VIRTUAL
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UNIVERSITY OF LIVERPOOL

# PROJECT REPORT

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# Table of Contents

# 1 INTRODUCTION

The purpose of this document is to identify current UK and international Virtual Engineering, (VE) and nuclear industry capabilities that are relevant to the development of an Integrated Nuclear Digital Environment that can enable the UK gain a competitive advantage over other countries well-established within the nuclear sector, by using our expertise in other industries to transform the design, construction, operation and decommissioning of nuclear plant. The development focus of this radical approach is to deliver safe and sustainable nuclear energy, ensuring safety standards are upheld whilst improving the economy of reactor design, build, operation, end-of-life and decommissioning. This will be achieved by enabling advanced modelling and simulation to be used to deliver evidence-based decision-making at all organisational levels including the stakeholder level.

This report forms the output of WP3. This covers the current state-of-the-art for multi-site working, multi-physics integrated modelling and VE in the nuclear industry, in order to define the starting point for developing the capability to meet the requirements defined in the WP2 Requirement Capture and Management report. This will be synthesized to produce a plan for development of the VE capability that integrates current UK analysis software and provides a platform for supporting current and future UK methods development activities defined in WP5 Architecture Design report [1].

# 2 PROJECT BACKGROUND

The Digital Reactor Design project, funded by BEIS, aims to identify, develop and demonstrate solutions to deliver a nuclear virtual engineering capability that incorporates virtual engineering and associated technologies from high-tech industries to enhance nuclear design and development programmes. The ultimate vision is an Integrated Nuclear Digital Environment (INDE) consisting of a series of interconnected multi-scale, multi-physics computational models linked to the real-world by data acquired during validation of prototypes, in-service monitoring and inspections of plant, post-shut-down inspections and in-situ monitoring of stored waste [2].

The project consortium will achieve this through building upon the existing and proven distributed simulation capability at the University of Liverpool's Virtual Engineering Centres which has arisen through links with other Universities, NASA, and industry through a number of collaborative programmes such as GAMMA[1], and HRAF[2] with the European Space Agency. Nuclear industry experience is brought into this capability from Wood PLC, National Nuclear Laboratory, EDF energy and Rolls Royce PLC, and is further supported by academic partners at the University of Cambridge, Imperial College and STFC Hartree Centre. A distributed simulation network will be developed allowing the integration of HPC, Virtual Reality, simulation codes and models from disparate geographical locations and is tool agnostic. It also allows the introduction of behaviour models on top of the CAD depictions to allow investigations and analysis of developing situations to create a virtual engineering visualization environment. This can be used to demonstrate visualization of simulation results to allow stakeholders to better understanding and interpretation of the outcome of high fidelity, high performance modelling and simulation tools. This will deliver a step change in

[1] http://www.aerospace.co.uk/technical/gamma-programme
[2] https://www.researchgate.net/project/HRAF-Pilot-1-Harwell-Robotics-and-Autonomy-Facility-Pilot-1

capability whereby strategic decisions can be underpinned by high fidelity simulation, reducing the pessimisms that result from our current position where this is currently impractical.

The network also allows remote viewing of simulations from multiple locations and can, with some development, allow real-time collaboration between participants. The infrastructure will handle the communication between all simulation entities of the system which is implemented based on IEEE 1516 "High-Level Architecture" [3], SISO "Real-time Platform Reference FOM" [4] and IEEE 1278 "Distributed Interactive Simulation" [5].

The Hartree Centre at Daresbury will provide High Performance Computing (HPC) expertise, the key technology necessary to underpin the level of computational modelling, complexity and required level of fidelity. This contribution, as well as the use of the VEC infrastructure, will assure the utilisation of already existing government-financed installations to achieve the maximum efficiency for current as well as future investments.

The project will aim to realise the benefits of integrated modelling as a means to improving state-of-the-art design and analysis of nuclear infrastructure, through:

- Innovation in the way in which the nuclear sector works: moving towards multi-site, multi-institution collaboration on complex, multi-disciplinary problems made possible through open access and remotely linked facilities with expert support.
- Transforming how analysis is performed in the nuclear sector by working towards fully integrated, high fidelity analysis with a single, unified problem description.
- Working towards innovation in nuclear design through bringing a state-of-the-art approach to the design lifecycle from other industries.

Our consortium aims to capitalise on the valuable complementary domain expertise and assets of the partners to provide a high-quality demonstration of the combined capability providing a coherent community of expertise. This is an essential resource for users who will want to draw from this body of expertise. It will be a key component in the building of the UK's national nuclear R&D infrastructure, complementing and working closely with other public facilities.

The infrastructure created by this project will deliver a framework that will enable the consortium partners, industry collaborators, academia and sector stakeholders (whether locally to each physical location or remotely) to share their modelling capabilities in a common environment to make the best use of a wide range of expertise and knowledge wherever it may reside. The framework developed will allow the evaluation and adoption of innovative tools and processes and promote co-innovation. The proposed framework, developed within the timescale of this project, will be applied to reactor core calculations.

The framework will be sufficiently flexible to ultimately enable new partners/supply chain organisations and sector bodies to participate as suits their needs and at different levels of participation (i.e. viewing, testing, training and scenario change). Importantly, the infrastructure developed will protect IP and therefore promote collaboration and exchange of ideas without exchange of developer knowledge.

# 3 CAPABILITY MAPPING

## 3.1 Aims

The aim of this capability mapping activity was to attempt to discover and document who does what within an overall reactor design process and with what tools and facilities.

A series of workshops for information gathering were organised. This information was used to define an initial organisation capability map and requested comments/amendments as necessary but was little changed. The final chart is given in Figure 1.

## 3.2 Capability Definition

The definition of capability was taken to be a combination of tools, process and people that could produce a necessary and acceptable output.

## 3.3 Methodology

At the beginning of the project three workshops were organised to collect information about the nuclear industry organisation. People necessarily operate within organisations and hence the initial focus, as reflected in Figure 1, was on organisational positioning within a process. From this it was anticipated that tools and facilities could be identified and also mapped.

## 3.4 Initial Views

### 3.4.1 People/Organisations

Each major organisation within the nuclear industry claims it has the staff to effectively do whatever is needed within the reactor design phase and across the reactor island. There appears to be no organisation that addresses the overall integration activity of the whole nuclear plant, with the possible exception of EDF.

Most of the major organisations within the UK Nuclear Sector have staff and expertise to cover all the roles identified in the Initial Requirements Document apart from the regulator role.

### 3.4.2 Current Process

Within the process stages of Figure 1 it appears that there is a coherent, consistent process across the life cycle of a nuclear power plant but based on current status this is not entirely the case.

There appears to be gaps between process stages and little account appears to be made of the needs of the future follow up activities from earlier phases. Projects phases tend today to be undertaken in silos and whilst there have been efforts in recent years to overcome this issue remains. Part of the reason for this is the vast quantity of information generated within a typical nuclear project. Information is typically held in documents and the process of passing large number of documents between projects is inefficient and likely results in a loss of fidelity of the information being transmitted. Whilst this is unlikely to be a nuclear exclusive problem, the complexity of nuclear projects from a regulatory perspective probably exacerbates it.

There is a clear need and trend for developing common data interfaces to bridge these gaps. In these circumstances the modelling and simulation of the following process stages need to be simplified, accept what is presently available to them and make the best of it.

The bulk of the activity within the current process is in analysis. New reactor designs are rare, unless one takes refuelling of a reactor core as a new design. There is, however, a continuous process of change via “Design Integrity / Design Authority”, where the design of the power station evolves during the 40+ years of operation, including integration of new systems, and replacement / retrofit of equipment. As a result, what is undertaken is impact analysis of possible changes in the fuel assembly arrangement, or of replacement of components to gain extra operational efficiencies etc. The level of fidelity achieved in individual analysis can be quite high, particularly if advanced tools (some of which are discussed later) are employed. For example it has been demonstrated in several studies, most recently in [6], that it is possible to undertake analysis of fuel performance down to the level of atomic scale diffusion, with such information available within licensing grade core codes. Such high fidelity analysis are becoming more and more frequent, as will be discussed later in this document with respect to international benchmarking, though typically they are taken in parallel to lower fidelity (lower perceived risk) analysis. These risks can be associated with the schedule of delivery (high fidelity analysis can take longer to deliver) and quality related (methods may have lower credibility than established methods). Emerging capabilities potentially give the designer and operator access to a large amount of information to both improve safety (accident tolerant fuels) and economic efficiency (high burnup). Whilst this technology can be used to solve day-to-day operational challenges, it cannot today effectively be used to look at process level challenges without first addressing the highlighted risks. This in turn contributes to the uncertainty and high cost of new build programmes.

Reactor design is performed on an infrequent timescale, with most reactors (at least in the western world). Nuclear new build has suffered from cost overruns and large delays, in part attributable to commencing construction without a finalized design. A potential gap is therefore the creation of a digital prototype, where a complete, virtual description of the reactor can be formulated prior to construction, and the construction process itself can be simulated. This has the potential to reduce greatly the cost and risk in the nuclear design process. What emerges as a critique of the current nuclear industry is one that is excellent at solving day-to-day problems associated with improving or maintaining safe economic operation but is incapable of effectively delivering the same economic benefits at a strategic level. It is important to note that the regulatory framework operated in the UK and elsewhere ensures that the same argument around economics does not apply to operational safety.

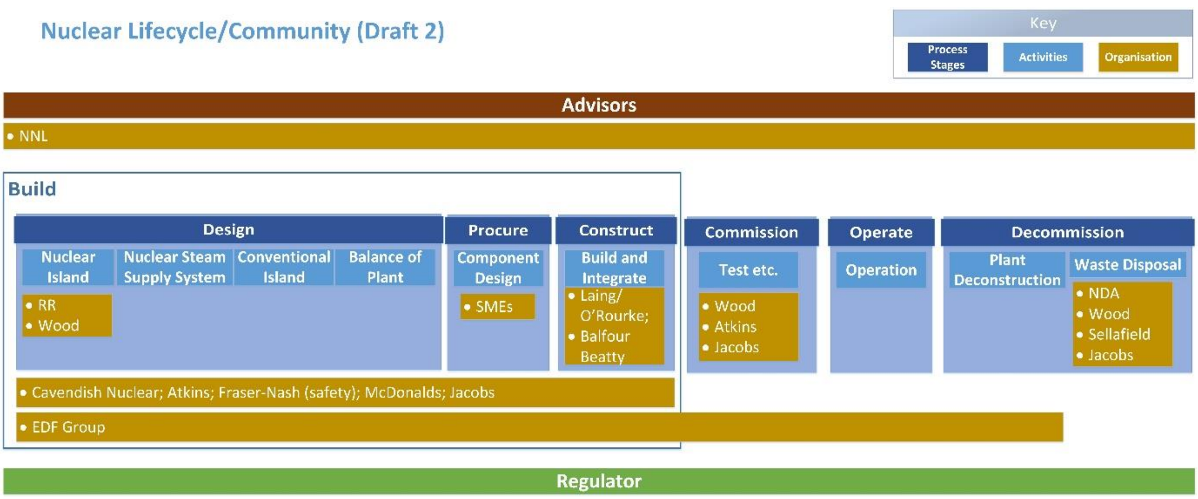


**Figure 1**: Initial Process/ Organisational Map

### 3.4.3 Tools

As demonstrated in the example given in the previous section, there is no shortage of tools within the nuclear industry, where 'tools' specifically refers to software codes. Many of these codes can solve very challenging operational problems to high fidelity. There is a set of recognised and licenced tools which form the core of the design analysis activities for each primary reactor type (AGR and PWR for UK) and through which ONR can be convinced of the acceptability of a change.

The method of use of the tools tends to be different between organisations, the tools themselves are isolated and the transfer of data between them is mediated by expert oversight and evaluation of output and the creation of specific (both to code and individual person) scripts to transform the output of one code into the input of another. In some cases neither the scripts nor the processes are well-documented, which complicates the knowledge transfer to future users. The industry is therefore dependent on maintaining Suitably Qualified Experienced Person (SQEP) status for a number of key experts associated with each code. Both the cost of maintaining this expertise and the demand on these individuals is high which imposes limits on where this knowledge can be effectively used. We expect that in future ONR would not accept future generations using codes as "black-boxes" without the underlying understanding of the codes, the physical processes they are modelling and their limits of applicability. The role of the SQEP'ed expert can evolve, but will certainly remain important. Capturing the some of the tacit knowledge of code developers and users is therefore a gap that needs to be addressed if we are to realise the benefits of integration and virtual engineering.

There appears to be no common taxonomy or ontology and little use of standard or reference models; in addition those organisations who have standard or reference models generally don't share them for commercial reasons. Standardisation of data inputs and outputs (or methods of exchanging data between codes) is not a uniquely nuclear problem but would go some way to addressing the current issues. Introduction of new tools and analysis methods is difficult since any changes in licenced software tools have to undergo significant verification and validation. Industry and regulators demand high reliability of each licensed tool and the 'arcane' structure of the analyses and processes in which they sit limits industry's ability to adapt develop them or adopt new tools. Together, these limitations make configuration management within complex design projects very difficult. Initiatives such as Building Information Modelling are being adopted with enthusiasm within the nuclear industry as this offers a future solution. The BIM nuclear taskforce has recommended a convergence of BIM with concepts such as INDE, [7]

The limitations of an existing code could be overlooked due the way that it is used to support a conservative prediction of performance. This means that the potential for use of modelling and simulation is not fully exploited due to a particular code having limited credibility. A tighter more integrated way of utilising these codes could expose these limitations requiring that industry invests in code improvements.

## 3.5 Computer Simulations

The computer simulation of processes running in nuclear reactors plays an important role in ensuring the safe, reliable and efficient operation of nuclear power plants. The simulation is the imitation of behaviour or operation of a real-world system or process and it is assumed that a computational model is used to perform the simulation. Computational models are mathematical models that are simulated using computation to study complex systems. Thus, the safety evaluation of normal nuclear power plant operation cannot be performed without the application of simulation tools that allow detailed calculations of the neutronics, thermal hydraulics, mechanics and other processes taking place in nuclear reactors. However, the roots of currently used software tools date back to projects initiated in the 1960s, especially in reactor physics and fuel/core management. The methods and procedures have been demonstrated to be highly computationally efficient and accurate enough to answer the current industrial demand. Nevertheless, there are still some approximations applied which create limitations on the applicability and reliability of the results for regulatory issues. In these cases, the historic approach is to add additional safety margins to account for the limitations of the models e. g. insufficient capturing of coupled physical effects. This approach is also called "a conservative approach". By definition, a conservative approach does not reduce safety, but it may contribute to operational and economic inefficiencies.

Currently, different strategies are used to develop the next generation of computer codes for nuclear application. On the one hand, there is the European approach used in the NURESIM program [7] which is mainly based on coupling of existing codes to achieve improved representation of coupled physical processes. NURESIM and its successors were successful programmes and the code suite, SALOME, that resulted from them continues to be utilised within EDF Energy. On the other hand, there is the US approach of the CASL program [8] which focusses on developing a tightly integrated framework based on a combination of some completely new high fidelity methods and existing codes and tools which are coupled to generate extremely detailed high-fidelity results. The resulting toolset, VERA is slowly gaining credibility across a range of US companies and is beginning to make an impact with the US regulator, who is prescriptive with respect to the codes used by site licensees.

## 3.6 Summary

The current capability mapping highlights some specific issues for the demonstration cases and the future longer-term development. Specifically the following points can be identified:

- There is a need for a highly qualified workforce for the next generation power plants and the industry needs to effectively utilise and maintain the high skill levels of SQEP'ed experts in nuclear reactor design;
- There is a requirement for updated quality assured processes to overcome issues of potentially overly 'conservative designs' to improve economic performance without having a detrimental effect on safety;
- There is a demand for the development of a system architecture for code coupling to facilitate the passing of high fidelity information/ data between functions of the whole reactor system;
- There is a need for code coupling to extend to high fidelity information, potentially down to the atomic scale, for some mission critical components of the system, particularly within the reactor core but extending to other areas where such increased fidelity can demonstrate clear value;
- The code coupling should form part of an overall integrated software framework, which is user-friendly and reduces or avoids knowledge requests on specific details from the user;
- It is important to develop a user-friendly graphical interface allowing to flatten the learning curve for the new specialists and to reduce human induced mistakes.

# 4 RELEVANT CODES INTEGRATION ACTIVITIES

Integrated reactor modelling or coupled modelling of the different physical and chemical phenomena occurring in a nuclear reactor has been, or is being, pursued in several corporate, national and international programmes. Generally speaking these involve the coupling of a number of unit models (or codes) within an integrated framework which overall provides a system level model of the reactor core. The overall aim of these efforts can be summarised as

- Improve efficiency by justifying the removal of extra safety factors which have previously been included as a result of insufficient modelling of coupled physical interactions.
- Incorporate the latest advances in reactor physics understanding to increase the accuracy of predictions;
- Improve validation by challenging the system codes and unit codes;
- Improve efficiency and reduce error traps when passing data from one calculation to another;

Broadly speaking integrated reactor platforms can be defined as fitting within two categories:

- Platforms intended for industrial application that couple license-grade codes within an integrated platform. Generally speaking the motivation is to provide more accurate and easier to use systems to set a future standard. Examples include Oak Ridge National Laboratory's VERA (baseline) [9] and AREVA's ARCADIA® code system [10].
- Platforms developed for research purposes and the development of new methods that are designed to test new technologies and approaches that are more advanced. The intention is that these will be verified and validated for incorporation into future industrial grade tools. An example would be Oak Ridge National Laboratory's VERA (advanced) and related developments under the US DOE NEAMES programmes.

There have been a number of notable attempts to integrate different tools and produce a digital environment for efficient nuclear power plant design at an international level, all as far as can be ascertained with limited success. The Table 1 provides some details of the resultant tools with an assessment of their uptake and reasons for non-use.

## 4.1 CASL Virtual Environment for Reactor Applications

The main national programme in the USA is the Consortium for Advanced Simulation of Light Water Reactors (CASL) programme (2010-), which involves the development of a Virtual Environment for Reactor Applications (VERA)[3] Modelling and Simulation (M&S) platform. The consortium is made up of a number of partners drawn from industry, government research institutes, national laboratories and university partners. There has been some international collaboration to date, particularly with the UK. In general, the development of the VERA platform is split into two development routes:

- Baseline VERA is based around existing industry standard tools for core reactor unit operations (neutronics, thermal hydraulics etc).
- Advanced VERA is concerned with the development of advanced codes, (such as BISON-CASL covering fuel performance and Insilico for neutron physics [11]).

It is important to note that both the CASL and related NEAMS (Nuclear Energy Advanced Modelling and Simulation Program)[4] are currently undergoing restructure and the formal programme structures as described in this report are changing.

As baseline VERA is based on industry standard license-grade tools, in principle it should be considered to be verified, and it is only subject to verification of the integration environment. The design of VERA [9] is based on the concept of boxes, which act as the containers for either the advanced or baseline models. There are, in addition, a series of coupling modules including DAKOTA [12] for uncertainty quantification and MOOSE [13] [14] for parallel and distributed computing on HPC platforms. There are a number of standard libraries for mesh and solution transfer and these handle coupling to industry codes, system codes and commercial CFD software. Common data formats are used for data storage (HDF5) with standard visualisation tools (e. g., Paraview) and a bespoke open source code VERA-VIEW [15] [16] is used for visualisation. The majority of the basic components are based on open-source projects; however, the overall project has limited release outside of the US due to restrictions on some of the component models. VERA is designed with a closely coupled star (or 'spaghetti') like integration architecture which was developed to deliver high performance on parallel computer systems. This architecture is inflexible and one cannot easily switch out elements of the VERA tool-set to for example include a license grade code. The choice of

[3] see www.casl.gov

[4] https://www.energy.gov/ne/nuclear-reactor-technologies/advanced-modeling-simulation

this architecture has to some extend slowed the process of adoption of VERA within industry, partially driven by the prescriptive way nuclear regulation operates in the US. It also effectively restricts VERA to the use of US tools, which may be limiting when considering a broader range of reactor designs.

CASL R&D is focused on enhancing understanding and predictability of challenge problems: key reactor phenomena that limit performance, and a number of multi-physics problems have been reported or are planned [17] [18]. One example is the departure from nucleate boiling which was demonstrated by Westinghouse and ORNL [19]. A further example is crud-induced power shift [20] which was demonstrated using industry standard codes. Industry has been very active in the development of VERA since its inception. Specific partners include the Tennessee Valley Authority (TVA) and Westinghouse, who have adopted VERA within their R&D division. VERA-Baseline has been reported as being used by Tennessee Valley Authority's to support the licensing case for the start-up of the Watts Bar Unit 2 reactor in 2016. Further validation benchmarks were undertaken in 2017, extending the number of reactor authorities that have become partners in the programme. These efforts represent a significant step towards industrial credibility that has seen Westinghouse invest in HPC capabilities to support increased usage of VERA. The CASL programme also has a strong focus on public engagement with information pertaining to the programme being publicly available on an internet site and through peer-reviewed publications.

Both CASL baseline and CASL advanced are reasonably demanding when it comes to computing requirements. Simulations are typically performed on systems of upwards of 32 cores, with 1000 core systems being the workhorse of the CASL R&D programme. US National supercomputing resources (such as ORNL Titan) have generally only been utilised for publicity purposes, with this publicity being used to support R&D into the computers themselves (or more specifically research into how such computers could be used in the future). VERA's computational requirements are by today's standards fairly modest, but have imposed another barrier to the adoption by industry that is only being recently solved by the utilisation of cloud services and low cost multi-core workstations. One of the perceived key weaknesses of VERA is the computational demand of running a whole core simulation which requires computational power that is out of reach of industrial users. However the evidence from the CASL partners is that once the need for High Performance Computing is demonstrated, industry will adopt it. Further industrial partners can always access the computing power of a partner research organisation as is the case between the partnership within Tennessee Valley Authority and ORNL.

## 4.2 NURESIM SALOME

The main international programmes in Europe have been the NURESIM, which ran between 2005-2008 and developed the SALOME code coupling platform, the NURISP project (2009-2012) and the NURESAFE (3rd stage 2013-2015) project. Together these projects resulted in the creation and development of the Nuclear Reactor Simulation (NURESIM) M&S platform [7] [21]. The final NURESAFE project involved 18 countries and 23 research and industrial partners from the European Union [21]. The Salome platform[5] is an open source integration platform for numerical simulations, which enables interoperability between a number of tools and data sources, namely: a computer-aided design (CAD) modeller, meshing algorithms, visualisation modules, computing codes and solvers. It consists of a number of software tools for pre-processing, post-processing, and code coupling. A GUI has been developed for end-user applications. It can be used as a standalone application for generation of CAD model, its preparation for numerical calculations and post-

[5] see http://salome-platform.org

processing of the calculation results. It can also be used as a platform for integration of the external third-party numerical codes to produce a new application for the full life-cycle management of CAD models. The main features of SALOME are:

- Supports interoperability between CAD modelling and computation software (CAD-CAE link).
- Makes easier the integration of new components into heterogeneous systems for numerical computation.
- Sets the priority to multi-physics coupling between computation software.
- Provides a generic user-friendly and efficient user interface, which helps to reduce the costs and delays of carrying out the studies.
- Reduces training time to the specific time for learning the software solution based on this platform
- Provides access to all functionalities via the integrated Python console.

SALOME includes a library that defines a standard data format called Model for Exchanging Data (MED). It is used to translate/transfer data between the codes. It is based on sequences of Hierarchical Data Format 5 (HDF5) data. The library also contains interpolation routines for code coupling applications where, for example, there may be a different spatial resolution between the codes. Further routines are available for temporal coupling to model phenomena such as transients. The unit codes are derived from existing software and include DyN3D[6] for deterministic core simulation [22], and COBRA-TF for sub-channel thermal hydraulics analysis [23]. Each of the unit codes are implemented in C++ programming classes, which provide the code coupling interfaces, which in turn can utilise interpolation and data exchange libraries.

A key feature of the NURESIM platform is the ability to couple a number of different codes (see Figure 2). The reason for this can be either to introduce the relevant multi-physics for a specific problem or to meet individual user's requirements with respect to regulatory requirements. The NURESIM project has undertaken a number of validation benchmark studies. For example, the coupled code DYN3D–SUBCHANFLOW was demonstrated for a mini-core Rod Ejection Accident, (REA) transient [21], and a boron dilution transient. This demonstrates neutron kinetics/thermal-hydraulics/fluid dynamics code coupling. Recently, the SALOME development team integrated ParaView[7] with the SALOME platform. The integration enables SALOME to benefit from the capability of the ParaView software to visualize large models. ParaView is currently the main visualization tool of the platform[8].

[6] see http://www.hzdr.de/db/Cms?pOid=11790&pNid=0
[7] see http://www.paraview.org
[8] https://blog.kitware.com/salome-an-open-source-simulation-platform-integrating-paraview/

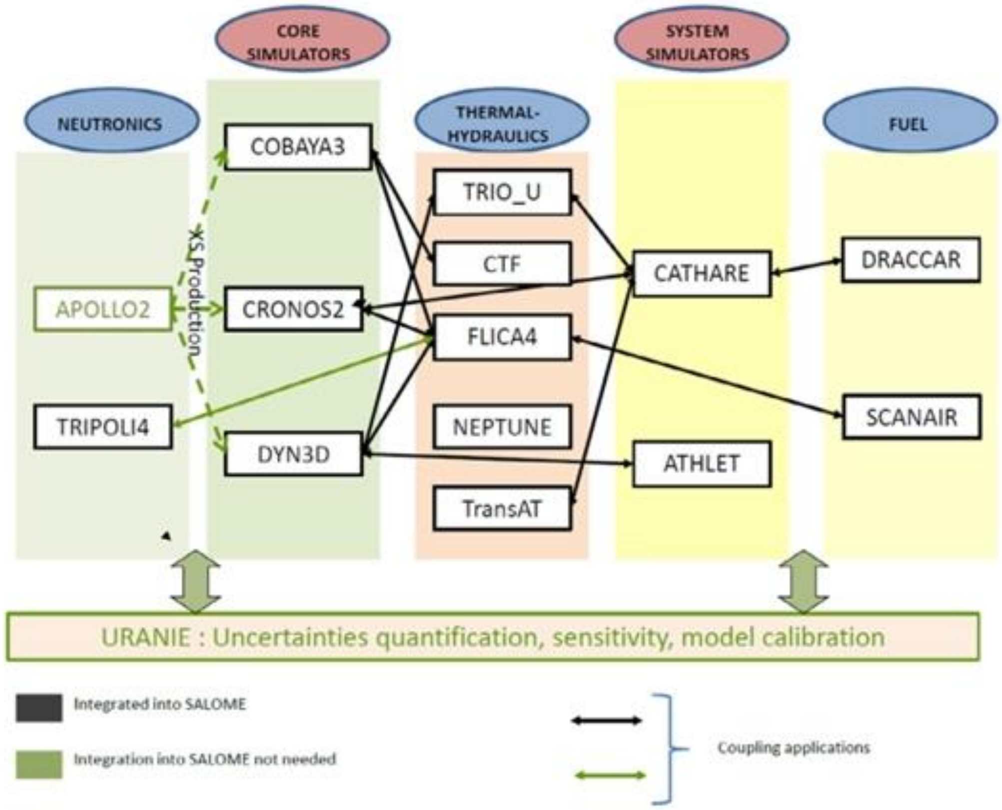


**Figure 2:** The NURESIM platform [21]

It also includes OpenTURNS[9], software for uncertainty quantification in simulation [24]. This allows the robust assessment of performances for complex systems and to comply with strict regulatory processes (security, safety, environmental control, health impacts, etc.) by taking into account uncertainties when dealing with complex numerical simulation frameworks. OpenTurns is being developed by several industrial companies (EDF, Airbus Group, and Phimeca Engineering) and academic institutions. It has been used in statistical assessments as part of the research programme funded by EDF Energy [25].

As a project funded through the European Framework programme, much of the information relating to the project is available through a web portal and through peer-reviewed publications. NURESIM SALOME is mostly used in research institutions as well as by EDF in France and in the UK, both for research and engineering purposes, providing a common interface between EDF teams.

## 4.3 Industrial Integrated Reactor System Codes

With respect to industrial integrated modelling platforms, there is paucity of publicly available information suitable for benchmarking of platforms, such as AREVA's ARCADIA®, and other efforts in China, such as Nuclear Power Institute of China's (NPIC) "Virtual Reactor". The only information available on these codes is in the form of presentations, conference papers and marketing materials. The main features of these platforms are the coupling of industry standard codes (including a core-simulator and fuel rod and thermal hydraulics unit codes) with a modern integrated software system consisting of a graphical user interface, workflow and a data management system [26]. There is a strong emphasis within the published literature on the ability to manage workflows within software

[9] http://www.openturns.org

such as ARCADIA®, which suggests the main driver is quality assurance and workflow optimisation. A professional approach to software engineering and design is also reflected in the marketing material for ARCADIA®, which matches the expectations of the intended industrial market for this software. There is no publicly available information on the NPIC system. There was an information exchange between NPIC and NNL in 2016/17 which provided some details of their R&D programme as overview. This exchange emphasised the focus on coupling industry standard codes within a professionally designed framework with the main emphasis being quality assurance and managed data-flows.

Rolls-Royce is running a project to integrate existing codes and methods named 'The DaVinci project' which was born out of discrete work tying together performance calculations and automating component analyses accompanied by cost modelling. DaVinci is split into two main streams focussing on component and system design. The solutions cover a range of needs: from running calculations built into Excel spreadsheets to programming interfaces for finite element analysis software. They are mainly built using commercially available software. In general, the tools are executed on individual desktop PCs by the end users. Cloud solutions are being investigated, where users execute workflows through a web portal using the Simulia Execution Engine, integrated into Isight software. This could provide a simplified mechanism to deploy the updates, and increased computing capacity; however, there are difficulties in terms of cyber-security and export control that require further work. Currently DaVinci is focussed on the design phase of the lifecycle of aerospace components, but there are plans to address manufacturing, certification and operation during later phases.

## 4.4 Summary

A benchmarking of nuclear industry focused code coupling activities has been carried out and the following learning points have been highlighted.

- A mission focused code integration programme is an important component of any organisational, national or international strategic activity in nuclear;
- An open, flexible architecture such as that adopted within the Salome platform is required to integrate a diverse range of unit-codes as will be required by UK industry;
- Significant leaning can be obtained from the US CASL programme where validation and credibility of the tools has been established through a focus on industry led challenge problems where the coupling can be validated at a system level.
- It is important to adopt common standards for data management and data exchange;
- An easy to use user interface is a common feature of all activities;
- There is an opportunity to collaborate with international partners in the US and Europe to share development of unit codes and to learn from experience on code coupling technologies;
- There is an opportunity to improve on the coupling architecture used within existing systems (which were designed >10 years ago) and adopt more open and more advanced industry standard technologies for virtual engineering;
    - Specifically architectures based on horizontal integration (Enterprise Service Bus) are more flexible that the star (or spaghetti) integration models adopted within VERA and Salome.
- There is a gap identified within other activities to extend the code coupling beyond the reactor island to encompass other major components of the system such as Balance of Plant in order to provide a whole system analysis.
- There is a further gap in that these codes support automated analysis but appear to offer few features to support automated design.

# 5 OPPORTUNITY ANALYSIS

In terms of the opportunities for the UK, public research needs are generally based on strategic roadmaps that address the key features needed by industry today and tomorrow. It is these strategic objectives that drive change in the industry. Specific projects leverage this underpinning investment. Thus when considering the opportunities it is important to think of the strategic political and economic objectives that digital reactor design can achieve. All of the programmes reviewed appear to view the capability as indirectly supporting a commercial model based on services or in support of the sale of other products and services. It is clear that within all of the integrated modelling suites reviewed here that there is a considerable drive from both national and commercial factors. CASL-VERA has a clear US government drive to support US industry and to reduce barriers to the adoption of nuclear power. Similar arguments can be made around SALOME and European Framework approach. For commercial suites, given the way these are marketed, the assumption is that the driver is to offer clients a comprehensive one-stop solution to their needs and the main strategic driver is the promotion of the business as a whole rather than an obvious commercial drive to sell a piece of software. In the case of the ARCADIA® [27] [28] [10] software, it addresses a strategic commercial need for fuel licensing and selling of fuel assemblies.

In the view of the development of the digital environment some major gaps have been identified. The digital environment has been proposed to allow modern approaches to support designing, prototyping, operating and decommissioning of nuclear plants to be adopted across a supply chain. The overall goal is that the environment should encourage innovation within the nuclear industry by reducing barriers to innovation. Those barriers include perceived technical risks. Hence, the following analysis of the technology gaps should address the requirements of this environment. These are in detail:

- An advanced level of computational modelling will require the use of High Performance Computing (HPC) that is widely available in academic research in support of the nuclear industry and has seen limited adoption within the industry for specific challenges.
- There is a need to overcome perceived technical risks associated with the use of high fidelity simulation to support industry relevant challenges.
  - These risks can be associated with lack of credibility of these models that could be solved by addressing needs for further validation.
  - The schedule risks associated with high fidelity simulation can be solved by focusing on ease of use and improved methods for data transfer.
- There is a need to understand how to validate emergent behaviour that is present in complex systems and that could arise as a result of coupling across multi-physics and multi-scale domains.
  - Notwithstanding this challenge, significant forward progress can be made by demonstrating code coupling against industry led challenge problems.
- Improved data transfer between the real world and the digital environment to assure the availability of validation data through the whole life-cycle of the nuclear system.
- Consistent data management within the digital environment to ensure sufficient knowledge management and long-term data preservation through the whole life-cycle of the nuclear system.
- The use of a digital prototype to facilitate virtual reactor design and assembly, in order to reduce the cost and risk of reactor design and construction.
- Digital reactor design software requires further virtual engineering features to support actual plant design.

- These include additional tools for design optimisation, including configuration management of components and decision making tools for cost analysis, design cycles and knowledge management.

In terms of the current technical considerations of the gap analysis, it is useful to compare the programmes against the reference for the UK Digital Reactor project. This is based the Integrated Nuclear Digital Environment [1]. This framework differentiated modelling across a range of physical and temporal scales in two directions. Firstly, models can be classified from the level of strategic descriptions down to sub components across the time scales from plant design through operation to decommissioning. Secondly models of individual challenge problems are represented by multi-physics and or multi-scale models that must be solved over different physical and temporal scales in order to solve a specific unit level problem at an appropriate fidelity. It is clear that in the case of the three examples discussed in this review that there is a strong emphasis on the latter needs – that is the requirement to solve challenging technical problems associated with reactor operation and licensing that requires the application of multiscale and multi-physics modelling. Within the collaborative projects, software design follows scientific computing principles, utilising tools emerging from the research community of High Performance Computing. However, for industry designed software tools, the software design principles appear to be grounded in commercial software development with more of a focus of quality control workflow management and a professionally designed user interface. Industry does however use academic and open source tools where appropriate.

A general feature of the research driven coupling frameworks VERA and SALOME is the focus on solving specific engineering/physics problems with respect to reactor operation. Advanced-VERA contains tools that are designed to model hypothetical future reactor designs giving some potential for these to be used to assess future designs. Whilst these challenge problems certainly relate to real world industrial problems, there may be other safety or economic factors that could come into play that are not directly addressed by the current tools. So for example, an integrated model may result in a high quality high fidelity prediction but industry may fall back on other methods or other variables outside the reactor analysis to support the actual decision.

There is an opportunity for the INDE framework to provide tools that support whole plant-lifetime analysis. That is from design (virtual prototype) through operational (digital twin) through decommissioning (decommissioning replica). International efforts in digital reactor design have primarily focused on automated analysis but do not directly provide a virtual engineering capability. This will require a more flexible open and more scalable platform that has been developed to date. A further opportunity relates to the interpretation and visualisation of results in the form that is usable by nuclear engineers not only nuclear reactor physics experts. There is an opportunity for UK companies to utilise HPC for reactor design. This will require the nuclear industry to adopt technologies such as the cloud to lower the barriers to access HPC. Sensitive nuclear data must be managed and perceptions on cloud security need to be challenged if this is to be successful.

Finally, there are clearly learning points from the CASL and NURESIM programmes with respect to legal, commercial and sociological factors. Collaboration is a key feature of these programmes, with a common software licensing model based around open source licensing for the protection and sharing of intellectual property. This model has not prevented the integration of commercially licenced codes within SALOME or Baseline VERA. Limited uptake can result from a lack of connection between developers and users. The opportunity is to integrate developer and user teams in a seamless manner. This approach has already been adopted within organisations such as EDF

(Salome) and NNL/ SL (process modelling). The opportunity is to extend this collaboration to be pan-organisational encompassing market leaders, research organisations and SME's.

Finally, international efforts to develop integrated reactor have taken place within the framework of wider collaborations on nuclear research. This is true to an extent in the UK, though there are likely to be some significant gaps. Firstly whilst there is a programme of R&D into advanced fuels, there is no obvious place for coordination in the current BEIS programmes for fuel related research and materials performance to support GEN-II+ and GEN-III designs. These are also not covered in the current materials programme (which focuses on manufacturing) or codes and standards programmes (focus on established methods, not state-of-the-art). In the US programme for example, the BISON fuel performance software was developed coupling lower length-scale materials modelling of both existing and future reactors. Whilst some responsibility lies with the fuel and reactor vendors it is incredible to conceive that UK PWR/ BWR reactors will operate for the next 100 years without substantial R&D to improve economic efficiency and safety to match that of advanced designs. It is very likely that further gaps will emerge and these need to be highlighted in the roadmap.

**Table 1**: Analysed projects overview

| Name of tool | Objectives | Current status | Who is using it | Learning points |
|---|---|---|---|---|
| VERA | Integrated toolset to support reactor safety, licensing and sustainability | Project live with sustainability plan and multi-year roadmap | Primarily US based research organisations (Advanced-VERA) and industry (Baseline-VERA) | • Industrial engagement<br>• Fixed toolset<br>• Shared IP based on open source licensing<br>• Lifecycle analysis<br>• Focus on technical challenge problems<br>• Limited focus on strategic considerations<br>• Based on scientific computing tools<br>• Needs HPC but industry will adopt it |
| SALOME | Integrated toolset to support reactor safety, licensing and sustainability | Project dormant after 3 rounds of funding | EDF | • Flexibility on tool-set<br>• Dissemination and outreach<br>• Open framework<br>• Shared IP based on Open Source Licensing<br>• Based on scientific computing tools<br>• Focus on technical challenge problems |
| ARCADIA | Integrated industrial toolset to support reactor safety, licensing | Commercial product | AREVA | • Emphasis on professional software engineering<br>• Workflow focus<br>• Industry standard codes<br>• Designed against software engineering principles |
| DaVinci | Integrated industrial toolset | Commercial product | Rolls-Royce | • Integrate from MS EXCEL spreadsheets to |

| | | | | |
|---|---|---|---|---|
| | to support reactor safety, licensing | | | programming for FEA software<br>• Built using commercially available software<br>• Individual tool execution<br>• No Cloud solution |

# 6 CONCLUSION

In recent years there has been substantial emphasis within the nuclear industry in moving towards more integrated, multi-physics modelling of nuclear reactors and fuel. However this still typically falls short of a complete, integrated multi-physics model of the entire reactor across its life cycle. In this report, lessons are drawn from other programmes in the area of integrated multi-physics modelling. A particular and unique focus of the present work is the intended incorporation of digital prototyping and digital twin technology, levering expertise from other industries, to capture and store all the data associated with a nuclear reactor in a manner allowing it to be queried in a structured way, alongside the use of integrated multi-physics modelling to form a holistic description of the reactor's state. Where current efforts mainly fall short is the lack of a holistic view of the reactor lifecycle. Thus whilst these tools have the potential or are being used to solve specific challenge problems during reactor operation, the impact in terms of improved economic performance of the whole system design is not yet adequately addressed.

This is therefore an opportunity for the UK to leap-frog other countries by using its expertise in other industries to transform the design, construction, operation and decommissioning of nuclear plant. In particular, the use of digital prototyping has the potential to transform the nuclear design and construction process in the nuclear industry and worldwide, by allowing a complete digital representation of the reactor to be created prior to its construction. Such processes are common in other industries. This could have dramatic benefits in preventing delays and cost overruns, and could hence enable the nuclear industry to be a more cost-effective supplier of electricity.

It is recognized that this is a substantial task, and that it may be many years before we have a 'complete' solution. It is also recognised that the potential timescales for development are long enough to mean that the framework needs to be flexible to accommodate what may come along, including further advances in digital technologies including but not limited to Big Data, Artificial Intelligence and Quantum Computing. To make this challenge tractable, a robust methodology has to be adopted for prioritising the development roadmap. This will need to take in to account the timing of investment based on the technology barriers and the value of the industry need. As nothing quite like this has been attempted, there will be a paucity of data (at least initially) to guide decisions. The methodology must therefore allow for feedback to update the methodology as we learn from successes and weaknesses. The nuclear industry has widely adopted technology readiness metrics such as Technology Readiness Levels and Scientific Readiness levels. It is however recognised that these metrics can fail to capture the interrelationship between technologies. These limits can be partially overcome by adopting systems engineering practices which identify the problems that need to be solved. This top down approach is also the philosophy adopted by the Integrated Nuclear Digital Environment.

This project therefore represents a first step towards this goal. Whilst we have chosen particular use cases to model in order to demonstrate and enable innovation through lifecycle simulation of nuclear reactors and their structural components, the main emphasis of this project is proving the concept of taking nuclear codes and integrating them into a framework. A key task within this project is to create a mechanism through which industrial needs are captured and understood.

Other aspects such as system engineering and design optimisation will follow in later phases of the programme.

## 6.1 Recommendations

The following recommendations have arisen from an analysis of the current UK capability and benchmarking of international activities.

- There is a clear need to develop an Integrated Nuclear Digital Environment to meet the goal of reducing the costs of providing safe and sustainable nuclear energy. It is recognised that currently UK industry is operating in silos without any clear identification of the process towards this ultimate end goal. Digitalization of industry processes and practices can clearly play a part to integrate these various components together to provide a comprehensive solution that can compete internationally. The development should focus on two key areas:
    - The strategic gap to be addressed by the framework is the exchange of information (data) across the nuclear lifecycle and configurational management and optimisation based on systems engineering principles. Further phases of this project should concentrate design effort on these areas once the basic concepts of the integration methodology have been identified in the current project.
    - Specific problems need to be addressed by integrating high fidelity modelling and simulation within the integrated modelling framework. Outputs from the current project will prove the basic concept of the model integration framework. In the next phase it is expected that the use cases will evolve from demonstrating the framework to solving real-world industry driven problems to demonstrate the capability. It would be expected that the next phase of the digital reactor design project would closely cooperate with both the advanced fuels and reactor physics BEIS programmes, and with industry partners, to define and implement specific solutions.
- The programme should continue to explore ways in which the tool could support ONR's mission to enforce safety across the industry.
- The effort to develop such a framework is substantial and can only be achieved in phases. It is recommended that a methodology based on systems engineering principles supported with metrics such as Technology Readiness Levels is used to prioritise the development of specific components within the digital environment to address specific technical issues and deliver the strategic goal.
    - The main deliverable of the current digital reactor design project is a strategic roadmap and this roadmap should make steps towards addressing the need for such a methodology.
- Licensing model for the framework needs to be addressed in the next phase of the project. It is clear that if the framework is to be widely adopted widely within industry it not only needs an open architecture, but it needs a licensing arrangement that is also based around collaboration and protection of intellectual property. An open source model is a strong contender but it is recognised that there are many types of open source license that have different benefits with respect to commercial exploitation. The current phase of the digital reactor project should review the options for licensing and this should be enacted in a future phase II of the project.
- It is recommended that the BEIS programme in digital reactor design should continue. The project to deliver a functioning INDE is technically challenging and Industry needs further support to develop the skills, IP framework and technology to go it alone in digital reactor design. Industry has already shown willingness having provided in-kind financial contribution to the current project. This will be built on in future phases.

- A review of BEIS programmes is required to determine if the existing scope and subjects covered within the current portfolio meet the needs of digital reactor design. Priority gaps include high fidelity materials simulation to address specific challenges related to core modelling. Further gaps will be identified during the remainder of the current digital reactor project and may lead to specific recommendations for revising the scope of existing projects or even establishing new projects.

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