A Novel Multiscale and Multiphysics Software Development for LWR Simulation in Support of the UK Nuclear Renaissance

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SUMMARY

- A multiscale and multiphysics software development, including a customized coupling environment and improved codes, is necessary to meet the needs of the nuclear community in the UK.
- This software development incorporates neutron transport, fluid mixing, and solid dynamics methods, and is designed to deliver results at the fuel pin or materials level using relatively few processors.
- Validation and verification of the multiscale and multiphysics software are being conducted to ensure it becomes state-of-the-art.

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1. INTRODUCTION

Nuclear reactors are a vital energy source for the United Kingdom (UK) to meet energy needs and reduce CO_2 emissions. The growing energy demand, driven by expanding electric infrastructure, has traditionally been met by fossil fuel power plants that emit significant amounts of CO_2 [1], and recently been supported by renewable power plants that are affected by adverse weather [2]. However, nuclear reactors offer a reliable and sustainable alternative with high output and no CO_2 emissions, unaffected by weather conditions.

The UK government is investing in new nuclear reactors to support energy supply [3]. Two Evolutionary Pressurised Water Reactors (EPR) by Framatome are under construction at Hinkley Point C, with plans for two more at Sizewell C, each generating 1.6 GWe and featuring advanced efficiency and safety systems [4]. The Advanced Modular Pressurised Reactor (AMR) by Rolls Royce, Modular Boiling Reactor (BWRX) by GE Hitachi, and Small Modular Pressurised Reactor (SMR) by Holtec are under design and could be built at various locations, each generating 470, 300, and 300 MWe, and including modularity and flexibility [5]. The Department of Business, Energy, and Industrial Strategy (BEIS) has launched a nuclear research and development program to enhance the efficiency and safety of reactors, focusing on advanced fuels, digital design, safety measures, recycling, manufacturing, and a national toolkit [6].

Nuclear simulation software is a vital tool for the UK to enhance the efficiency and safety of nuclear reactors. Reactor design and operation, supported through the modelling of physical phenomena, have relied on conservative safety margins due to the simplicity of simulation methods and computational limitations. However, the advancement of simulation methods and computational resources could enable less conservative safety margins maintaining safety and improving performance.

The UK government is also investing in new simulation software to improve reactor design and operation [7]. Simulation software can be categorized based on requirements: “State-of-the-science” includes new methods not widely used in academia. “State-of-the-art” encompasses methods commonly used in academia and partially in industry. “Acknowledged rules of technology” consists of standard methods used in both academia and industry. To be effective for the nuclear community in the UK, simulation software should meet several key needs: reduce conservative safety margins, enable data transfer between software, improve the simulation of coupled physical phenomena, and be user-friendly.

Coupling in simulation software refers to how different codes depend on each other and share information [8].There are two types of coupling: loose and tight. In loose coupling, simulations of coupled physical phenomena occur separately in different codes. It can be divided into internal coupling, which merges codes with significant changes, and external coupling, which keeps codes separate with minimal changes. In tight coupling, simulations of coupled physical phenomena occur simultaneously within one code. Coupling can also be one-way or two-way. In one-way coupling, data flows only in one direction from one code to another, while in two-way coupling, data flows back and forth between the codes.

Historically, nodal codes have been used to simulate simplified coupled reactor physics using neutron diffusion, non-mixing fluid, and solid dynamics. They offer results at the fuel assembly level after fuel assembly homogenization [9], or at the fuel pin level after fuel pin power reconstruction [10], neglecting some coupled physical phenomena. Past computational limitations hindered detailed simulations of coupled reactor physics due to complex shapes, materials, large system sizes, and long calculation times. These methods and limitations have contributed to conservative safety margins in reactor design and operation.

Recently, improved codes have been developed to simulate advanced or fully coupled reactor physics using neutron transport and mixing fluid–solid dynamics. They offer results at the fuel pin level after fuel pin homogenization, or at the material level without homogenization, capturing more coupled physical phenomena [11–13]. Present computational resources as clusters can enhance detailed simulations of coupled reactor physics with complex shapes and materials, large system sizes, and short calculation times. These new methods and resources could contribute to less conservative safety margins in reactor design and operation.

Now, coupling software environments (CSE) such as Simulation Numerique par Architecture Logicielle en Open Source et a Methodologie d'Evolution (SALOME) [14], Virtual Environment for Reactor Applications (VERA) [15], and Multi-physics Object Oriented Simulation Environment (MOOSE) [16] are being created to couple different codes or physics using a simple interface or a fully integrated framework. Also, Multiscale and Multiphysics software developments (MMSD) such as Nuclear Reactor Simulator (NURESIM) and Consortium for Advanced Simulation of Light Water Reactors (CASL) are being created to simulate improved or full coupled reactor physics using the improved codes and CSE. These CSE and MMSD meet some of the needs of the nuclear community in the UK.

1.1. NURESIM and CASL

The NURESIM [17] MMSD was developed and is being updated by multiple partners with funding from the European Atomic Energy Community (EURATOM), which can be observed in Figure 1.

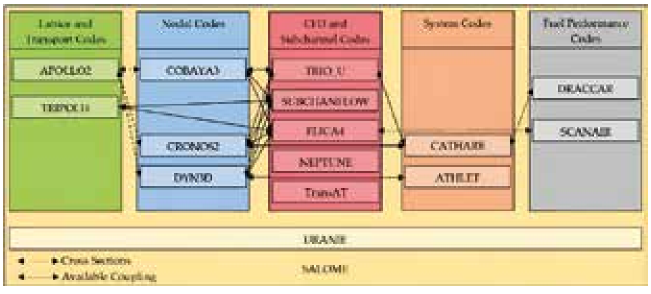


FIGURE 1: NURESIM.

NURESIM includes SALOME to couple nodal, subchannel, system, and fuel performance codes, providing simplified or improved reactor physics [18–20]. It also incorporates lattice, transport, and computational fluid dynamics (CFD) codes, and other software to generate cross sections, verify results and for uncertainty quantification. Despite being state-of-the-art, NURESIM does not meet all the needs of the nuclear community in the UK as it lacks neutron transport methods for reasons other than to verify results, not providing full coupled reactor physics.

The CASL [21] MMSD was developed and is being updated by multiple partners with funding from the United States Department of Energy (USDOE), which can be observed in Figure 2.

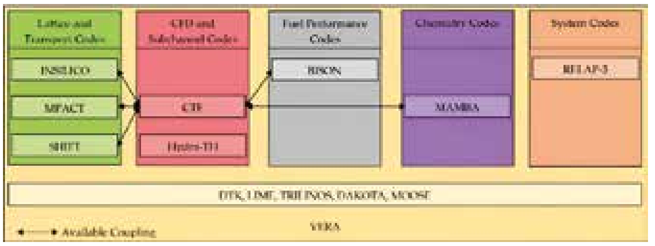


FIGURE 2: CASL.

CASL includes VERA to couple transport, subchannel, fuel performance, chemistry, and system codes, providing improved or full coupled reactor physics [22–24]. It also incorporates transport and CFD codes, and other software to verify results and for meshing, solving, uncertainty quantification, and coupling. Despite being state-of-the-art, CASL does not meet all the needs of the of the nuclear community in the UK as it requires thousands of processors not typically available to produce results in under a day, providing full coupled reactor physics in all the reactor core.

1.2. Alternative Multiscale and Multiphysics Software Development

An alternative MMSD [25] is being developed by the University of Liverpool (UOL) with funding from the Engineering & Physical Sciences Research Council (EPSRC), which can be observed in Figure 3.

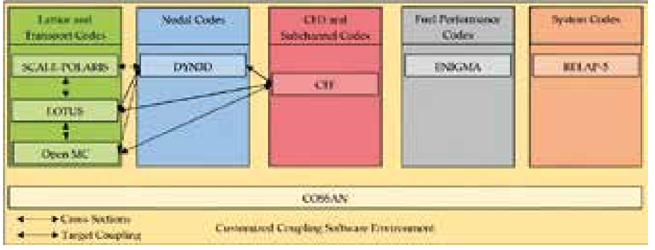


FIGURE 3: Alternative MMSD.

This MMSD includes a customised CSE to couple the LOTUS transport, the DYN3D nodal, and the CTF subchannel codes, providing simplified, improved or full coupled reactor physics. It also incorporates the SCALE-POLARIS lattice and Open MC transport codes to generate cross sections and verify results. It could also include other codes in the future. It will meet the needs of the UK nuclear community, even though the CSE and improved codes are still under development. It uses advanced neutron transport methods not just for verification but to improve nuclear reactor efficiency and safety. It requires only a few processors to produce results in under a day, making it affordable as it can be run on a personal computer. It provides full coupled reactor physics in the fuel assemblies of interest, with boundary conditions obtained from simplified coupled reactor physics in all the reactor core, allowing the use of improved methods while minimizing computational resources usage. It is optimised for research purposes but can be extended for industrial purposes. A reactor core with fuel assemblies where boundary conditions are applied is shown in Figure 4.

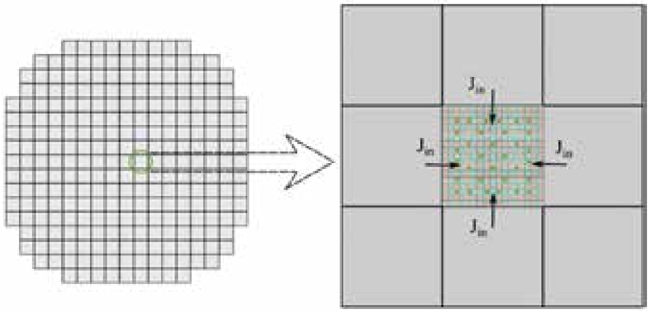


FIGURE 4: Reactor core at the fuel assembly level and fuel assembly at the fuel pin or materials levels.

1.3. Validation and Verification

Validating and verifying this MMSD is essential for it to become state-of-the-art. This process involves comparing the codes and their couplings to experimental data or other code results, typically using benchmarks that contain them. Validation and verification can target either the software or its solution [26]. Software validation and verification focuses on identifying and fixing errors in methods or source code, while solution validation and verification ensures the accuracy of inputs and outputs. Validation and verification can also be performed from academic and industrial perspectives. Academically, codes and couplings are tested to demonstrate their principles and use, usually resulting in local deployment. Industrially, they are further developed and tested for broader applications, leading to wider deployment.

1.4. Aim and Objectives

The aim is to develop this alternative MMSD, along with its validation and verification. This includes several objectives:

- Verify the accuracy and methodology of LOTUS in providing neutronics at the material level.
- Validate and verify the accuracy and methodology of CTF and FLOCAL (module of DYN3D) in delivering thermal hydraulics at the heater rod level.
- Implement a one-way coupling between DYN3D and CTF and verify the coupling and improved feedback at the fuel pin level.
- Implement a two-way coupling between DYN3D and CTF and verify the coupling and improved coupled reactor physics at the fuel pin level.
- Develop a multi-way coupling between LOTUS, CTF, and DYN3D and verify the coupling and full coupled reactor physics at the fuel pin or materials level.

2. MULTISCALE AND MULTIPHYSICS SOFTWARE DEVELOPMENT

The alternative MMSD is presented, along with its validation and verification. The process begins with a review of the theory including neutronics, thermal hydraulics, and coupled reactor physics and the codes used encompassing SCALE-POLARIS, LOTUS, Open MC, DYN3D, and CTF. Next, the benchmarks covered in the validations and verifications are introduced, including the PSBT, FLOCAL developer, KAIST, and customised benchmarks.

Neutronics verification of LOTUS follows, detailing methods applied in LOTUS and Open MC and presenting results for a 17x17 fuel assembly. Thermal-hydraulics validations and verifications of CTF and FLOCAL are then conducted, including methods used in both codes and results obtained for 5x5 and 2x1 bundles.

The one-way coupling between DYN3D and CTF and its verification are then covered encompassing methods used in SCALE-POLARIS, DYN3D, and CTF, coupling scripts created for the coupling, and resulting data for a 17x17 fuel assembly. Next, the two-way coupling between DYN3D and CTF and its verification are performed including modifications to DYN3D, the customised CSE developed for the coupling, methods employed in SCALE-POLARIS, DYN3D, and CTF, and results for a 17x17 fuel assembly.

Finally, the multi-way coupling between LOTUS and CTF with DYN3D and its verification are addressed including modifications to Open MC, the customised CSE that enables the coupling, methods used in all relevant codes, and results for a 3x3 quarter core with reflectors composed of 17x17 fuel assemblies or a 34x34 quarter core without reflectors.

2.1. Theory and Codes

Accurate simulation of the physical phenomena in a nuclear reactor relies on the interaction between neutronics and thermal hydraulics, which are represented in codes such as SCALE-POLARIS, LOTUS, Open MC, DYN3D, and CTF. Hence, the theory and codes used are initially presented in this MMSD.

In neutronics, the neutron transport equation describes the neutrons balance in a nuclear reactor, including processes like streaming, absorption, scattering, fission, and decay. Due to its complexity, an analytical solution is not feasible, so a numerical solution is obtained using deterministic or probabilistic approximations. Deterministic approximations apply mathematical methods to solve the mentioned equation. Probabilistic approximations apply statistical methods to represent the phenomena associated to the previous equation.

In thermal hydraulics, the fluid and solid dynamics equations describe the fluids and solids behaviour in a nuclear reactor including processes like advection, pressure losses, turbulence, phase changes, and heat transfer. Due to their complexity, analytical solutions are not possible, so numerical solutions are obtained using deterministic approximations. These approximations use mathematical methods to solve the mentioned equations.

In coupled reactor physics, the power equation and cross-section feedback describe the relations between power density and fission reaction rate, as well as between cross sections and the fuel temperature, moderator temperature and density, and boron concentration. The complexity of these relations also prevents analytical solutions, requiring numerical approximations.

SCALE [27,28] is a comprehensive deterministic and probabilistic neutronics analysis code system developed and maintained by Oak Ridge National Laboratory (ORNL). Methods in the POLARIS module include Multi-Group (MG), Embedded Self-Shielded Method (ESSM), Method of Characteristics (MOC), homogenisation, steady and transient states. SCALE offers configurable accuracy and computational performance and has been extensively validated and verified. As state-of-the-art software, it is well-suited for generating cross-sections for other neutronics codes across multiple levels.

LOTUS [29,30] is a deterministic transport code for neutronics analysis developed at Rheinisch-Westfälische Technische Hochschule Aachen (RWTH) and further developed by UOL. It supports methods like MG, Current Coupled Collision Probability with orthonormal polynomial expansion (CCCPO), flexible treatment of albedo boundary conditions, and steady state. LOTUS delivers high accuracy with moderate computational performance and has undergone partial verification. As state-of-the-science software, it is selected for modelling neutron transport at the fuel pin and materials levels.

Open MC [31,32] is a probabilistic transport code for neutronics analysis developed at the Massachusetts Institute of Technology (MIT) and maintained by UChicago Argonne. It implements methods like Continuous Energy (CE) or MG, Monte Carlo (MC), and steady state. Open MC is recognized for very high accuracy—albeit with lower computational performance—and is extensively validated and verified. As state-of-the-art software, it is ideal for verifying other neutronics codes at the materials level.

DYN3D [33,34] is a deterministic nodal code for neutronics and thermal hydraulics analysis developed by Forschung Dresden Rossendorf (FDR) and updated by Helmholtz Zentrum Dresden Rossendorf (HZDR). Methods in the NK (Neutron Kinetics) and FLOCAL (Thermal Hydraulics) modules encompass MG, diffusion, Nodal Expansion Method (NEM), fuel pin power reconstruction, control rods, fluid mixture, channel, pressure losses, boiling, heat transfer regime, fuel rods, steady and transient states. DYN3D offers lower accuracy, but high computational performance and is widely validated and verified. As part of the acknowledged rules of technology, it is appropriate for modelling simplified coupled reactor physics at the fuel assembly and pin levels.

CTF [35,36] is a deterministic subchannel code for thermal hydraulics analysis developed by Pacific Northwest Laboratories (PNWL) and updated by Pennsylvania State University (PSU) and North Carolina State University (NCSU). It applies methods like two fluids three fields, subchannel, flow regime, pressure losses, drag, turbulent mixing, boiling, entrainment, heat transfer regime, fuel rods, steady and transient states. CTF offers high accuracy and moderate computational performance and is extensively validated and verified. As a state-of-the-art code, it is selected for modelling mixing fluid and solid dynamics at the fuel pin level.

2.2. Benchmarks

Necessary data to model the physical phenomena in a nuclear reactor includes the geometry, materials, and boundary conditions available in benchmarks like the PSBT, KAIST, FLOCAL developer, and customized benchmarks. Hence, the benchmarks used are initially presented in this MMSD.

The PSBT benchmark [37,38] is a validated and verified benchmark by the OECD (Organisation for Economic Cooperation & Development) for light water reactor (LWR) thermal hydraulics, previously covered using CTF [39,40]. It includes a 5x5 bundle with heater rods, guide tubes, and a wide range of boundary conditions. The FLOCAL developer benchmark is a proposed benchmark by HZDR for LWR thermal hydraulics not covered before. It includes a 2x1 bundle with heater rods and a single set of boundary conditions. The PSBT 5x5 bundle and FLOCAL developer 2x1 bundle geometries can be observed in Figure 5.

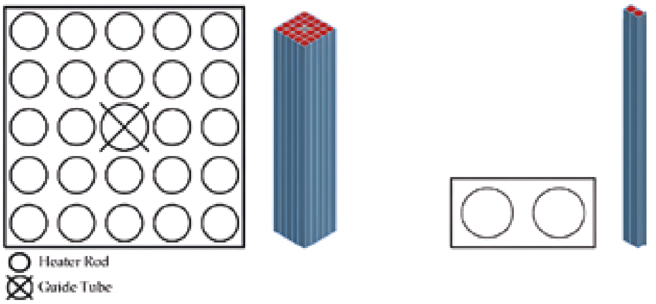


FIGURE 5: PSBT 5x5 bundle and FLOCAL developer 2x1 bundle geometry.

The KAIST-1A benchmark [41] is a less verified benchmark than the PSBT benchmark by KAIST (Korean Advanced Institute of Science & Technology) for pressurised water reactors (PWR) neutronics previously assessed using other neutronics codes [42,43]. It includes a 17x17 fuel assembly with fuel pins, burnable absorber pins, guide tubes, and several boundary conditions. The modified KAIST-1A benchmark is a variation of the original benchmark. It includes different boundary conditions. The KAIST-1A MOX benchmark is another verified benchmark [44]. It includes a 17x17 fuel assembly with fuel and Mixed Oxide Fuel (MOX) pins, guide tubes, and different boundary conditions. The KAIST 17x17 fuel assembly geometry can be observed in Figure 6.

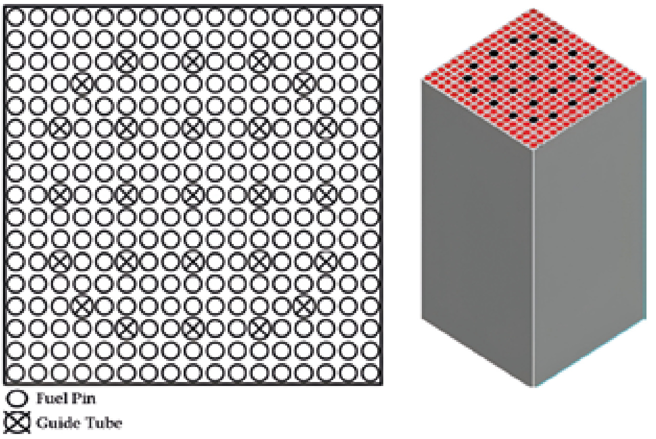


FIGURE 6: KAIST 17x17 fuel assembly geometry.

The customised benchmark is a proposed benchmark for PWR neutronics and thermal hydraulics. Initially, it includes a 3x3 quarter core with reflectors, fuel assemblies, burnable absorber assemblies, and global boundary conditions to obtain local boundary conditions. Finally, it includes 17x17 fuel assemblies and a 34x34 quarter core without reflectors with fuel pins, burnable absorber pins, guide tubes and the previously obtained local boundary conditions. The customised 3x3 quarter core with reflectors, 17x17 fuel assembly and 34x34 quarter core without reflectors geometry can be observed in Figure 7.

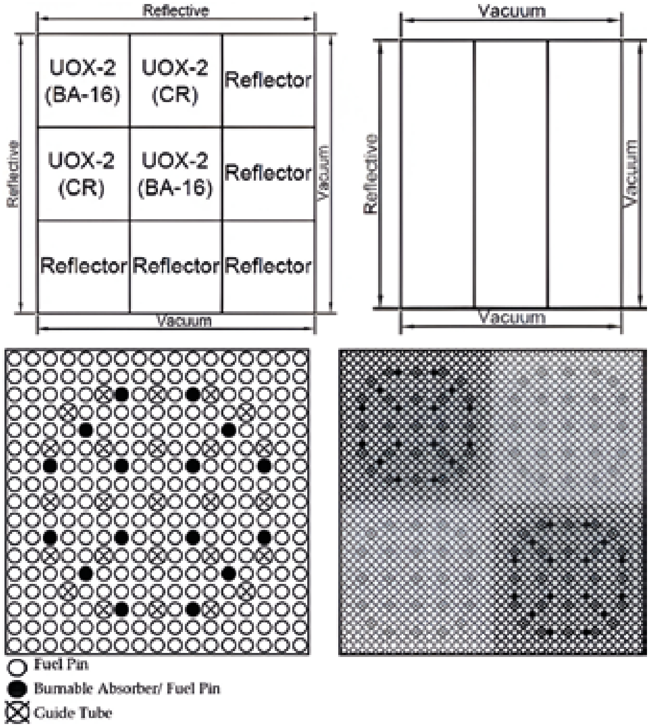


FIGURE 7: Customised 3x3 quarter core with reflectors, 17x17 fuel assembly and 34x34 quarter core without reflectors.

2.3. Code Validations and Verifications

Validation and verification of the codes in this MMSD are essential to ensure their improved accuracy and methodology soundness and justify their selection to provide neutronics or thermal hydraulics at the fuel pin or materials levels. Accordingly, targeted validations and verifications of the codes were conducted as part of this MMSD.

The development and application of LOTUS to provide neutronics at the fuel pin and materials levels are central to this research. High accuracy and a flexible methodology can be achieved through the CCCPO, variable order of expansion, and albedo boundary conditions. Hence, a verification of the accuracy and methodology available in LOTUS to provide neutronics at the materials level was performed through the KAIST MOX benchmark [45].

In Open MC, cross sections for the 17x17 fuel assembly were created using methods like ACE and MC. LOTUS and Open MC then simulated the 17x17 fuel assembly using methods such as MG or CE, CCCPO or MC, variable order of expansion, and full reflection. Power distribution differences between LOTUS and Open MC are presented for the 17x17 fuel assembly in Figure 8.

LOTUS provides similar accuracy and a flexible methodology in a 17x17 fuel assembly through the transversal power distribution differences when compared to Open MC. Differences occurred due to the variable order of expansion, error cancellation between MG and CE, and the CCCPO and MC methods. Other local verifications of LOTUS are also available [30,46].

The accuracy and methodology available in CTF and FLOCAL to provide thermal-hydraulics at the heater rod level are not so well known in research. Variable accuracy and methodology can be achieved by including different crossflow and turbulent mixing. Therefore, a validation and verification of the accuracy available

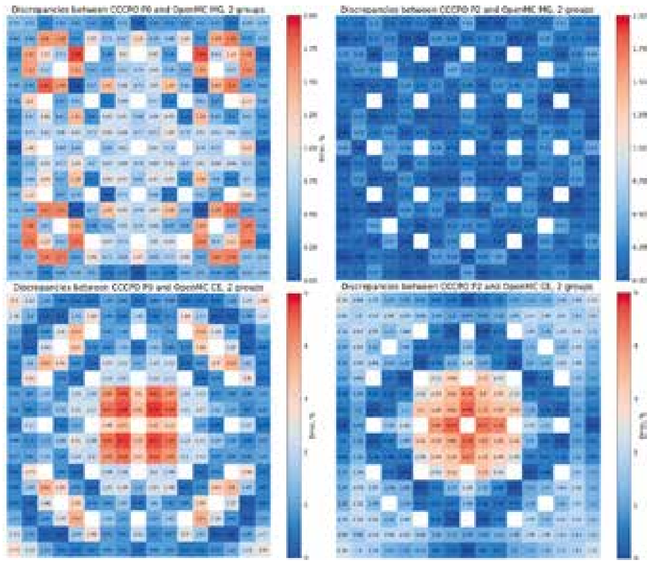


FIGURE 8: 17x17 fuel assembly LOTUS vs Open MC power distribution differences.

in CTF and a verification of the methodology available in CTF and FLOCAL to provide thermal-hydraulics at the heater rod level were done separately through the PSBT and FLOCAL developer benchmarks [47].

In CTF and FLOCAL, the 5x5 and 2x1 bundles were simulated, through subchannel or channel, nucleate boiling, different crossflow, and turbulent mixing methods. Void fraction mean values and errors for CTF, experimental data and other codes are presented for the 5x5 bundle in Figure 9.

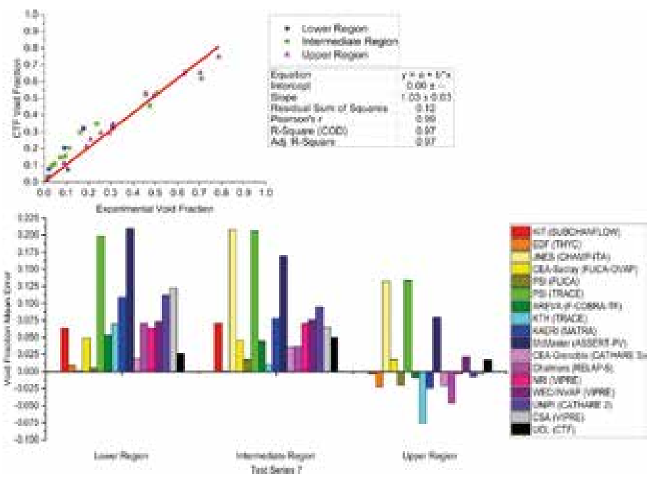


FIGURE 9: 5x5 bundle CTF vs experimental and CTF vs other codes void fraction mean error.

CTF provides high accuracy in a 5x5 bundle through the void fraction mean values and errors when compared to experimental data and other thermal hydraulics codes. Differences occurred due to the nucleate boiling, crossflow, and turbulent mixing methods, and the different nature of the codes. Void fraction distributions for CTF and FLOCAL are presented for the 2x1 bundle in Figure 10.

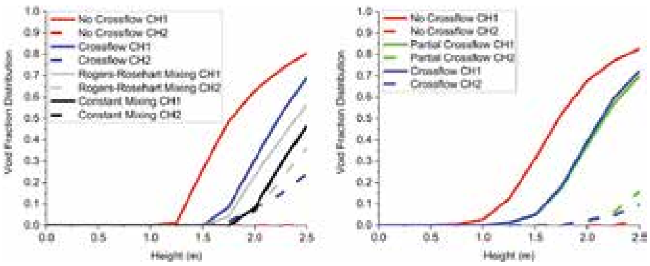


FIGURE 10: 2x1 bundle CTF vs FLOCAL void fraction distribution.

CTF provides a wider methodology in a 2x1 bundle through the void fraction distribution compared to FLOCAL. Other methods in FLOCAL, apart from the no-crossflow method, were only available during its development. Differences occurred due to the range of fluid mass, momentum, energy transfer, turbulent mixing, subchannel, or channel methods.

2.4. Coupling Verifications

Verification of the couplings in this MMSD is essential for it to become state-of-the-art, these being gradually implemented to show the improved or full coupled reactor physics at the fuel pin or materials levels. Accordingly, verifications of the couplings were carried out in this MMSD.

Simplified coupled reactor physics at the fuel pin level involves 3D neutron diffusion and non-mixing fluid and solid dynamics. These are available in DYN3D after performing fuel pin power reconstruction or fuel pin homogenisation. However, improved feedback can become available after transferring the power distributions in a one-way coupling between DYN3D and CTF at the fuel pin level. Hence, a verification of the coupling and improved feedback at the fuel pin level in the one-way coupling between DYN3D and CTF was performed through the KAIST benchmark [48] and coupling scripts.

Cross sections for the 17x17 fuel assembly were generated in SCALE-POLARIS through methods like ESSM and MOC for two energy groups. The 17x17 fuel assembly was simulated in DYN3D and CTF using methods like two energy groups, NEM, full reflection, channel or subchannel, nucleate boiling, and in CTF, crossflow and turbulent mixing.

The coupling scripts extract, normalise, and import the power distributions from DYN3D to CTF. Convergence was achieved only in each code. The one-way coupling between DYN3D and CTF is available in Figure 11.

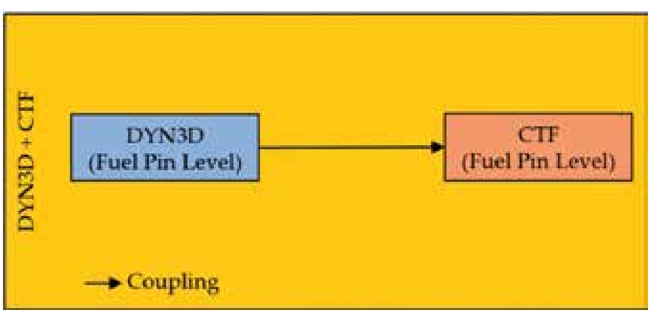


FIGURE 11: One-way coupling between DYN3D and CTF.

Fluid temperature mean values and distributions for DYN3D and the one-way coupling between DYN3D and CTF are presented for the 17x17 fuel assembly in Figure 12.

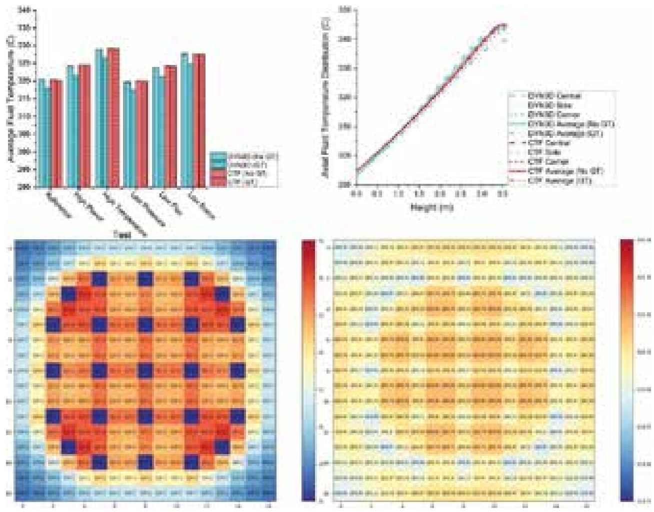


FIGURE 12: 17x17 fuel assembly DYN3D vs DYN3D + CTF average fluid temperature value and distributions.

The one-way coupling between DYN3D and CTF provided improved fluid temperature distributions in the 17x17 fuel assembly when compared to DYN3D. Differences occurred due to the variation of boundary conditions, different methods such as the channel or subchannel, nucleate boiling, and the absence or presence of crossflow and turbulent mixing.

Improved coupled reactor physics at the fuel pin level involves 3D neutron diffusion with mixing fluid and solid dynamics. These are not available in DYN3D, requiring the decoupling of NK from FLOCAL and recoupling to CTF. Then, improved coupled reactor physics can become available after transferring the power and feedback distributions until achieving convergence in a two-way coupling between DYN3D and CTF at the fuel pin level. Therefore, a verification of the coupling and improved coupled reactor physics at the fuel pin level in the two-way coupling between DYN3D and CTF was done through modifications to DYN3D, the customized CSE, and the modified KAIST benchmark [49].

The generation of cross sections for the 17x17 fuel assembly for two energy groups was performed in SCALE-POLARIS through the ESSM and MOC methods. The simulation of the 17x17 fuel assembly was performed in DYN3D and CTF through two energy groups, NEM, partial reflection, channel or subchannel, heat transfer, and without or with crossflow and turbulent mixing methods.

Modifications to DYN3D allow the decoupling of NK from FLOCAL and recoupling of CTF to DYN3D. The customized CSE executes a loop that runs DYN3D, followed by power exportation, under relaxation and importation, and then runs CTF, followed by feedback exportation, under relaxation and importation. The loop is executed until achieving convergence between codes.

The two-way coupling between DYN3D and CTF can be observed in Figure 13.

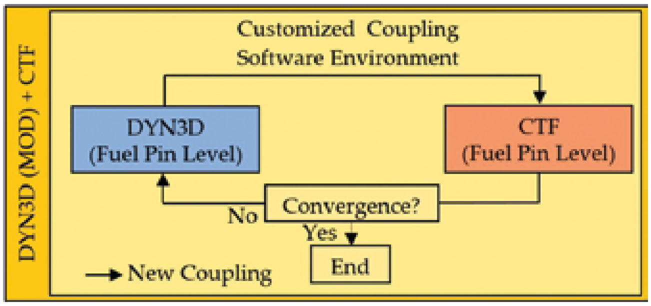
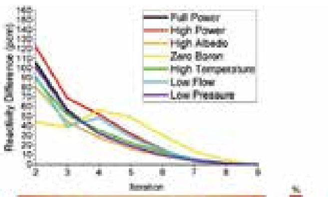


FIGURE 13: Two-way coupling between DYN3D and CTF.

Effective multiplication factor, convergence, average traversal power distributions and differences between DYN3D and the two-way coupling between DYN3D are presented for the 17x17 fuel assembly in Figure 14.

Test	UOX-2 (CR) Fuel Assembly	
	Effective Multiplication Factor	
	DYN3D + CTF	DYN3D
Full Power	1.23733	1.23923
High Power	1.23097	1.23387
High Albedo	1.23855	1.24018
Zero Boron	1.33532	1.33922
High Temperature	1.23445	1.23635
Low Flux	1.23594	1.23796
Low Pressure	1.23715	1.23897



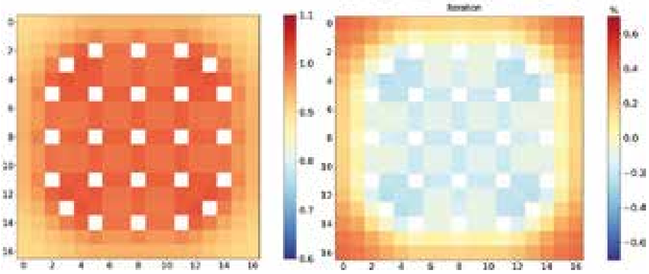


FIGURE 14: 17x17 fuel assembly DYN3D vs DYN3D + CTF effective multiplication factor, convergence, power distribution and differences.

The two-way coupling between DYN3D and CTF provided improved effective multiplication factor values and convergence, transversal power distributions and differences in the 17x17 fuel assembly when compared to DYN3D. Differences and convergence occurred due to the variation of boundary conditions, different fuel rod, nucleate boiling, interphase, crossflow, turbulent mixing, channel, subchannel, and under-relaxation methods.

Full coupled reactor physics at the fuel pin or materials level involves 3D neutron transport, mixing fluid and solid dynamics. For a reactor core, this would lead to long computational times, although for fuel assemblies with additional boundary conditions, this would lead to lower computational times. Only 2D neutron transport is available in LOTUS, while 3D neutron diffusion is available in DYN3D, and 3D neutron transport is available in Open MC, so a combination of 2D transversal neutron transport or diffusion and 1D axial neutron diffusion can be obtained through power 2D to 3D conversion. Also, 3D mixing fluid and solid dynamics are available in CTF, while 3D non-mixing fluid dynamics are available in DYN3D, which can be used for cross section interpolation and 3D to 2D conversion. Partial albedo boundary conditions are available from DYN3D and can be included for neutron leakage in LOTUS or DYN3D but not in Open MC, requiring modifications to adjust neutrons' outgoing weight at the boundaries. Total power and mass flow boundary conditions are available from DYN3D and can be included for the thermal conditions in CTF. Finally, full or improved coupled reactor physics can become available after transferring the boundary conditions, power and feedback distributions until achieving convergence in a multi-way coupling between LOTUS, DYN3D, or Open MC and CTF at the fuel pin or materials level with DYN3D at the fuel assembly level. Hence, a verification of the coupling and full coupled reactor physics in the multi-way coupling between LOTUS and CTF with DYN3D was performed through the customized CSE, modifications to Open MC, and the customized benchmark [50].

In SCALE-POLARIS, cross sections for the 3x3 quarter core with reflectors, 17x17 fuel assemblies, and 34x34 quarter core without reflectors were generated for two energy groups using methods like ESSM and MOC. In DYN3D, the 3x3 reactor core with reflectors was simulated using methods like two energy groups, NEM, asymmetric reflection, channel, and heat transfer. In LOTUS, DYN3D or Open MC, the 17x17 fuel assemblies and 34x34 quarter core without reflectors were simulated using methods like two energy groups, CCCP or NEM or MC, and asymmetric reflection. In CTF, the 17x17 fuel assemblies and 34x34 quarter core without reflectors were simulated using methods like subchannel, heat transfer, crossflow, and turbulent mixing.

Modifications to Open MC allow partial albedo boundary conditions. The customized CSE runs DYN3D followed by albedo, total power and mass flux exportation, reformat and importation. Then, the customized CSE executes a loop that includes feedback generation, format, under-relaxation, cross-section interpolation, 3D to 2D conversion, and importation. Later, the customized CSE runs LOTUS, DYN3D, or Open MC. Then, the customized CSE continues the loop, including power reformat, 2D to 3D conversion, and importation. After, the customized CSE runs CTF. Finally, the customized CSE continues the loop, including feedback exportation. This loop is executed until achieving convergence between codes.

The multi-way coupling between either LOTUS, DYN3D, or Open MC and CTF with DYN3D can be observed in Figure 15.

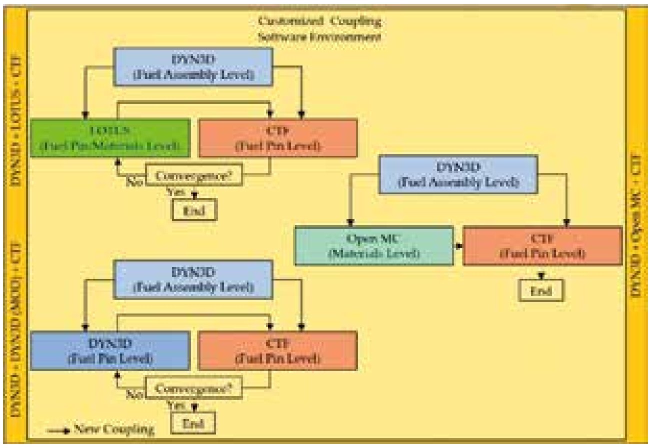


FIGURE 15: Multi-way coupling between LOTUS + CTF + DYN3D, DYN3D + CTF + DYN3D, Open MC + CTF + DYN3D.

Boundary conditions from DYN3D are presented for the 3x3 quarter core with reflectors in Figure 16.

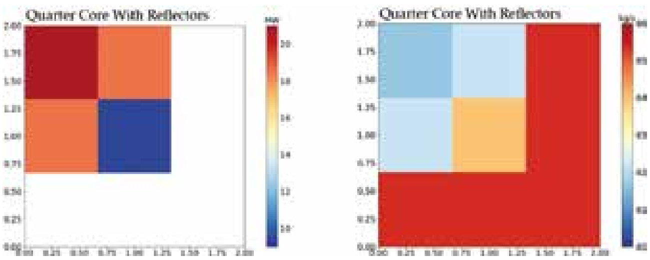


FIGURE 16: 3x3 quarter core with reflectors DYN3D average power and mass flow boundary conditions.

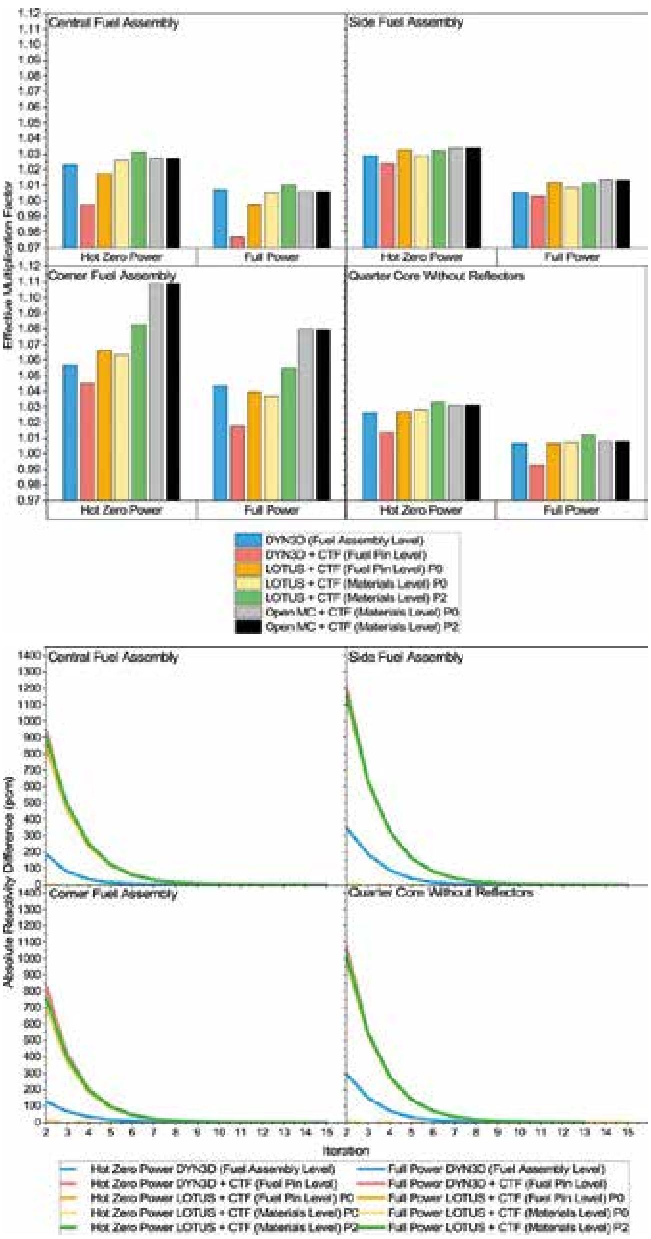


FIGURE 17: 17x17 fuel assembly and 34x34 quarter core without reflectors LOTUS + CTF vs Open MC + CTF vs DYN3D + CTF vs DYN3D effective multiplication factor and convergence.

Effective multiplication factor, convergence, average traversal power distribution and differences between the multi-way coupling between either LOTUS, DYN3D, or Open MC and CTF with DYN3D are presented for the 17x17 fuel assemblies and 34x34 quarter core without reflectors in Figures 17 and 18.

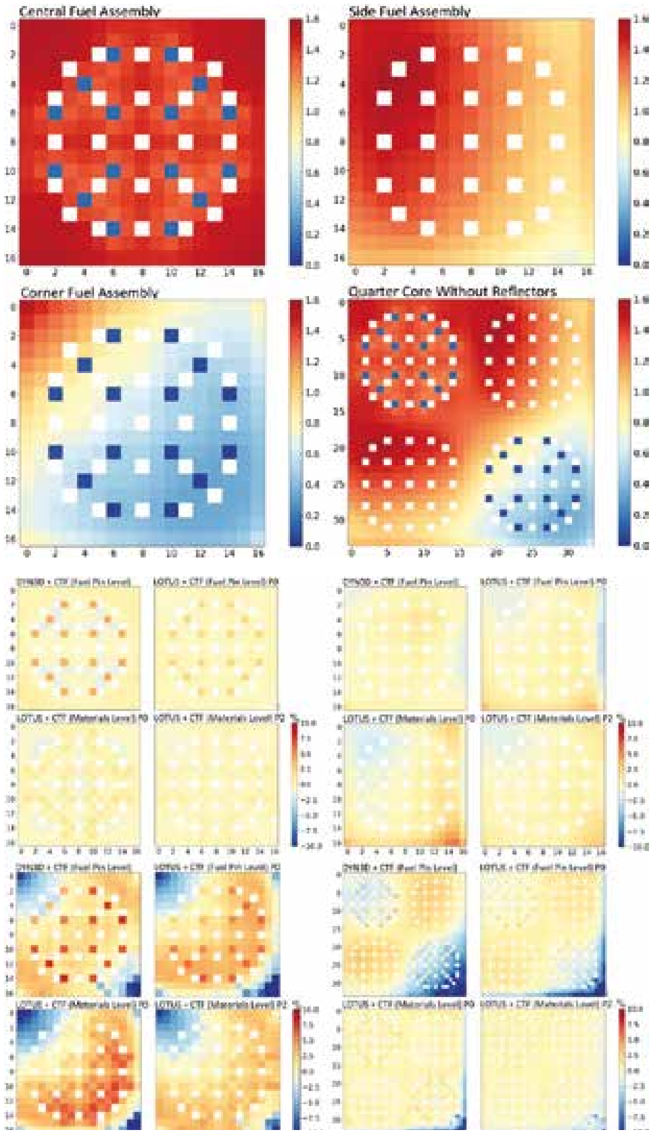


FIGURE 18: 17x17 fuel assembly and 34x34 quarter core without reflectors LOTUS + CTF vs Open MC + CTF vs DYN3D + CTF power distributions and differences.

The multi-way coupling between LOTUS and CTF with DYN3D provided effective multiplication factor values and convergence, transversal power distributions and differences in a 3x3 quarter core with reflectors composed of 17x17 fuel assemblies or a 34x34 quarter core without reflectors. These values, convergence, and distributions were improved when compared to a multi-way coupling between DYN3D and CTF with DYN3D or similar when compared to a multi-way coupling between Open MC and CTF with DYN3D. Differences and convergence occurred due to the different albedo distributions at the outer boundaries, power redistribution, variation of boundary conditions, and methods such as the CCCP or NEM or MC, cross section homogenization, feedback under-relaxation, subchannel or channel, and power under-relaxation

3. CONCLUSIONS

Overall, the aim of an alternative MMSD, and its validation and verification, has been answered through the objectives. A customised CSE is implemented to couple the nuclear codes using a simple interface that supports parallelisation within an HPC, and visualisation of results as in NURESIM and CASL. Nodal and subchannel codes are used to provide simplified and improved coupled reactor physics at the fuel assembly and fuel pin levels similar to NURESIM. Transport and subchannel codes are employed to achieve full coupled reactor physics at the fuel pin and materials levels like in CASL.

Advanced neutron transport methods are not just used for verification, allowing to better improve nuclear reactor efficiency and safety in contrast to NURESIM. A small number of processors is required to deliver results in less than a day, making it affordable to be run in a personal computer unlike CASL. Full coupled reactor physics are provided only for the fuel assemblies of interest by applying LOTUS and CTF with boundary conditions derived from applying DYN3D in all the reactor core, allowing the use of improved methods while minimizing computational resources usage as opposed to NURESIM and CASL.

Initially, the verification of the accuracy and methodology in LOTUS supported its selection for providing neutronics at the materials level. Subsequently, the validation and verification of the accuracy and methodology in CTF and FLOCAL further explained their selection for providing thermal hydraulics at the heater rod level.

Then, the one-way coupling between DYN3D and CTF and its verification demonstrated improved feedback at the fuel pin level in contrast to simplified feedback in DYN3D. The one-way coupling between DYN3D and CTF required computational times of 20+ minutes, while DYN3D required 1-2 minutes to simulate the 17x17 fuel assemblies using 1 processor. Later, the two-way coupling between DYN3D and CTF and its verification showed improved coupled reactor physics at the fuel pin level as opposed to simplified coupled reactor physics in DYN3D. The two-way coupling between DYN3D and CTF required computational times of 1–3 hours to simulate the 17x17 fuel assemblies compared to 1-2 minutes for DYN3D using 1 processor.

Finally, the multi-way coupling between LOTUS and CTF with DYN3D, and its verification, justified its use for delivering full coupled reactor physics at the fuel pin and materials levels across all iterations. Similarly, it further explained the use of the multi-way coupling between DYN3D and CTF with DYN3D to provide improved coupled reactor physics at the fuel pin level across all iterations. Additionally, it supported the use of the multi-way coupling of Open MC and CTF with DYN3D to verify the full coupled reactor physics, although limited only to the last iteration. The associated computational times were as follows:

- LOTUS and CTF with DYN3D: 3 to 24 hours (all iterations)
- DYN3D and CTF with DYN3D: 1 to 8 hours (all iterations).
- Open MC and CTF with DYN3D: 6 to 36 hours (only last iteration).

These simulations were performed for 17×17 fuel assemblies and a 34×34 quarter core without reflectors, utilizing parallelisation across 36 processors. It should be noted that the computational times are not optimised as a high level of discretization was used for research purposes which can be reduced for industrial purposes.

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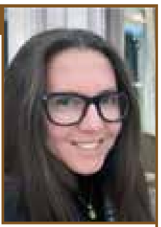

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ACRONYMS

AMR	Advanced Modular Reactor
BEIS	Department of Business, Energy, and Industrial Strategy
BWRX	Modular Boiling Water Reactor
CASL	Consortium for Advanced Simulation of LWRs
CCCPO	Current Coupled Collision Probability with Orthonormal Polynomial Expansion
CE	Continuous Energy
CFD	Computational Fluid Dynamics
CSE	Coupling Software Environment
EPR	Evolutionary Pressurised Reactor
ESSM	Embedded Self Shielded Method
EURATOM	European Atomic Community
FDR / HZDR	Forschung Dresden Rossendorf / Helmholtz Zentrum Dresden Rossendorf
KAIST	Korean Advanced Institute of Science and technology
LWR	Light Water Reactor
MC	Monte Carlo
MG	Multi Group
MIT	Massachusetts Institute of technology
MMSD	Multiscale and Multiphysics Software Development
MOC	Method of Characteristics
MOOSE	Multi Object Oriented Simulation Environment
NCSU	North Carolina State University
NEM	Nodal Expansion Method
NURESIM	Nuclear Reactor Simulation
OECD	Organisation for Economic Cooperation & Development
ORNL	Oak Ridge National Laboratory
PNWL	Pacific Northwest Laboratories
PSU	Pennsylvania State University
PWR	Pressurised Water Reactor
RTWH	Rheinisch Westfälische Technische Hochschule Aachen
SALOME	Simulation Numerique par Architecture Logicielle en Open Source et a Methodologie d'Evolution
SMR	Small Modular Reactor
UK	United Kingdom
UOL	University of Liverpool
USDE	United States Department of Energy
USM	University Sains Malaysia
VERA	Virtual Environment for Reactor Applications

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