of this strategy particularly challenging. To the authors' knowledge, despite some efforts in this direction (Jareteg et al., 2014), no such implementation in OpenFOAM has been achieved to date.

Although dedicated matrix preconditioners, accelerators, and its parallel scalability could be used to speed up convergence, OpenFOAM tends to be preferable over legacy tools mainly in cases where the geometry of the core cannot be simulated with structured meshes, or when a multi-physics coupling is of interest. A case where the multi-physics capabilities of OpenFOAM were employed to address a specific neutronic challenge is given once again by the simulation of MSRs, where, in order to take into account the precursors drift in the circulating fuel, one needs to complement the precursors equations by an advection term, with velocities that can be determined by a thermal–hydraulic solver.

An interesting feature of the neutronics solvers developed with OpenFOAM is the possibility to readily employ its moving-mesh features. Thanks to this functionality, one can take a displacement field from another OpenFOAM solver, or from an external solver, and use it to deform the mesh used for neutronics. This can be employed in the attempt to improve predictions of expansion reactivity feedback, for instance in fast reactors (Fiorina and Mikityuk, 2015; Fiorina et al., 2019).

Finally, it is worth mentioning that a first attempt has been carried out to implement the Method of Characteristics in OpenFOAM (Cosgrove and Shwageraus, 2017). The solver has 1-D and 2-D capabilities, but computational performances turned out to be relatively poor. The author suggested the use of OpenMP parallelization and the implementation of a faster ray-tracing routine as possible ways to improve performances, but unfortunately this activity was discontinued. To the authors' knowledge, no attempts have been made to develop solvers

[2] It is worth mentioning here that this same set of equations would nonetheless result in different discretized equations, since velocity and pressure are normally solved on a staggered grid in system codes, while OpenFOAM employs collocated finite volumes, with a mesh staggering that can only be emulated via a Rie-Chow interpolation.

based on spherical harmonics (beside P1 and SP3), while an implementation has been proposed for the Transient Fission Matrix approach (Laureau et al., 2017).

Regarding fuel burnup, one could easily employ the available linear solvers of OpenFOAM to obtain a cell-by-cell, or cellZone-by-cellZone simulation of the isotopic evolution of the fuel. However, for improved performances, one may need to implement dedicated methods such as the method of matrix exponential with exclusion of the fastest-decaying isotopes, or the Chebyshev rational approximation method.

4.4. Fuel behavior and other thermo-mechanical problems

In its standard distributions, OpenFOAM includes a solver for linear elastic displacement of a solid, including thermal deformation. In addition, significant efforts have been spent, in the frame of the FOAM-extend project, to create an extensive library of solvers for various non-linear thermo-mechanical problems (Cardiff et al., 2018). An example of application to the creep deformation in CANDU pressure tubes can be found in (Corzo and Ramajo, 2020). Another application is related to the prediction of thermal deformations in fast reactors, which, as mentioned, can be coupled to neutronics solvers and the moving-mesh capabilities of OpenFOAM to allow for detailed prediction of reactivity feedbacks. Finally, a recent but promising application relates to fuel performance modelling (see Section 6.4).

Using OpenFOAM for the analysis of thermal mechanics implies adopting a finite volume discretization for Computational Solid Mechanics (CSM). While finite volumes are very popular in the field of CFD, CSM is most often associated with the finite element methods, with two- and three-dimensional nuclear fuel performance codes typically based on finite elements. However, it has been shown (Idelsohn and Oñate, 1994) that finite elements and finite volumes share several features and that there is no clear-cut division between the two in terms of application range. In fact, interest is growing toward the use of finite volumes for CSM, showing that there is no obvious difference in terms of performance and accuracy, with both methods having their own strengths and weaknesses (Cardiff and Demirdžić, 2018). Finite-element methods offer improved accuracy with lower mesh resolution; however, the resulting matrices are typically relatively dense, in some cases requiring direct solvers. Finite-volume methods, on the other hand, tend to yield relatively sparse matrices that can be solved readily using iterative solvers. In a sense, the simplicity of the resulting matrix compensates for the relatively low order of the method.

One particular drawback that has been observed in the use of OpenFOAM for CSM is associated with the segregated solution algorithm employed for vector equations, which can experience slow convergence in some applications. In addition, a technical aspect that is worth mentioning is that the displacement-based equations for thermal-mechanics feature a discontinuous derivative at the interface between different materials. It follows that one should develop specific treatments in case of multi-material applications. One may follow an approach similar to the one developed in (Clifford, 2013) for pressure in porous media or develop dedicated internal boundary conditions as proposed in (Tuković et al., 2013).

The greatest advantage of the cell-centered finite-volume method turned out to be once again its simplicity and conservative formulation. For non-mathematicians, the possibility of simply defining and manipulating field values, physical properties and correlations at the cell-centers, and fluxes at their faces, saves time, and simplifies code maintenance and testing.

5. Advanced modelling capabilities in OpenFOAM

Thanks to its characteristics in terms of code development, OpenFOAM is a powerful framework for the formulation, development and testing of new approaches and methodologies. In this context, the coupling with other codes and the implementation of reduced order modelling can be mentioned as two notable examples.

5.1. Coupling with other codes

OpenFOAM has several features that make it well suited for coupling with other codes, namely:

- The use of finite volumes, which allows for an intuitive exchange of information;
- The use of general unstructured meshes, which allows tailoring of the geometry and mesh to that of other codes;
- The availability of several mesh conversion tools to convert meshes from and to an OpenFOAM-readable format;
- The availability of mesh-to-mesh projection algorithms, which facilitate the transfer of information among different meshes in a consistent and mathematically rigorous way;
- The availability of an octree mesh search algorithm, which allows to rapidly identify which cell contains a specific point in space;
- The use of object-oriented C++, which makes OpenFOAM suited for cross-compilation with several existing scientific codes, with the only caveat that the GNU-GPLv3 license of OpenFOAM is incompatible for cross-compilation with proprietary codes and with some of the other existing open-source licenses;
- The availability of surface based (inlet/outlet) coupling schemes, such as externalCoupled boundary conditions.

As an example, these features allow for a straightforward coupling with Monte Carlo codes based on delta-tracking. In particular, single cells in OpenFOAM can be used for tallying various quantities that result from a Monte Carlo simulation (viz., fission power), with these quantities naturally representing the integral value over the cell volume, as required by a finite volume simulation. In turn, the octree mesh search algorithm of OpenFOAM can be used to assign each collision to a specific cell. Of course, Monte Carlo codes based on surface tracking can also be coupled with OpenFOAM, though the several surfaces that are employed in finite-volume meshes tend to make this kind of coupling computationally expensive. Examples of coupled OpenFOAM-Monte Carlo simulations can be found in (Sorrell and Hawari, 2019; Aufiero et al., 2015; Leppänen and Aufiero, 2014; Scolaro et al., 2019). Similar to the case of Monte Carlo codes, a finite volume approach is well suited also for coupling with solvers based on collision probability (Wu and Rizwan-Uddin, 2016).

Another example is the coupling of 2-D or 3-D OpenFOAM-based solvers for fuel behavior with legacy 1.5-D solvers. One can achieve this by: creating a simple OpenFOAM geometry based on the axial slices and radial mesh of the 1.5-D solver; transferring information cell by cell to this mesh; employing a weighted-volume mesh-to-mesh projection algorithm to transfer this information to the (typically finer) mesh that is used for OpenFOAM simulations. An example of this coupling can be found in (Scolaro et al., 2021).

As a last example, one may want to couple OpenFOAM with system codes to complement them with high-fidelity simulations of specific components. This kind of coupling can be achieved by using boundary conditions in OpenFOAM to pass information from and to the system codes. An example is the coupling of OpenFOAM and the ATHLET system code (Herb and Chiriac, 2016) in the framework of the developments related to the AC2 code package at GRS in Germany (Wielenberg et al., 2019).

Finally, the generic coupling scheme preCice developed at TUM in Germany (Bungartz et al., 2016) provides a framework that limits the effort in coupling OpenFOAM and other tools to the creation of a code specific adaptor.

5.2. Reduced order modelling

Although most of the OpenFOAM-based research in the nuclear field

has been directed towards high-fidelity models, it is worth mentioning that OpenFOAM has represented an important playground for the development of software and methods for Model Order Reduction (ROM), resulting in a significant scientific output. Model Order Reduction refers to a relatively large set of methodologies that are employed to reduce the computational footprint of numerical analysis. According to the specific application needs, two approaches are available for obtaining a reduced order model, namely: a non-intrusive one which relies on advanced interpolation and fitting of available data; or an intrusive one where the reduced order model is derived from the projection of the governing equations onto a reduced space. Among various techniques for the creation of the reduced space, proper orthogonal decomposition (POD) has recently received some attention in the nuclear field. It was initially introduced in a fluid dynamics context aiming at extracting coherent structures from turbulent flows. In particular, POD is used to provide a set of basis functions that identify a low dimensional space representative of the problem of interest, starting from some solutions obtained through experiments or more often from a high-fidelity model.

A POD library was developed in the past in the frame of the FOAM-extend project and can be easily adapted to other OpenFOAM distributions for reduced order modelling applications. This library allows the creation of the orthogonal basis (based on cross-correlation), starting from the outcomes of one or more simulations (i.e., the snapshots). In addition to this, OpenFOAM allows performing all the intrusive operations required in the development of projection-based ROM such as: access to the governing equations; matrix manipulation; and Galerkin or Petrov-Galerkin projections.

OpenFOAM-based POD techniques were used for modelling temperatures in prismatic high-temperature reactors (Clifford, 2013), for control-oriented studies of the hydraulics of Lead Fast Reactors (LFR) (Lorenzi et al., 2017; Sartori et al., 2016), for neutron diffusion (German and Ragusa, 2019); for the parametric multi-physics analysis of the Molten Salt Fast Reactor (German et al., 2019), for control rod movement (Sartori et al., 2016); as well as for more general thermal-hydraulic applications (German et al., 2019; German et al., 2020).

6. Examples of advanced solvers and applications

Following its capabilities to model the most relevant phenomena in the field of nuclear reactor safety (Section 4), thanks to its features in terms of code coupling, and making use in some cases of ROM techniques (Section 5), OpenFOAM has revealed itself as a valuable option for nuclear reactor safety analysis, as witnessed by the several single- and multi-physics solvers developed by various authors in the last decade.

In most cases, OpenFOAM-based solvers have been developed to investigate highly complex phenomena involving non-trivial geometries and a non-linear interaction of several physics. The reasons for choosing OpenFOAM in these situations are twofold. First, the use of finite volumes allows for an intuitive implementation of models, which can help specialists in a domain to develop relatively sound solvers in other domains. In this sense, one should also note that OpenFOAM is distributed with several solvers for thermo-fluid dynamics (including Lagrangian solvers). This provides a good starting point in a field that is otherwise complex in terms of implementation details. The second reason that favored the use of OpenFOAM for complex multi-physics applications is the availability of all the necessary ingredients, namely:

- unstructured meshes providing complete geometrical flexibility;
- multi-mesh (or multi-region) treatment to allow for the representation of different phenomena at different scales or levels of details;
- mesh-to-mesh projection to streamline coupling of the different physics;
- the possibility to subdivide the mesh into cell zones to allow for different material properties and equations;
- the availability of coupled boundaries that can be used to allow communication between boundaries in the same mesh or different meshes;
- the AMI (Arbitrary Mesh Interface) algorithm for face-to-face projections between non-conformal meshes.

One may also add the open availability of a large variety of solvers and routines, either from the official OpenFOAM distributions, or via in-kind contributions from the community.

This section includes a selection of examples to showcase how OpenFOAM can be used to address important problems in the field of nuclear reactor analysis. We try to highlight the salient aspects, modelling challenges, and the possible added value with respect to other approaches.

6.1. Multi-physics and multi-scale modelling of advanced reactor technologies

As already mentioned, in the last couple of decades OpenFOAM has enjoyed a wealth of applications for modelling nontraditional reactor types. This follows from the geometric flexibility allowed by unstructured meshes, as well as from the possibility to easily implement new equations and models.

6.1.1. High-Temperature Gas-cooled Reactors

Both pebble-bed and prismatic HTGRs are characterized by multiple distinct spatial scales, starting with the TRISO-coated particles on the smallest scale, followed by the fuel elements at the intermediate scale, and finally the reactor core and pressure vessel at the largest scale. These designs present a challenge for computer simulations since one ideally needs to know the behavior of the reactor at all locations and scales to understand the response under design and beyond design conditions, but direct simulation on all scales is currently intractable. A hierarchical multi-scale methodology was developed by (Clifford, 2013) towards addressing this problem. The heat transfer at the lower length scales was modelled independently, assuming an infinite array of unit cells, and homogenized to obtain effective homogeneous material properties for the coarser scales, as well as ROMs to represent the fine-scale behavior. By repeatedly applying the homogenization scheme and stepping out to the largest scales, the full reactor could be modelled consistently with the ability to reconstruct the temperature profiles at any time, location, and scale. This multi-scale solution was coupled to a coarse-mesh CFD solver that included a new model for the turbulent mixing and thermal dispersion in porous media based on the traditional k-ε turbulence model. This work leveraged several advanced functionalities available in OpenFOAM. Support for multiple arbitrary meshes in a single solver facilitated the modelling of different geometries at different scales. Specialized homogenization equations were constructed and solved in OpenFOAM using vector PDEs, and effective homogeneous material properties were calculated using field operations. Corrections for discontinuities and gaps were readily treated using customized equation operators. OpenFOAM's flexible boundary condition design allowed thermal radiation across open regions to be incorporated within the homogenization process itself. The availability of classes for POD, and the ability to access the underlying equation terms, facilitated the construction of ROMs for the fine-scale behavior. Time-integration of the ROMs was achieved using OpenFOAM's built-in ODE solvers. Finally, the object-oriented design of the framework facilitated on-demand reconstruction of the fine-scale solutions. Exemplary results that were obtained for the MHTGR-350 MW Benchmark Model are reported in Fig. 1.

6.1.2. Molten salt reactors

The uncommon features of liquid-fueled MSRs pushed researchers to develop new solvers for reactor analysis in the attempt to overcome the limitations of legacy tools. This effort was motivated by the scarce

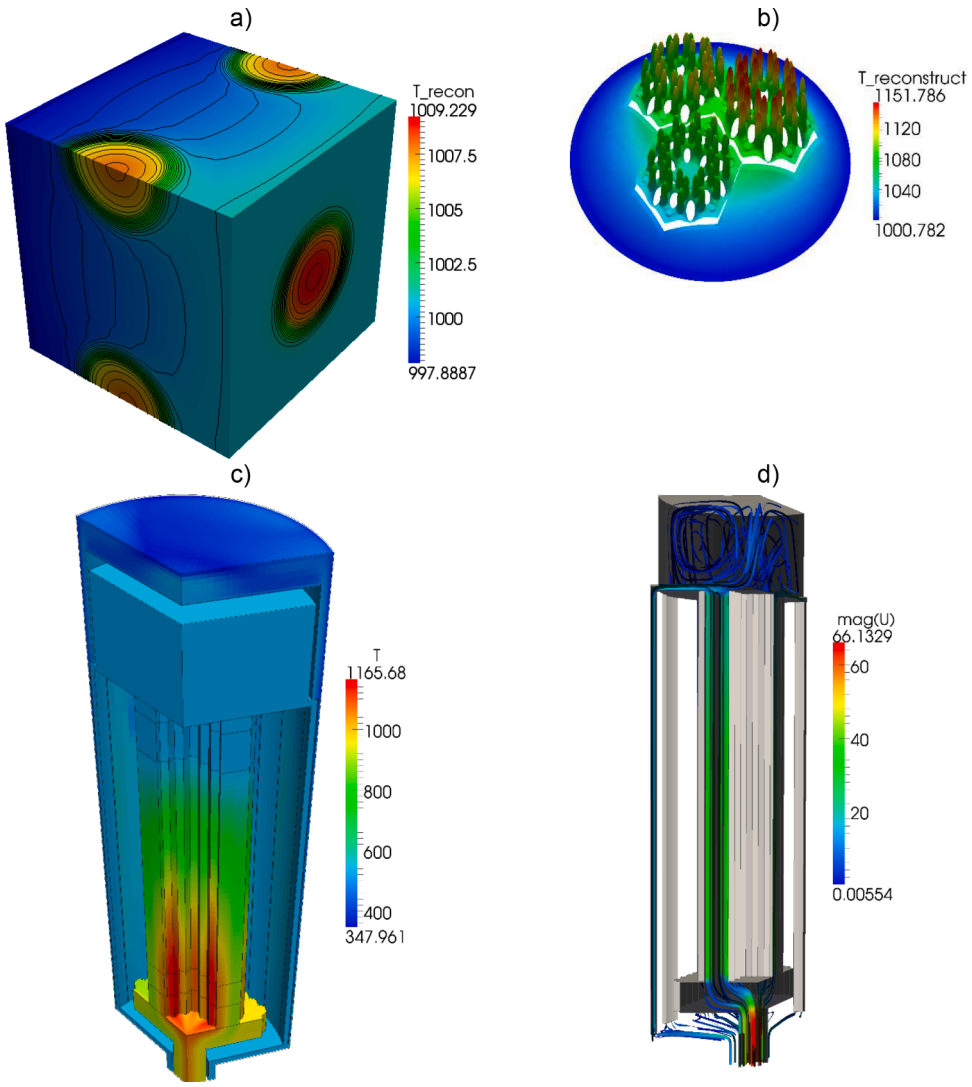

Fig. 1. Example of results obtained in (Clifford, 2013) for the MHTGR-350 MW Benchmark Model: a) ROM reconstructed solution for TRISO coated particles; b) ROM reconstructed solution for a fuel element; c) Temperature distribution in the core; and d) Velocity distribution in the core.

experience on these nuclear systems compared to commercial reactors and the peculiar characteristic of a circulating fuel. The latter poses some modelling challenges such as the drift of the delayed neutron precursors, the strong coupling between neutronics and thermal hydraulics, and the internal heat generation in the fluid. Especially for non-moderated MSRs, the capability of correctly assessing the fluid flow distribution turned out to be essential, calling for the use of CFD modelling approaches instead of more traditional system or sub-channel approaches. In addition, flexibility and access to governing equations was required to implement the modifications needed to describe the moving precursors and the volume heat source in the fluid fuel.

For these reasons, OpenFOAM was selected at the Politecnico di Milano (PoliMi) for creating a simulation tool capable of considering the salient aspects of MSR modelling. PoliMi developed a first solver for the Molten Salt Fast Reactor (MSFR) during the EVOL project (Aufiero, 2014). This included a one-group diffusion equation for the neutronics, a balance equation with advection–diffusion terms for the transport of delayed neutron precursors, a decay heat energy balance equation, as well as incompressible RANS equations with standard turbulence models, Boussinesq approximation, and energy equation for the thermal-hydraulics (Fig. 2). An improved version of the MSFR solver was later developed during the SAMOFAR project aimed at studying the effect of the online sparging system for fission product removal. A

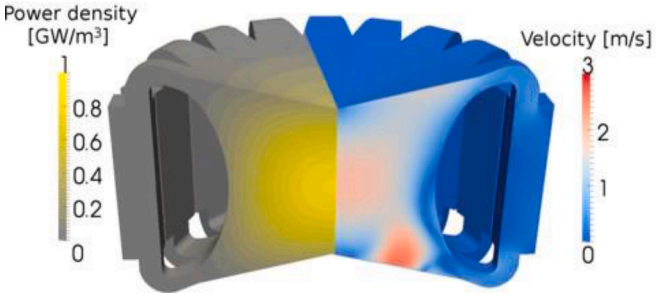

Fig. 2. Velocity and power density fields in the MSFR after the single pump failure accident obtained in first OpenFOAM solver for MSR (Aufiero, 2014).

correct bubble spatial distribution is in fact essential to obtain a correct evaluation of the void reactivity feedback coefficient due to the importance of the spatial and spectral effects (Fig. 3). The neutronics modelling of the MSFR solver was then extended with multi-group neutron diffusion and the simplified P3 (SP3) neutron transport approach (Cervi et al., 2019), and its thermohydraulic modelling with a Euler-Euler compressible two-phase thermo-hydraulic model (Cervi et al., 2019a).

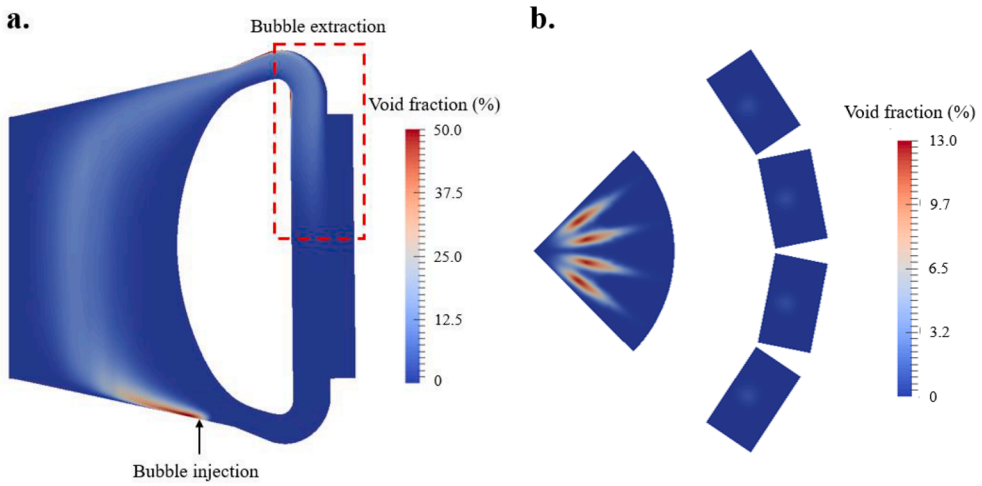

Fig. 3. Core average void fraction in the MSFR in case of injection of helium bubbles for fission product removal, axial (a) and radial (b) section. Results are obtained with the two-phase OpenFOAM solver for MSR presented in (Cervi et al., 2019a).

6.1.3. Fluoride-salt-cooled high-temperature reactors

The work in (Aufiero and Fratoni, 2016) is a good example of an advanced use of OpenFOAM and of its coupling with an external tool. It proposed a new approach to the multi-physics modeling of pebble-bed fluoride-cooled high temperature reactors (PB-FHRs) that accounted for the full dimensionality of the neutron transport problem, with explicit description of the pebbles random packing in the core, and random distribution of the TRISO particles inside the pebbles. In particular, the sphere distribution was obtained via an OpenFOAM based Discrete Element Modeling of the pebble bed, complemented by a porous-medium CFD solver to account for the temperature variation in the molten salt. The position and temperature of each pebble was then adopted directly in a Monte Carlo neutron transport calculation. The data exchange between the neutronics and the thermal-hydraulics solver was simplified by the scoring of Monte Carlo collisional estimators for the fission power deposition directly on the finite-volume grid adopted for spatial discretization of the set of coupled PDEs in the CFD problem. The tool allowed for an accurate simulation of the initial fuel loading and the approach to criticality of an FHR, considering the peculiar cone-shaped fuel assembly structure that forms as pebbles are loaded from the center of the bottom graphite reflector. The detailed pebble power distribution and coolant temperature field (Fig. 4), as well as the effect of asymmetric control rod insertion, were also presented as useful results that can be easily achieved with the proposed approach, with respect to simplified 2D or neutron diffusion-based solver.

6.2. General-purpose multi-physics: The GeN-Foam solver

Starting from the pioneering work on HTGRs and MSRs presented in the previous section, the GeN-Foam solver (Fiorina et al., 2015; Radman et al., 2021a; GeN-Foam Repository, 2021) has been developed at the EPFL and at the PSI to address more generally the problem of the multi-physics analysis of nuclear reactors. GeN-Foam includes functionalities for investigating pin- and plate-type fuels, as well as liquid-fueled

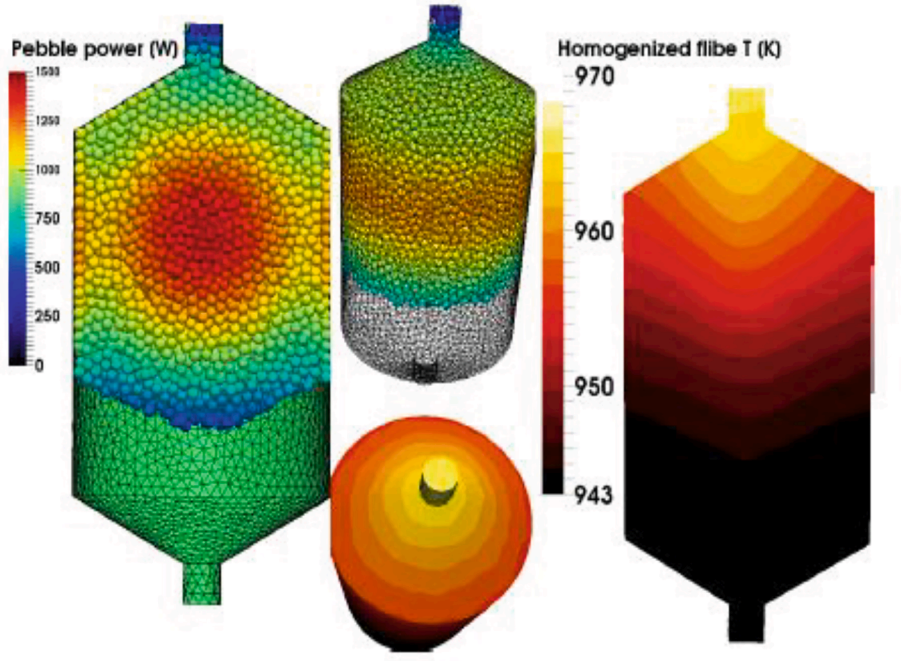

Fig. 4. Coupled Serpent–OpenFOAM results for an FHR (Aufiero and Fratoni, 2016).

reactors. It allows for the fine- and coarse-mesh modelling of single- and two-phase flows. With regard to neutronics, a standard multi-group diffusion solver has been complemented with SP3 and SN solvers, as well as with a simple solver for point kinetics (Mattioli et al., 2021; Radman et al, in press). All physics take advantage of moving meshes to account for thermal deformations. By benefitting in particular from the previous work of (Clifford, 2013) and (Aufiero, 2014), the development of GeN-Foam had mainly to overcome two methodological challenges, namely: the combined fine- and coarse-mesh (porous medium) simulation of both single- and two-phase flow; and the simulation of core deformations and their impact on reactivity.

The fine- and coarse-mesh simulation of single- and two-phase flow required the development of a new solver (Radman et al., 2021a, b) that combines a series of improved solution strategies and algorithms including: the use of a PIMPLE algorithm for pressure–velocity coupling; the adoption of the Multidimensional Universal Limiter with Explicit Solution (MULES) algorithm for the solution of the phase continuity equations[3]; an improved implementation of the partial elimination algorithm to improve convergence of the pressure–velocity coupling; and the implementation of dedicated baffles to simulate the heat exchange across wrappers in coarse-mesh simulations. As an example of applications, Fig. 5a shows the simulation of sodium flow in a sodium fast reactor subassembly featuring windows for sodium stabilization (Radman et al., 2019), while Fig. 5b shows the results of the multi-dimensional detailed reanalysis of the KNS experiment on sodium boiling (Radman et al., 2021).

Simulation of core deformations required setting up two thermo-mechanical solvers in order to separately evaluate the radial deformation of core structures and the axial deformation of the fuel. The mesh-to-mesh projection algorithms available in OpenFOAM have been employed to transfer this information to a target mesh. With the deformation field transferred to the target mesh, it was then possible to interpolate it from cell centers to mesh points and employ this information to deform the mesh and to parametrize the physical properties (viz., the cross sections) based on the local deformation. Finally, a thermo-mechanical model for contact was introduced to perform heterogeneous core simulations with explicit modelling of the mechanical interaction among single subassemblies. As a practical example, Fig. 6 shows some results obtained for the European Sodium Fast Reactor (ESFR). In particular, Fig. 6a shows an example of a homogenous simulation (Fiorina and Mikityuk, 2015), where the direct coupling with thermal hydraulics, the mesh deformation, and the local parametrization of cross-sections allowed to estimate a fuel expansion reactivity feedback that is 50% lower with respect estimations based on uniform axial and radial expansions. Fig. 6b shows a similar study, but based on a heterogeneous representation of the subassemblies, which allows for a higher-fidelity simulation of displacements and the explicit simulation of core flowering and core compaction (Fiorina et al., 2019).

6.3. Containment modelling: the containmentFOAM solver

The analysis of containment response during an accident is usually performed on the basis of established 1-D system codes (e.g., ASTEC or MELCOR) for a broad range of possible scenarios. Such codes are well validated against a large number of experiments and contain a large number of physical models, which are either based on similarity mechanics or empirical correlations. Nevertheless, containment atmosphere mixing, aerosol transport and possible combustion processes in a complex compartmented geometry are intrinsically 3D processes and can only be covered by conservatism in system codes.

[3] The MULES can be considered as a particular implementation of a Flux Corrected Transport (FCT) technique, which aims at a discretization of the advection terms that is less diffusive than a low-order scheme, (e.g. upwind) while not resulting in a potentially unbounded phase fraction.

In recent years, CFD is increasingly employed to complement legacy codes with a higher level of spatial resolution and modeling details, in particular with an explicit representation of relevant geometric aspects affecting the flow and transport phenomena. However, as mentioned in section 4.2, a full-scale containment model must employ a well-balanced level of details and describe the strong interactions of various phenomena in a primarily buoyancy driven flow.

In containmentFOAM (Kelm et al., 2021), the containment atmosphere is described as a single phase (reacting) multi-component flow. A dedicated multiSpeciesTransport library was built on top of the OpenFOAM thermo and turbulence libraries for calculation of diffusive mass fluxes and corresponding enthalpy transport. Furthermore, this library serves as a basis to integrate multi-phase phenomena such as wall condensation, fog formation and transport or aerosol transport (Vijaya Kumar et al., 2021). These phenomena are reduced to a single transport equation by utilizing a mixture model along with a drift flux approach and they interact with the gas phase via volumetric source terms, e.g., for the transfer of latent enthalpy or decay heat. It should be remarked that direct access to the solution algorithm enables a flexible and stable implementation of these source terms. Turbulent transport within the predominantly mixed and free convection flow is modeled by extending the available k-ω SST turbulence model with specific source terms to account for production and dissipation of turbulent kinetic energy in density gradients. The initially cold containment structures represent significant heat sinks and are represented within the multi-region framework. As the flow is wall-bounded and driven by wall heat transfer, a scalable and consistent wall treatment was implemented extending established wall functions. Gas radiation significantly affects heat transfer in humid atmospheres and is modeled using a non-gray spectral model and a Monte Carlo transport solver which was integrated into the thermophysical library utilizing the Lagrangian library for tracking the photon transport (Liu et al., 2019). The operational behavior of passive auto-catalytic recombiners (PAR) for combustible gas management is integrated by coupling containmentFOAM with the mechanistic 2D PAR model REKODIREKT, using a domain decomposition approach and the file-based coupling scheme available in the externalCoupled boundary condition of OpenFOAM. In a containment, different compartments are initially separated by means of doors or burst foils. Depending on pressure and temperature differences they can open new flow paths. This is modeled utilizing the activeBaffle functionality in OpenFOAM.

Fig. 7 showcases a recent application of containmentFOAM to the reanalysis of the ISP-37 VANAM-M3 experiment (Firnhaber et al., 1996). Subsequent to the illustrated preconditioning and pressurization of the multi-compartmented Battelle Model Containment by superheated steam injection, a hygroscopic NaOH aerosol is released, and its distribution and deposition is studied.

Even though analysis of combustion processes and resulting loads is currently not further evaluated in containmentFOAM, the available combustion models in OpenFOAM can be utilized within its pressure-based solver. An alternative option is to use the computed fields as an initial condition for a specialized solver like ddtFOAM, which is based on a density-based Riemann solver and enables accurate capturing of shock waves. In ddtFOAM, combustion is modeled via a reaction progress variable and a sub-grid model for auto-ignition, which employs tabulated delay times obtained from a detailed chemical mechanism. The use of adaptive mesh refinement enables efficient application to large scale geometries (Hasslberger et al., 2015). Recently, it was demonstrated that such 3D under-resolved CFD methods can be applied to analyze and estimate the risk of Flame Acceleration (FA) and even Deflagration to Detonation Transition (DDT) at containment scale (Hasslberger et al., 2017).

6.4. Fuel modelling: the OFFBEAT solver

The evolution of the nuclear fuel during irradiation is characterized by complex multi-scale and multi-dimensional phenomena. Traditional

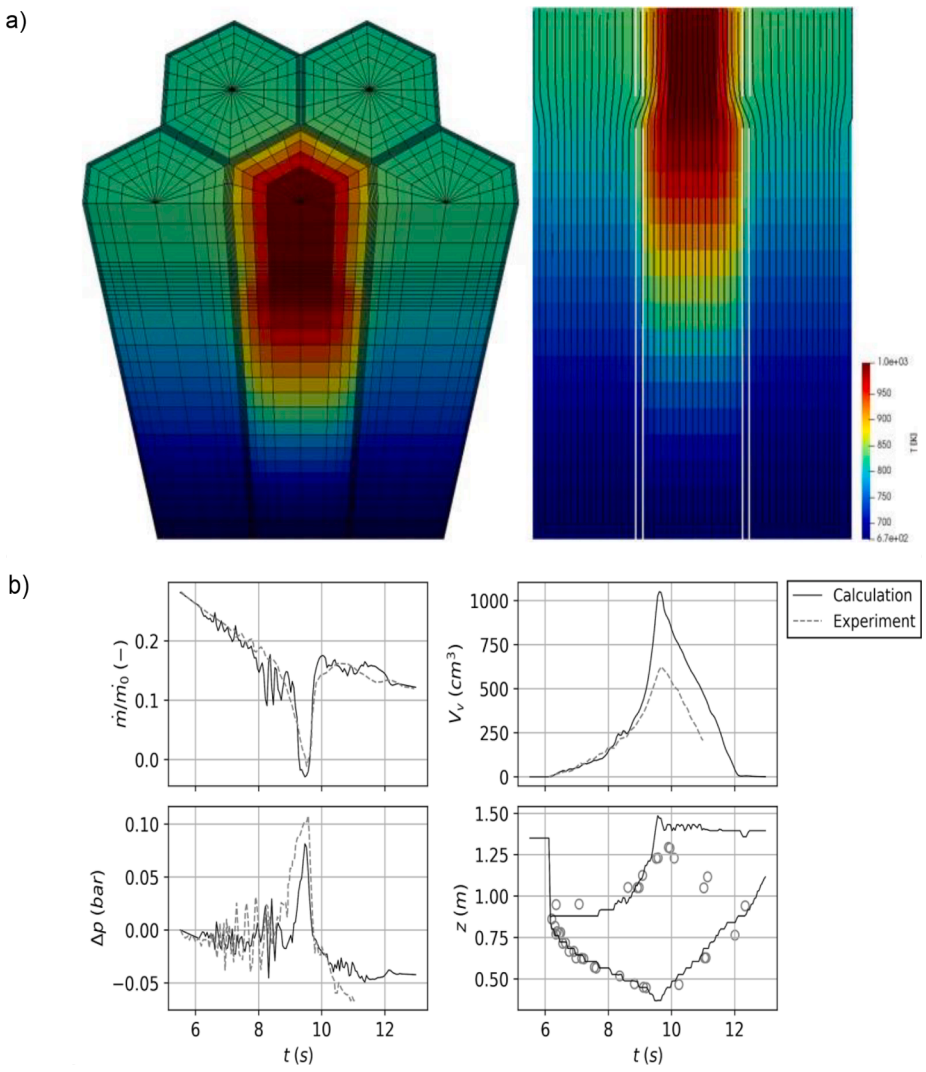

Fig. 5. a) Simulation of sodium flow in a boiling-stabilized sodium fast reactor. b) Reanalysis of the KNS experiment: normalized inlet mass flow (top left); total vapor volume (top right); absolute pressure change (bottom left); maximum and minimum axial vapor extent (bottom right).

fuel behavior analysis codes have reduced this complexity by following the so-called 1.5-D or quasi-2-D approach, while relying on experimental correlations to describe the most important mesoscale phenomena. However, in the last two decades, the fuel performance community has shown a growing interest towards the development of higher fidelity tools with multi-dimensional, multi-physics and multi-scale capabilities. In this framework and motivated by a recent fuel failure in a Swiss BWR, the EPFL and the PSI have started the collaborative development of a new multi-dimensional fuel performance code based on OpenFOAM. OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT) (Scolaro et al., 2020) aims to enhance our understanding of the mechanisms behind poorly-known local effects in the fuel and assessing their impact on fuel integrity.

OFFBEAT follows a displacement-based solution strategy, which results in a Laplacian-based formulation that fits well a finite-volume discretization algorithm. Starting from the available small-strain linear-elastic solver of OpenFOAM, its thermo-mechanical capabilities have been extended to nonlinear phenomena such as creep and plasticity, as well as for time-dependent phenomena such as swelling, densification, relocation, and axial growth. Essentially, this translated into adding new strain components in the equations for displacement. In addition, various models have been included to deal with time, temperature, and irradiation dependency of various properties, according to available correlations. Two major methodological challenges that were addressed are the fission gas release and the simulation of thermo-mechanical interaction between fuel and cladding.

The challenge of simulating fission gases is mainly associated with their release and subsequent buildup in the gap. Their release was initially treated via traditional correlations. Later, the developers have benefitted from the C++ programming and the compatible license of the SCIANTIX code (Pizzocri et al., 2020) to couple it with OFFBEAT, thus allowing for a more mechanistic description of fission gas release. The buildup of gases in the gap and plena was instead treated by developing a dedicated class capable of calculating the available gap volume on-the-fly starting from the position and displacement of the surfaces surrounding the gap (Scolaro et al., 2020).

With regard to the thermo-mechanical interaction of fuel and cladding, the modelling of the heat conduction and of the mechanical contact between fuel and cladding has been obtained by developing two dedicated coupled boundary conditions for temperature and displacement. Both coupled boundaries make use of the AMI algorithm available in OpenFOAM to cope with non-conforming meshes between fuel and cladding. Although the simulation of mechanical contact can be easily obtained via the standard penalty method, this approach sometimes exhibits slow convergence and can be unstable in some cases mainly due to its explicit nature. As described in detail in (Scolaro et al., 2021), an innovative semi-implicit algorithm has been developed that can significantly improve convergence.

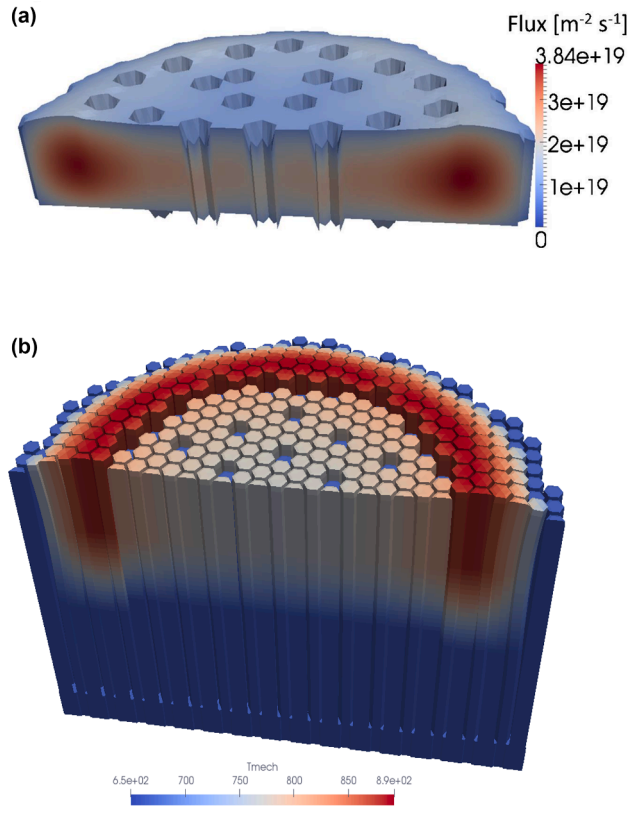

Fig. 6. a) Homogeneous simulation of core axial deformations in the ESFR. b) Simulation of core flowering in the ESFR.

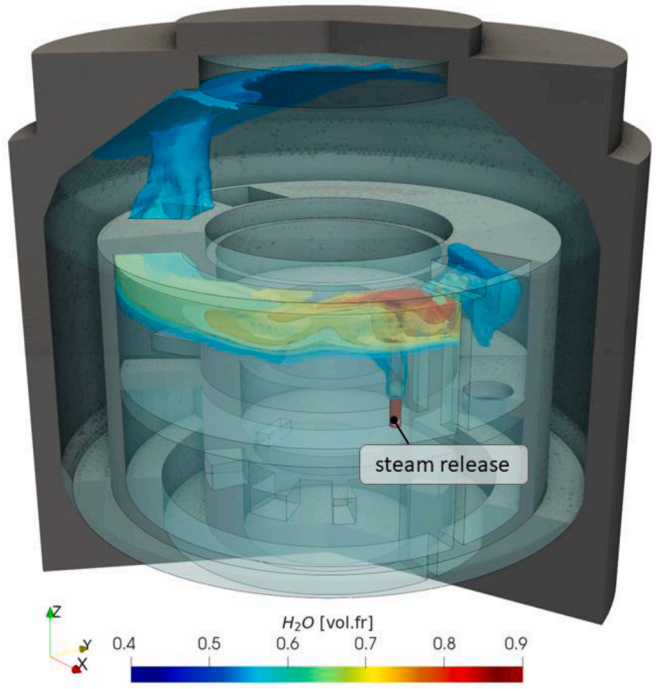

Fig. 7. ISP-37 VANAM-M3 test: Steam injection into the multi-compartmented Battelle Model Containment (volume ~ 615 m^3).

Beside a rapid development allowed by the availability of most of the necessary functionalities, the choice of basing OFFBEAT on OpenFOAM has also yielded some important benefits such as:

- The capability to treat most of the problem dimensionalities of interest, including 1.5-D, 2-D r-z, 2-D r-theta and 3-D geometries. It also allows for 2.5-D r-theta simulations, in the sense that it allows for the simulations of multiple, 2-D r-theta slices, coupled between them via the gap pressure.
- A massive parallel scalability, which allows OFFBEAT to tackle large-scale 3-D problems.
- An intuitive finite volume discretization, which in turn allows for quick integration of new models and streamlined coupling with other codes, such as Serpent2 and TRANSURANUS.
- A straightforward coupling with the CFD solvers of OpenFOAM.

As an example, OFFBEAT was used for a high-fidelity simulation of pellet cladding interaction, including the formation of ridging in the cladding and the impact of a missing pellet surface (Scolaro et al., 2019) (Fig. 8a), as well as for an investigation of the effect of eccentricity on in-pile fuel behavior experiments (Fig. 8b) (Scolaro et al., 2021).

7. Conclusions and future perspectives

In the last two decades, the use of OpenFOAM as a multi-physics library for nuclear applications has grown from a sporadic use in specific projects to being one of the preferred choices to tackle the analysis of operating and innovative reactor concepts; to investigate specific and highly complex problems; as well as to experiment with new numerical methodologies.

These research activities have exposed some of the pros and cons of this approach. Typically reported downsides include a relatively steep learning curve, a non-obvious workflow, and some limitations associated with the use of finite volumes and segregated solution algorithms. Advantages include a cost-free and open-source license; a strong community support; a wide range of existing solvers; flexibility for code tailoring and for developing new applications; an intuitive discretization strategy based on the finite volume method; and a well-structured object-oriented programming with an intuitive multi-level API, with positive impact on the quality of new solvers, on the time required for new developments, and on the possibility of users with various experience to perform code modifications.

Because of these features, the use of OpenFOAM for multi-physics applications has proven to be a good choice for PhD research projects, where the student has the flexibility to trade the time required for a proficient use with a large flexibility to develop new algorithms and investigate specific phenomena. OpenFOAM has also proven beneficial for research groups and communities with strong interests in specific technologies (viz., HTGRs, MSRs, FHRs) or phenomenologies (viz., LWR containment H2 mixing and mitigation, sodium flow in windowed assemblies, core deformation in SFRs), whose analysis can benefit from the use of innovative numerical methodologies. In these cases, the flexibility of OpenFOAM often allowed these research groups to obtain first-of-a-kind results, while its object-oriented programming allowed for an optimal code development strategy with limited maintenance needs and well-encapsulated new developments.

More recently, the use of OpenFOAM is starting to involve a broader community of students and researchers. This is the result of the positive feedback loop that is typical of an open-source development paradigm, where a growing number of users results in new solvers, tutorials, documentation, and in-kind support that can facilitate the involvement of an increasingly broader community. This combines with an improved documentation of the base library itself to greatly simplify the first steps in using OpenFOAM. As a result, it is not uncommon today to see master thesis research based on OpenFOAM. A lower entry step, the open-source license, and an intuitive API are also starting to be recognized as interesting features for education and training, as they discourage counterproductive black-box approaches and improve understanding.

The commercial application of OpenFOAM in industrial design, safety assessment or in support of licensing certainly benefits from a

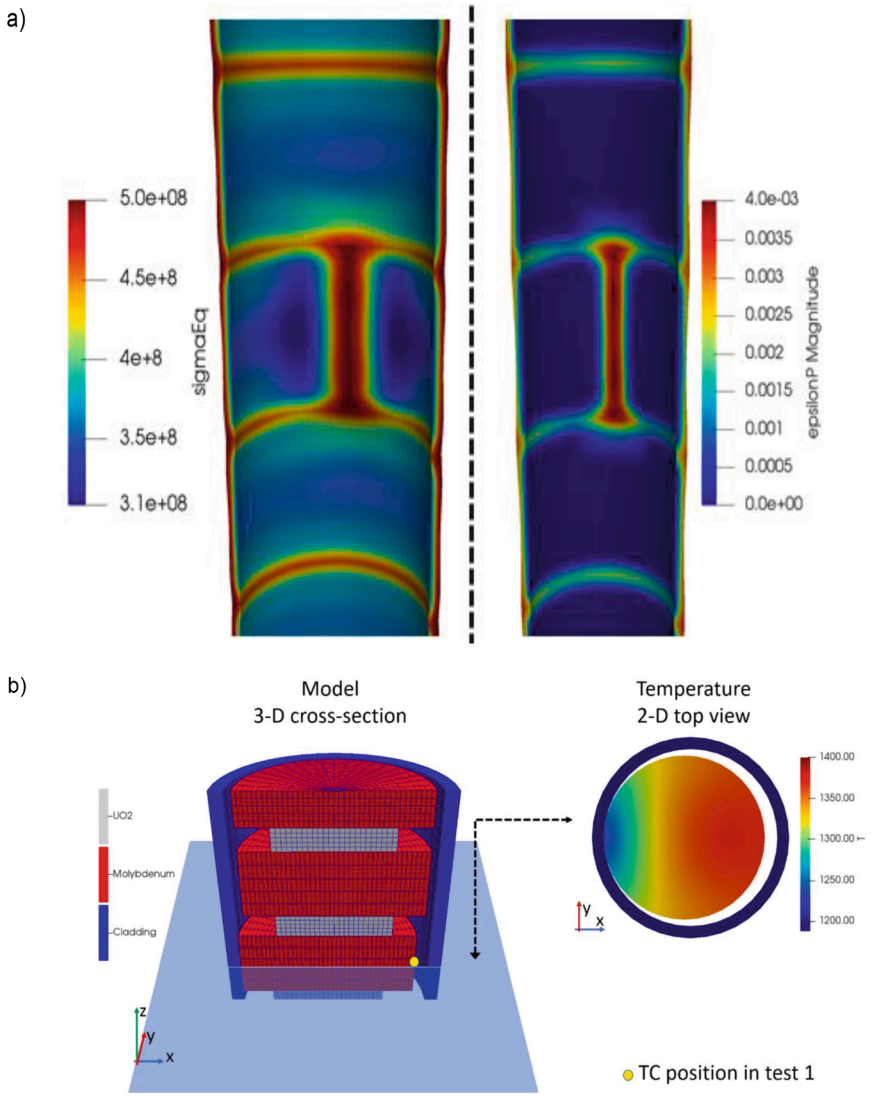

Fig. 8. a) 3-D thermo-mechanical simulation of a pin, including a missing pellet surface (sigmaEq and epsilonP represent the Von Mises stresses and the plastic deformations, respectively). b) Cross section of a 100% eccentricity model used for the stack S41 from the HBRP experiment (left); detail showing the 2-D temperature distribution on a radial slice at the center of the eccentric molybdenum disc (right).

transparent and reviewable code. However, the general flexibility in implementing and using any combination of models and numerical methods impairs comparability and rating of results. Consequently, use of OpenFOAM for production calculations demands a certain level of standardization along with well-documented best practices associated with a thorough validation.

Recognizing the increasing interest in the open-source developments worldwide and the growing need for standardization, the Open-source Nuclear Codes for Reactor Analysis (ONCORE) initiative has been launched in 2020 (IAEA, "ONCORE,", 2021; Fiorina et al., 2020). It is an IAEA-facilitated international collaboration framework for the development and application of open-source multi-physics simulation tools to support research, education, and training for the analysis of advanced nuclear power reactors. In addition, the ESI group has established in 2020 the OpenFOAM technical committee for nuclear applications (OpenFOAM Technical Committees, 2021). This committee aims at establishing a streamlined communication channel between the nuclear community and the OpenFOAM developers.

These and other initiatives are helping connect a growing, but sometimes fragmented, community and provide the coordination that is necessary for a consistent development effort towards a novel open-source multi-physics platform that could represent an important asset for research and education in nuclear science and technology.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The authors wish to thank Ivan Spisso for providing us with an overview of the ongoing efforts to improve the scalability of OpenFOAM.

This work is partly motivated by the IAEA Open-source Nuclear Codes for Reactor Analysis (ONCORE) initiative, a collaborative framework for the development and application of open-source multi-physics to support research, education, and training in nuclear science and technology.

References

Altahhan, M., Bhaskar, S., Ziyad, D., Balestra, P., Fiorina, C., Hou, J., Smith, N., Avramova, M., 2020. Preliminary design and analysis of Liquid Fuel Molten Salt Reactor using multi-physics code GeN-Foam. Nuclear Engineering and Design 369, 110826. https://doi.org/10.1016/j.nucengdes.2020.110826.

Aufiero, M., Fratoni, M., 2016. Development of multiphysics tools for fluoride-cooled high-temperature reactors. In: Physics of Reactors 2016, PHYSOR 2016: Unifying Theory and Experiments in the 21st Century, pp. 2116–2127.

Aufiero, M., Cammi, A., Geoffroy, O., Losa, M., Luzzi, L., Ricotti, M.E., Rouch, H., 2014. Development of an SP3 neutron transport solver for the analysis of the Molten Salt Fast Reactor. Chem. Eng. Sci. 111, 390–401. https://doi.org/10.1016/j.ces.2014.03.003.

Aufiero, M., Fiorina, C., Laureau, A., Rubiolo, P., Valtavirta, V., 2015. Serpent-Openfoam coupling in transient mode: Simulation of a godiva prompt critical burst. Mathematics and Computations, Supercomputing in Nuclear Applications and Monte Carlo International Conference, M and C+SNA+MC 2015.

Aufiero, M., 2014. Development of advanced simulation tools for circulating-fuel nuclear reactors. PhD Thesis. Politecnico di Milano, Italy.

Bungartz, H.J., et al., 2016. preCICE – A fully parallel library for multi-physics surface coupling. Comput. Fluids 141, 250–258. https://doi.org/10.1016/j.compfluid.2016.04.003.

Cardiff, P., Demirdžić, I., 2018. Thirty years of the finite volume method for solid mechanics," Oct. 2018, [Online]. Available: http://arxiv.org/abs/1810.02105.

Cardiff, P., et al., 2018. "An open-source finite volume toolbox for solid mechanics and fluid-solid interaction simulations," Journal, vol. 00, pp. 1–45, Aug. 2018, Accessed: Aug. 26, 2020. [Online]. Available: http://arxiv.org/abs/1808.10736.

Cervi, E., Lorenzi, S., Cammi, A., Luzzi, L., 2019. Development of an SP 3 neutron transport solver for the analysis of the Molten Salt Fast Reactor. Nucl. Eng. Des. 346, 209–219. https://doi.org/10.1016/j.nucengdes.2019.03.001.

Cervi, E., Lorenzi, S., Luzzi, L., Cammi, A., 2019a. Multiphysics analysis of the MSFR helium bubbling system: A comparison between neutron diffusion, SP3 neutron transport and Monte Carlo approaches. Ann. Nucl. Energy 132, 227–235. https://doi.org/10.1016/j.anucene.2019.04.029.

Cervi, E., Lorenzi, S., Cammi, A., Luzzi, L., 2019b. Development of a multiphysics model for the study of fuel compressibility effects in the Molten Salt Fast Reactor. Chem. Eng. Sci. 193, 379–393. https://doi.org/10.1016/j.ces.2018.09.025.

Clifford, I.D., Ivanov, K., 2010. PBMR 400MW Benchmark Calculations Using the Simplified P3 Approach. Proceedings of HTR2010, Prague, Czech Republic.

Clifford, I., Jasak, H., 2009. Application of Multi-Physics Toolkit to Spatial Reactor Dynamics. International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics (M&C), Saratoga Springs, NY, USA.

Clifford, I.D. "A Hybrid Coarse and Fine Mesh Solution Method for Prismatic High Temperature Gas-Cooled Reactor Thermal-Fluid Analysis," PhD Thesis, PennState University, 2013. [Online]. Available: https://pdfs.semanticscholar.org/7096/4dc2d72b27aeab25fbd83746b564622f4623.pdf.

Corzo, S.F., Ramajo, D.E., 2020. Numerical simulation of high-temperature creep deformation in Zr-2.5%Nb pressure tubes of CANDU reactors. Int. J. Press. Vessels Pip. 179, 104029 https://doi.org/10.1016/j.ijpvp.2019.104029.

Cosgrove, P., Shwageraus, E., 2017. Development of MoCha-Foam: a new Method of Characteristics Neutron Transport Solver for OpenFOAM. International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering - M&C, Jeju, Korea.

Culpo, M., "Current bottlenecks in the scalability of OpenFOAM on massively parallel clusters," *PRACE white paper*, pp. 1–13, 2011, [Online]. Available: https://www.prace-ri.eu/IMG/pdf/Current_Bottlenecks_in_the_Scalability_of_OpenFOAM_on_Massively_Parallel_Clusters-2.pdf%5Cnpapers3://publication/uuid/55A0715F-3674-45DE-9A64-D3F9CE41031A.

"Elmer FEM," 2021. http://www.elmerfem.org.

"FeniCS," 2021. https://fenicsproject.org.

Fiorina, C., 2019. Impact of the volume heat source on the RANS-based CFD analysis of Molten Salt Reactors. Ann. Nucl. Energy 134, 376–382. https://doi.org/10.1016/j.anucene.2019.06.024.

Fiorina, C., Mikityuk, K., 2015. Application of the new GeN-Foam multi-physics solver to the European Sodium Fast Reactor and verification against available codes. ICAPP 2015, Nice, France.

Fiorina, C., Clifford, I., Aufiero, M., Mikityuk, K., 2015. GeN-Foam: A novel OpenFOAM® based multi-physics solver for 2D/3D transient analysis of nuclear reactors. Nucl. Eng. Des. 294, 24–37. https://doi.org/10.1016/j.nucengdes.2015.05.035.

Fiorina, C., Aufiero, M., Pelloni, S., Mikityuk, K., 2014. A time-dependent solver for coupled neutron-transport thermalmechanics calculations and simulation of a Godiva promptcritical burst. In: International Conference on Nuclear Engineering, Proceedings, ICONE. https://doi.org/10.1115/ICONE22-30395.

Fiorina, C., Amati, G., Ruggiero, V., Spisso, I., 2018. Partnership for Advanced Computing in Europe SHAPE Project Milano Multiphysics: Evaluation of the Intel Xeon Phi performances for high fidelity nuclear applications. Accessed: Sep. 01, 2020. [Online]. Available: https://prace-ri.eu/wp-content/uploads/WP267.pdf.

Fiorina, C., Radman, S., Koc, M.-Z., Pautz, A., 2019. Detailed modelling of the expansion reactivity feedback in fast reactors using OpenFOAM. International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering - M&C, Portland, US.

Fiorina, C., Kerkar, N., Mikityuk, K., Rubiolo, P., Pautz, A., 2016. Development and verification of the neutron diffusion solver for the GeN-Foam multi-physics platform. Ann. Nucl. Energy 96. https://doi.org/10.1016/j.anucene.2016.05.023.

Fiorina, C., Hursin, M., Pautz, A., 2017. Extension of the GeN-Foam neutronic solver to SP3 analysis and application to the CROCUS experimental reactor. Ann. Nucl. Energy 101, 419–428. https://doi.org/10.1016/j.anucene.2016.11.042.

Fiorina, C., et al., 2021. An initiative for the development and application of open-source multi-physics simulation in support of R&D and E&T in nuclear science and technology. EPJ Web Conf., Volume 247, PHYSOR2020 – International Conference on Physics of Reactors: Transition to a Scalable Nuclear Future. https://doi.org/10.1051/epjconf/202124702040.

Firnhaber, M., Kanzleiter, T.F., Schwarz, S., Weber, G., 1996. International standard problem ISP37: VANAM M3 - A Multi compartment aerosol depletion test with hygroscopic aerosol material: comparison report." OECD/NEA.

"FreeFEM," 2021. https://freefem.org/.

Gaston, D., Newman, C., Hansen, G., Lebrun-Grandié, D., 2009. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. Nucl. Eng. Des. 239 (10), 1768–1778. https://doi.org/10.1016/j.nucengdes.2009.05.021.

GeN-Foam Neutronics, "GeN-Foam/classes/neutronics · master · foam-for-nuclear project / GeN-Foam · GitLab." Available at: https://gitlab.com/foam-for-nuclear/GeN-Foam/-/tree/master/GeN-Foam/classes/neutronics (accessed Nov. 21, 2021).

"GetFEM," 2021. http://getfem.org/.

GeN-Foam Repository, 2021. "GeN-Foam Repository". https://gitlab.com/foam-for-nuclear/GeN-Foam/-/tree/develop.

GeN-Foam Tutorials, 2021. "Tutorials/2D_FFTF, develop branch, foam-for-nuclear project, GeN-Foam, GitLab." https://gitlab.com/foam-for-nuclear/GeN-Foam/-/tree/develop/Tutorials/2D_FFTF (accessed Aug. 31, 2021).

German, P., Ragusa, J.C., Fiorina, C., Tano Retamales, M., 2019. Reduced-order modeling of parametrized multi-physics computations for the molten salt fast reactor. In: International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, M and C 2019, pp. 1808–1817.

German, P., Tano, M.E., Ragusa, J.C., Fiorina, C., 2019. Reduced-order modeling of fluid flows in closed-loop systems. In: Transactions of the American Nuclear Society. https://doi.org/10.13182/T31281.

German, P., Ragusa, J.C., Fiorina, C., 2019. Application of multiphysics model order reduction to doppler/neutronic feedback. EPJ Nucl. Sci. Technol. 5, 17. https://doi.org/10.1051/epjn/2019034.

German, P., Ragusa, J.C., 2019. Reduced-order modeling of parameterized multi-group diffusion k-eigenvalue problems. Ann. Nucl. Energy 134, 144–157. https://doi.org/10.1016/j.anucene.2019.05.049.

German, P., Tano, M., Ragusa, J.C., Fiorina, C., 2020. Comparison of Reduced-Basis techniques for the model order reduction of parametric incompressible fluid flows. Prog. Nucl. Energy 130. https://doi.org/10.1016/j.pnucene.2020.103551.

Hasslberger, J., Boeck, L.R., Sattelmayer, T., 2015. Numerical simulation of deflagration-to-detonation transition in large confined volumes. J. Loss Prev. Process Ind. 36, 371–379. https://doi.org/10.1016/j.jlp.2014.11.018.

Hasslberger, J., Kim, H.K., Kim, B.J., Ryu, I.C., Sattelmayer, T., 2017. Three-dimensional CFD analysis of hydrogen-air-steam explosions in APR1400 containment. Nucl. Eng. Des. 320, 386–399. https://doi.org/10.1016/j.nucengdes.2017.06.014.

Herb, J., Chiriac, F., 2016. One- and Two-Phase Coupling of OpenFOAM with the Thermal-Hydraulic Code ATHLET for Nuclear Safety Analyses. 11th OpenFOAM® Workshop, Guimarães, Portugal.

Hu, T., Cao, L., Wu, H., Du, X., He, M., 2017. Coupled neutronics and thermal-hydraulics simulation of molten salt reactors based on OpenMC/TANSY. Ann. Nucl. Energy 109, 260–276. https://doi.org/10.1016/j.anucene.2017.05.002.

IAEA ONCORE, 2021. "IAEA ONCORE INITIATIVE,", Available at: https://www.iaea.org/topics/nuclear-power-reactors/open-source-nuclear-code-for-reactor-analysis-oncore.

Idelsohn, S.R., Oñate, E., 1994. Finite volumes and finite elements: Two 'good friends'. Int. J. Numer. Meth. Eng. 37 (19), 3323–3341. https://doi.org/10.1002/nme.1620371908.

Introini, C., Cammi, A., Lorenzi, S., Baroli, D., Peters, B., 2017. A 3D CFD Model for the Study of Natural Circulation in the Pavia TRIGA Mark II Research Reactor. NENE 2017, 1–9.

Jareteg, K., Vinai, P., Demazière, C., 2014. Fine-mesh deterministic modeling of PWR fuel assemblies: Proof-of-principle of coupled neutronic/thermal-hydraulic calculations. Ann. Nucl. Energy 68, 247–256. https://doi.org/10.1016/j.anucene.2013.12.019.

Kampili, M., Kelm, S., Dehbi, A., Allelein, H.-J., 2019. Development of a Continuous Random Walk model based on normalized Langevin equation in OpenFOAM for turbulent dispersion of particles and validation against DNS statistics. 7th ESI OpenFOAM Conference, Berlin, Germany.

Kelm, S., et al., 2021. The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H2/CO Mitigation and Aerosol Transport. Fluids 6 (3), 100. https://doi.org/10.3390/fluids6030100.

Kirk, B.S., Peterson, J.W., Stogner, R.H., Carey, G.F., 2006. libMesh : a C++ library for parallel adaptive mesh refinement/coarsening simulations. Eng. Comput. 22 (3–4), 237–254. https://doi.org/10.1007/s00366-006-0049-3.

Kliem, S., Tromm, W., Reinecke, E.-A., 2018. Reactor safety research within the Helmholtz Association. Kerntechnik 83 (5), 400–406. https://doi.org/10.3139/124.110888.

Laureau, A., Heuer, D., Merle-Lucotte, E., Rubiolo, P.R., Allibert, M., Aufiero, M., 2017. Transient coupled calculations of the Molten Salt Fast Reactor using the Transient Fission Matrix approach. Nucl. Eng. Des. 316, 112–124. https://doi.org/10.1016/j.nucengdes.2017.02.022.

Laureau, A., Lederer, Y., Krakovich, A., Buiron, L., Fontaine, B., 2018. Spatial analysis of unprotected transients in heterogeneous sodium fast reactors. Ann. Nucl. Energy 115, 554–564. https://doi.org/10.1016/j.anucene.2018.01.029.

Le, D., Labahn, J., Beji, T., Devaud, C.B., Weckman, E.J., Bounagui, A., 2018. Assessment of the capabilities of FireFOAM to model large-scale fires in a well-confined and mechanically ventilated multi-compartment structure. J. Fire Sci. 36 (1), 3–29. https://doi.org/10.1177/0734904117733427.

Leppänen, J., 2014. Development of a CAD based geometry model in serpent 2 Monte Carlo code. Trans. Am. Nucl. Soc. 111, 663–667.

Leppänen, J., Aufiero, M., 2014. "Development of an unstructured mesh based geometry model in the Serpent 2 Monte Carlo code — VTT's Research Information Portal," 2014. Accessed: Jan. 22, 2021. [Online]. Available: https://cris.vtt.fi/en/publications/development-of-an-unstructured-mesh-based-geometry-model-in-the-s.

Liu, X., Kelm, S., Kampili, S.M., 2019. Development and verification of a Monte Carlo radiation solver for thermal radiation. 14th OpenFOAM Workshop, Duisburg, Germany.

Lorenzi, S., Cammi, A., Luzzi, L., Rozza, G., 2016. POD-Galerkin method for finite volume approximation of Navier-Stokes and RANS equations. Comput. Methods Appl. Mech. Eng. 311, 151–179. https://doi.org/10.1016/j.cma.2016.08.006.

Lorenzi, S., Cammi, A., Luzzi, L., Rozza, G., 2017. A reduced order model for investigating the dynamics of the Gen-IV LFR coolant pool. Appl. Math. Model. 46, 263–284. https://doi.org/10.1016/j.apm.2017.01.066.

Martineau, M., Posey, S., Spiga, F., 2020. AmgX GPU Solver Developments for OpenFOAM. Available at: https://www.esi-group.com/sites/default/files/resource/other/1672/8th_OpenFOAM_Conference_NVIDIA_Posey.pdf.

Mattioli, A.S., Fiorina, C., Lorenzi, S., Cammi, A., 2020. Derivation and implementation in OpenFOAM of a point-kinetics model for Molten Salt Reactors. ANS Winter Meeting. American Nuclear Society, Whashington DC, US. Available at: https://www.esi-group.com/sites/default/files/resource/other/1672/8th_OpenFOAM_Conference_NVIDIA_Posey.pdf.

OpenFOAM Technical Committees, 2021. "OpenFOAM Technical Committees". https://www.openfoam.com/governance/technical-committees.php#tm-nuclear.

"OpenFOAM," 2021. www.openfoam.com.

"OpenFOAM Foundation," 2021. www.openfoam.org.

Pizzocri, D., Barani, T., Luzzi, L., 2020. SCIANTIX: A new open source multi-scale code for fission gas behaviour modelling designed for nuclear fuel performance codes. J. Nucl. Mater. 532, 152042 https://doi.org/10.1016/j.jnucmat.2020.152042.

Radman, S., Fiorina, C., Pautz, A., 2019. Preliminary development of a coarse-mesh sodium boiling model for OpenFOAM based multi-physics solvers. 8th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH 2019), Portland, OR.

Radman, S., Fiorina, C., Pautz, A., 2021. Development of a Novel Two-Phase Flow Solver for NuclearReactor Analysis: Validation against Sodium Boiling Experiments. Nuclear Engineering and Design.

Radman, S., Fiorina, C., Mikityuk, K., Pautz, A., 2019. A coarse-mesh methodology for modelling of single-phase thermal-hydraulics of ESFR innovative assembly design. Nucl. Eng. Des. 355 https://doi.org/10.1016/j.nucengdes.2019.110291.

Radman, S., Fiorina, C., Pautz, A., 2021. Development of a Novel Two-Phase Flow Solver for Nuclear Reactor Analysis: Algorithms, Verification and Implementation in OpenFOAM. Nucl. Eng. Des. 379, 111178. https://doi.org/10.1016/j.nucengdes.2021.111178.

Radman, S., Fiorina, C., Song, P., Pautz, A., n.d. Development of a point-kinetics model in OpenFOAM, integrationin GeN-Foam, and validation against FFTF experimental data. Annals of Nuclear Energy. in press.

Sartori, A., Cammi, A., Luzzi, L., Rozza, G., 2016. A multi-physics reduced order model for the analysis of Lead Fast Reactor single channel. Ann. Nucl. Energy 87, 198–208. https://doi.org/10.1016/j.anucene.2015.09.002.

Scolaro, A., Clifford, I., Fiorina, C., Pautz, A., 2020. The OFFBEAT multi-dimensional fuel behavior solver. Nucl. Eng. Des. 358 https://doi.org/10.1016/j.nucengdes.2019.110416.

Scolaro, A., Robert, Y., Fiorina, C., Clifford, I., Pautz, A., 2019. Coupling methodology for the multidimensional fuel performance code offbeat and the Monte Carlo neutron transport code SERPENT. GLOBAL 2019 - TOP FUEL 2019 Conference, Seattle, US. https://www.scopus.com/inward/record.uri?eid=2-s2.0-85081089291&partnerID=40&md5=1a5a962f0eb915c2ed4788b023a3da4.

Scolaro, A., Fiorina, C., Clifford, I., Pautz, A., 2019. Multi-dimensional Creep Analysis Using the Novel OFFBEAT. Technical Meeting on Progress on Pellet Cladding Interaction and Stress Corrosion Cracking: Experimentation, Modelling and Methodologies Applied to Support the Flexible Operation of Nuclear Power Plants, Aix-en-Provence (France). Availabe at: https://www-pub.iaea.org/MTCD/publications/PDF/TE-1960web.pdf.

Scolaro, A., Fiorina, C., Van Uffelen, P., Clifford, I.D., Pautz, A., Schubert, A., 2021. Coupling Methodology Between TRANSURANUS and the Multi-Dimensional Fuel Performance Code OFFBEAT. ANS Winter Meeting. American Nuclear Society, Whashington DC, US. ANS Winter Meeting.

Scolaro, A., Fiorina, C., Clifford, I., Pautz, A., 2021. Development of a semi-implicit contact methodology for finite volume stress solvers. Int. J. Numer. Meth. Eng. 1–30 https://doi.org/10.1002/nme.6857.

Scolaro, P., van Uffelen, C., Fiorina, A., Clifford, Schubert I., Pautz, A., 2021. Investigation on the effect of eccentricity for fuel disc irradiation tests. Nucl. Eng. Technol. 53, 1602–1611.

Sorrell, N.C., Hawari, A.I., 2019. TREAT M2 experiment modeling for transient benchmark analysis. Ann. Nucl. Energy 128, 398–405. https://doi.org/10.1016/j.anucene.2019.01.026.

Spisso, I., Amati, G., Ruggiero, G., Fiorina, C., 2018. PPorting, optimization and bottleneck of OpenFOAM in KNL environment. Tech. rep., Intel eXtreme Performance Users Group (IXPUG). Available at: http://tiny.cc/ry47kz2018.

Tuković, Ž., Ivanković, A., Karač, A., 2013. Finite-volume stress analysis in multi-material linear elastic body. Int. J. Numer. Meth. Eng. 93 (4), 400–419. https://doi.org/10.1002/nme.4390.

Vijaya Kumar, G., et al., 2021. Implementation of a CFD model for wall condensation in the presence of non-condensable gas mixtures. Appl. Therm. Eng. 187, 116546. https://doi.org/10.1016/j.applthermaleng.2021.116546.

Wan, C., Hu, T., Cao, L., 2020. Multi-physics numerical analysis of the fuel-addition transients in the liquid-fuel molten salt reactor. Ann. Nucl. Energy 144, 107514. https://doi.org/10.1016/j.anucene.2020.107514.

Wielenberg, A., et al., 2019. Recent improvements in the system code package AC2 2019 for the safety analysis of nuclear reactors. Nucl. Eng. Des. 354 https://doi.org/10.1016/j.nucengdes.2019.110211.

Wu, H., Rizwan-Uddin, 2016. A tightly coupled scheme for neutronics and thermal-hydraulics using open-source software. Annal. Nucl. Energy 87 (P2), 16–22. https://doi.org/10.1016/j.anucene.2015.08.004.