Modelling and Simulation Activities in Support of the UK Nuclear R&D Programme on Digital Reactor Design

A. Levers
University of Liverpool

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MODELLING AND SIMULATION ACTIVITIES IN SUPPORT OF THE UK NUCLEAR R&D PROGRAMME ON DIGITAL REACTOR DESIGN

B. Lindley, D. Allen, A. Bowen J. Lillington, A. Smethurst, P. Smith
Wood
Dorchester, UK

D. Bowman, L. Dwyer, K. Lai, A. Levers, K. Vikhorev
University of Liverpool
Virtual Engineering Centre
Warrington, UK

D. Litskevich, B. Merk, E. Patelli, E. Patterson
University of Liverpool
Liverpool, UK

M. Bankhead, A. Peakman
National Nuclear Laboratory
Warrington, UK

S. de Haas, C. Jackson
Rolls-Royce
Derby, UK

J. Draup, E. Galenne
EDF Energy
London, UK

G. Parks, E. Shwageraus
University of Cambridge
Cambridge, UK

M.D. Eaton
Imperial College London
London, UK

L. Mason, A. Toland
STFC
Warrington, UK

ABSTRACT

The UK Department of Business, Energy and Industrial Strategy (BEIS) recently launched an R&D programme in Digital Reactor Design, incorporating the development of a Nuclear Virtual Engineering Capability with an integrated Modelling and Simulation programme. A key challenge of nuclear reactor design and analysis is the system complexity, which arises from a wide range of multi-physics phenomena being important across multiple length scales. This project constitutes the first step towards developing an integrated nuclear digital environment (INDE) linking together models across physical domains and incorporating real world data across all stages of the nuclear lifecycle. Simulation case studies will be developed within the INDE framework, delivering an enhanced modelling capability while ensuring the framework has immediate application. For these case studies have been specified that are relevant to design and operation phases for AGR and PWR type reactors. The AGR case considers the through-life structural performance of graphite bricks. This involves modelling of multi-scale, multi-physics phenomena in the support of reactor operations. The PWR case study is based on core multiphysics modelling, with potential relevance to operating and future PWRs, and in particular in the design of SMRs.

UK PROGRAMME ON DIGITAL REACTOR DESIGN

BEIS recently launched a new programme in nuclear energy as a first stage in a strategic initiative to preserve long term nuclear capabilities in the UK. This includes an integrated five-year integrated R&D programme in Digital Reactor Design. It incorporates development of a Nuclear Virtual Engineering Capability, with an integrated Modelling and Simulation programme; along with Thermal Hydraulics Model Development, and specification of a Thermal Hydraulic Rig **[1]**. The integrated programme of virtual engineering and modelling and simulation activities are the subject of the present paper, with specific focus on the modelling and simulation activities. The scope of the present project comprises the first two years of this programme.

This programme follows on from the recommendations of the UK Nuclear Innovation and Research Advisory Board (NIRAB) [2], which included the development of “digital tools and the fundamental scientific understanding needed to design and build future generations of reactors in an accelerated and cost effective way, with emphasis on ever increasing safety." This included a specific recommendation to "establish a Nuclear Virtual Engineering Centre featuring state-of-the-art virtual engineering tools and techniques."

The overall goals of this programme are [1]:

- By 2020 to establish the UK as a partner engaged in collaborative design projects for new reactors (Generation IV and SMR), building on its existing and growing design expertise
- By 2030, for maturing R&D to result in deployment of new plant with significant UK design content and manufactured parts
- By 2050, for R&D to have facilitated UK industry to be a significant partner in the global deployment of Gen III+, Gen IV and SMR technologies.

The specific objectives of the modelling and simulation programme described in this paper are to deliver improved understanding and safety of through life performance of reactor components, develop and enhance predictive modelling capability, and develop innovative, validated, multi-scale and multi-physics models to predict the through-life structural performance of key reactor components. It is anticipated that this will be completed in early 2019.

It is targeted to deliver these objectives through implementation of the modelling and simulation programme within the nuclear virtual engineering capability, with a view to increasing uptake of modern digital engineering practices within the UK nuclear industry and establishing a collaborative network of UK wide facilities for virtual engineering. This is further discussed in Ref [3]. Overall, the aim is to facilitate a step change in the way that nuclear design and development are delivered.

The integrated programme of virtual engineering and modelling & simulation is being delivered by a multidisciplinary team spanning industry, academia and national facilities. The team is led by Wood, a leading nuclear consultancy and Technical Support Organization (TSO), and brings together the Virtual Engineering Centre at the University of Liverpool, Rolls-Royce (a reactor vendor and designer), EDF Energy (the UK nuclear operator), the UK's National Nuclear Laboratory, the Hartree Centre, Imperial College London and the University of Cambridge. This team represents a cross-section of the various capabilities and end users within the nuclear industry, working towards ensuring usable end products with immediate and demonstrable benefits.

Other BEIS R&D programmes are being implemented in parallel as part of an overall nuclear innovation strategy, including programmes on Advanced Nuclear Fuels, Fuel Recycling and Nuclear Materials, Advanced Manufacturing and Modular Build. Ultimately, it is intended to draw synergies across the various projects, facilitating collaborative working across UK nuclear organizations to the general benefit of 'UK plc'.

TOWARDS AN INTEGRATED NUCLEAR DIGITAL ENVIRONMENT

To achieve the goals outlined above, it is intended to work towards the creation of an Integrated Nuclear Digital Environment (INDE) as proposed in Ref. [4] (Figure 1), which introduces concepts utilized in other high tech industries. The nuclear reactor lifecycle consist of design and construction, operation, end-of-life and waste disposal phases. It is proposed to replicate each of these within the INDE, incorporating real-world data at each stage. The INDE is being developed primarily by the Virtual Engineering Centre within the current programme, and the linking between physics simulations is being performed using the High Level Architecture standard [5].

A key feature and challenge of nuclear reactor analysis is system complexity, which arises from a wide range of multi-physics phenomena being important across multiple length scales. Reactor design and operations must take into account different physical domains and can rely on subject matter experts within these different disciplines, which include core physics, thermal-hydraulics, fuel performance, chemistry and structural integrity. Design or operating limits may arise through complicated interaction of different physical phenomena and there is an increased trend in nuclear engineering towards multiphysics modelling, rather than modelling on a discipline-by-discipline basis. The purpose of this is to more accurately capture multiphysics phenomena, quantify uncertainties with increased confidence, and therefore work towards reducing uncertainties and hence improve reactor performance.

Reactor vendors and operators have various systems in place or in development to perform coupled simulations for reactor or core reload design, supporting operations and fault studies. These systems may include couplings of core and primary circuit models, and coupling of neutronics, thermal-hydraulics and fuel performance within the core itself. There are also various R&D efforts in this area, including the CASL project which integrates a wide range of high fidelity, multi-physics, multi-scale models [6]; the NURESIM platform, which links together a large number of primarily European codes [7]; the NEAMS workbench [8]. It is a goal of the present project to engage and learn from these efforts through development of international links.

It is, however, rare to model the whole plant at the system level (encompassing nuclear island, turbine island and balance of plant), except in the case of training simulators, which typically utilize simplified models. There are instances of software with capability to model an entire reactor system, with application to safety case calculations [9].

A key requirement of the current project is to utilize and enhance existing, verified code systems which are utilized within the UK nuclear industry, and therefore to enhance the modelling and simulation capability of 'UK plc'. Ultimately, there is also a requirement for the virtual engineering capability to be code agnostic so that it can be used with other tools, or with the current tools as they are upgraded in the future.

A digital environment for a nuclear reactor would consist of an interconnected set of multi-scale, multi-physics models, including detailed physics models of components (e.g. the fuel pins), combined to give a complete model of the overall nuclear plant. Information required for plant monitoring and predictive maintenance would also be included, including simulation of I&C.

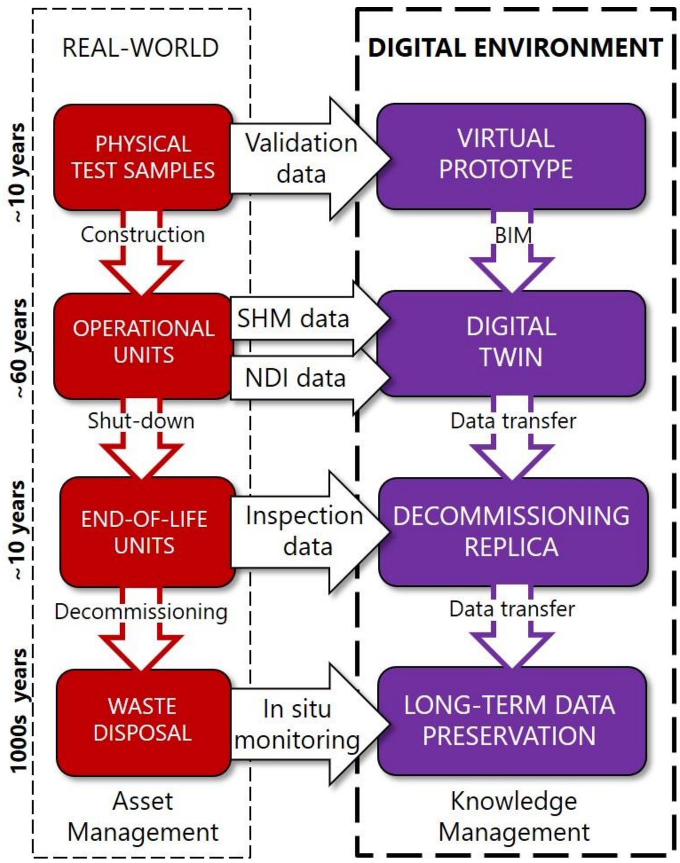

Figure 1: Integrated Nuclear Digital Environment (Ref. [4])

In reactor design, there are various drivers for the creation of such an environment. Optimization of a reactor design requires an understanding of constraints and trade-offs across physical disciplines. Innovations introduced in one discipline to improve performance (e.g. in the fuel), could for example introduce practical constraints or otherwise compromise other aspects of the design. Hence data integrity is essential and requires a consistent representation of the design across different disciplines; automatically and rapid data transfer across disciplines; and automated archiving of cases along with effective configuration control. A virtual prototype encompassing these capabilities would allow improved quality assurance through reduced reliance on human intervention in data processing. It would also facilitate rapid iteration cycles, allowing greater exploration of the design space and overall improved, safer designs. This also has the potential to reduce timescales and costs, improve reliability, and facilitate a move towards small-scale mass production.

Ultimately, such a design capability would be utilized alongside integrated computational optimization of the design, as is considered in other industries. Consistent treatment of uncertainties across physics domains is also a key challenge, and the subject of much recent research in the nuclear industry [10].

The virtual prototype should act as a single source of truth for all information in the design. This would include a consistent geometric description of the design, used in various representations across disciplines. A need for CAD integration with physics models in some form naturally follows from this.

When moving from the design to operations phase, the virtual prototype would evolve into a digital twin, with different instances for each individual reactor. This would incorporate information from the reactor itself, and combine simulation with plant data to provide a complete description of the plant.

While it is common in the nuclear industry to perform simulations which incorporate plant data (e.g. using detector measurements during a core follow simulation), and to use data to draw insights (e.g. use of data from the plant to predict component failures), this tends to be isolated by discipline.

It is also typical in the nuclear industry to perform simulations mirroring the current state of the plant, and to simulate the future behavior of the reactor, along with ‘what if’ scenarios (reload analysis, fault studies in the safety case). While such information may exist, it might not be possible to query it in a structured way as a consequence of the way it is stored within archives or reports.

A key feature of a digital twin for a reactor would be to store all the data recorded from operations and generated through simulations, and to include a structured way of querying the data. This will facilitate drawing insights from the data.

An important requirement is to enable remote working between sites and organizations, as all stages of the nuclear lifecycle are typically supported across multiple sites. This brings associated safety, security and IT challenges. A potential barrier to developing such a framework is the lack of pre-existing legal structures to facilitate collaborative working between industry and academia, particularly with respect to movement of data.

A major challenge in developing a generalized capability is the diverse range of reactor types which have been proposed, designed and built. These have diverse materials, geometry and key physical phenomena. The UK fleet at present consists predominantly of AGRs: gas-cooled, graphite-moderated reactors, where both the coolant chemistry and structural behaviour of the graphite is complicated. There is also a single PWR, which is water-cooled, and hence has a different chemical regime and different fuel geometry. PWRs and AGRs also have different limiting transient scenarios, for example loss of coolant is more limiting in a PWR than in an AGR, while transient scenarios of importance in an AGR include the reactivity effect of water ingress.

In the near term, a number of Generation III/III+ new build initiatives for a range of water-cooled reactor technologies are being progressed in the UK. This is expected to include BWRs which differ fundamentally from PWRs in having two phase flow in the core, a new set of issues to the UK. In addition there is the possibility of building one or more SMR designs in the UK, which may also differ significantly from large designs.

In the longer term, Generation IV reactors may be built, for example sodium-cooled fast reactors (of which the UK operated two at Dounreay), or molten-salt reactors (for which the liquid fuel results in fundamentally different physical phenomena and chemical regime).

A goal of the current project is to facilitate generality of the developed capability across reactor types.

IMPLEMENTATION OF THE MODELLING AND SIMULATION PROGRAMME

In the present programme, a framework for the INDE is being developed, to facilitate future developments. This is being pursued through integration of the nuclear virtual engineering capability and modelling and simulation tasks. This is being accomplished through interaction between these tasks: an architecture is being developed for the INDE framework, and this will be used to perform the application cases. Where there are limitations in the INDE framework to perform such modelling, feedback will be provided to the INDE framework development team to be incorporated in a future evolution of the framework.

Initially simple cases, for example simplified physics models from a single physical domain, will be modelled. This will utilize the initial capabilities available within the INDE framework architecture. Over time, the complexity of the physics simulations will be increased, and the architecture will be iterated to allow the simulations to be run within the INDE framework.

Simulation case studies have been developed to cover different stages of the nuclear lifecycle, in particular reactor design and reactor operation. The case studies have also been selected to be representative of AGR and PWR applications.

This approach has been determined to drive the development of the INDE framework in a manner that:

- Is consistent with actual applications as the case studies are being used to drive its development, including simplified versions of these in the early phases of the project;
- Encourages communication between developers and users – in particular, it is possible to incorporate user feedback from an early stage;
- Provides immediate benefits, by being used to solve modelling and physics problems which are of immediate relevance to the UK nuclear industry;
- Is applicable across multiple stages of the nuclear life cycle – by specifying application cases from different lifecycle stages;
- Is applicable across reactor types – by specifying application cases for different reactor types;
- Is code agnostic.

AGR APPLICATION CASE STUDY

An AGR problem has been selected as one of the two major application cases for the modelling and simulation task. As discussed, AGRs comprise all but one of the UK's current nuclear generating fleet, and are moving towards the end of their life. One potentially life-limiting factor for the AGRs is the structural performance of the graphite bricks in the core.

Under irradiation, the graphite bricks exhibit complicated and time dependent shape changes which result in thermal stresses. This is complicated by oxidation of the graphite by the CO_2 coolant.

The assessment of the structural performance of the graphite bricks is a complicated multiphysics, problem, requiring consideration of phenomena ranging from 3D core scale to detailed models of individual graphite bricks. The irradiation in the bricks requires a core flux solution. This is derived through a coupled neutronic-thermal-hydraulic calculation using the PANTHER core simulation code [11]. The core simulation uses parameterized macroscopic cross-sections for fuel stringers which are derived using a 2D neutron transport calculation, for example using the WIMS reactor physics code [12].

The core neutron flux is then used in a radiation damage and nuclear heating assessment, which requires a 3D neutron transport calculation utilizing a detailed geometric description of the reactor (a typical model is shown in Figure 2). The MCBEND code is typically used for this [13].

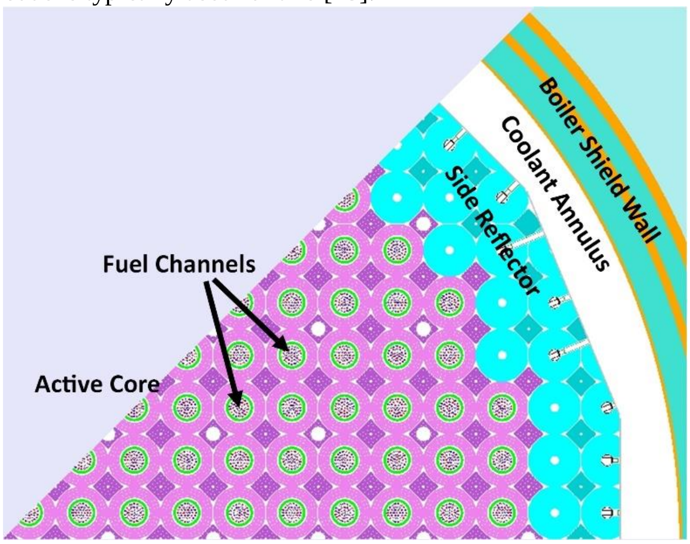

Figure 2: AGR core slice model

A 3D distribution of the graphite brick neutron damage, graphite weight loss and temperature is then calculated using the FEAT-GRAPHITE code [14] that has been developed specifically for the purpose. The graphite stress also results in feedback to the core physics simulation, as the reduction in moderator affects the neutron spectrum and 3D flux solution. In practice however, this is a relatively weak effect.

Finally, stress analysis of individual bricks is performed using a finite element code such as code aster [15] to derive brick shapes and brick stresses. This includes a probabilistic fracture mechanics calculation to help reduce inherent uncertainty in structural integrity assessments.

The overall calculation flow is shown in Figure 3.

The particular case to be solved is intended to represent an actual operating AGR, giving opportunities to verify and validate the INDE framework through comparison to existing data, to provide a tool for future use within the AGR programme, and to perform real world calculations with end-user applications. This could include a predictive simulation of future behavior of the AGR towards end of life. To this end, the case study is being developed through close collaboration between Wood and EDF Energy, the UK's nuclear operator.

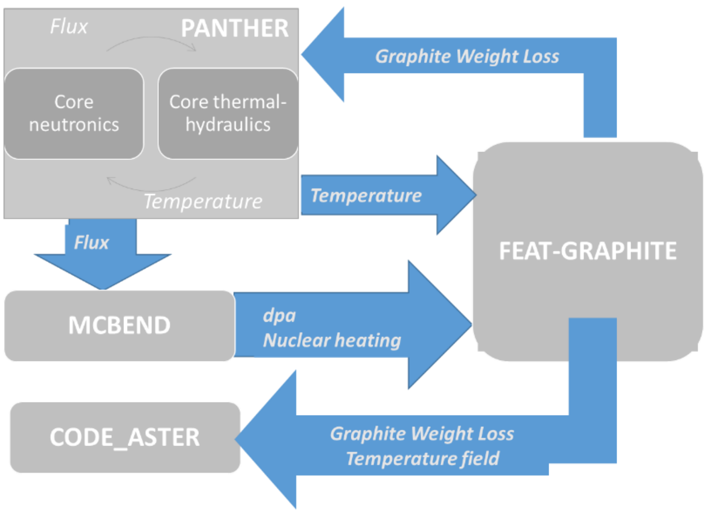

Figure 3: AGR Modelling and Simulation Case Study

PWR APPLICATION CASE STUDY

A PWR problem has been selected as the second major case study for the modelling and simulation task. This has multiple drivers:

- The UK has a single operating PWR, Sizewell B
- There are multiple plans for PWR new build in the UK, in particular Hinkley Point C.
- Prospects for SMR design, development and construction in the UK and abroad.

There has been extensive development in the area of high fidelity, multiphysics modelling of PWR cores in recent years, driven by a desire to predict multiphysics phenomena [6], and to develop an understanding of uncertainties in order to reduce them. Of particular interest at present is the modelling of the rod ejection accident (REA) scenario. In this postulated transient, a control rod is ejected from the core in a very short space of time. While negative temperature feedback shuts down the transient, the power spike has the potential to damage the fuel, and hence a limit is specified for the allowable increase in enthalpy of the fuel pin, in order to prevent fuel failure. This is typically the limiting reactivity insertion accident in a PWR; and in recent years the worth of control rods has increased to allow higher performance core design, while the increase in enthalpy of the fuel pin during the transient can be viewed as more limiting than previously thought, necessitating more detailed analysis [16] [17].

REA analysis is a multi-scale, multiphysics problem encompassing:

- Core steady-state and transient neutronics;
- Accurate modelling of thermal-hydraulic feedback, plus an assessment of whether departure from nucleate boiling occurs and/or departure from nucleate boiling ratio;
- Fuel performance modelling, including irradiation performance of the fuel up to the point of the postulated transient, and potentially transient thermal-mechanical modelling of the fuel.

One example of recent work in REA multiphysics modelling is the specification and solution of the Light Water Reactor Uncertainty Analysis in Methods (UAM) benchmark [10], which aims to treat uncertainties across these physical domains in a consistent manner, with application to an REA analysis problem.

In this project, it is intended to couple the PANTHER core simulation code, utilizing cross-sections prepared by WIMS lattice calculations, and the ENIGMA fuel performance code [18], with potential extension to also including an appropriate subchannel code such as COBRA-TF [19] or VIPRE [20]

A potential application case for this capability is in the design of the UKSMR [21], being developed by a consortium led by Rolls-Royce. The specification for this use case is therefore being developed by Rolls-Royce in collaboration with Wood and NNL. It is targeted to bring immediate benefits in facilitating analysis of PWRs and SMRs in the UK, as well as developing a strategic capability bringing together and enhancing the PWR core analysis capabilities of the UK.

FUTURE APPLICATION TO GENERATION IV

A potential future application of the INDE framework is to support the analysis of revolutionary Generation IV designs of reactor. There are many such concepts being developed worldwide, including several in the UK [22] [23]. The UK is also engaging in international programmes on the development of Generation IV reactor technologies [24] [25].

A major barrier to the deployment of revolutionary reactor technologies is a lack of experimental data, including in the development of validated models. Innovative designs can also pose challenges in modelling unique physics phenomena. A further major barrier is the cost of licensing, which can run to hundreds of millions and take several years, increasing the timeframe for return on investment.

It is hoped to address such challenges through development of a virtual prototyping capability, which could:

- Make best use of available validation data;
- Incorporate and utilize high fidelity, multiphysics, multi-scale models which have enhanced predictive capability, to mitigate limited experimental data;
- Integrate fuel cycle models with reactor models – this is particularly important for designs which consider reprocessing and fuel recycling;

- Provide a digital means of developing safety cases, hence reducing the time and resources required to produce them.

CONCLUSIONS

The UK R&D programme on digital reactor design sits within a wider nuclear R&D programme. In particular, the modelling and simulation task is integrated synergistically with the development of a nuclear virtual engineering capability.

Within the digital reactor design programme, the virtual engineering capability will be delivered through creation of an INDE. Within the present project, the first step towards this goal will be realized.

The modelling and simulation case studies will be solved in an incremental and iterative manner within the developed INDE framework, allowing the framework to be developed in a way that makes it fit-for-purpose, and provides immediate benefits on the timeframe of the project. Simulation case studies have also been selected in a way to demonstrate and test the INDE frameworks capabilities, notably consideration of diverse reactor types across the nuclear life cycle.

An AGR application case study has been specified based on the through-life structural performance of graphite bricks. This involves modelling of multi-scale, multi-physics phenomena in the support of reactor operations.

A PWR application case study has been specified based on integrated multiphysics modelling of a PWR reactor core, with potential application to operating and future PWRs, and in the design of SMRs.

NOMENCLATURE

AGR	Advanced Gas-cooled Reactor
BIM	Building Information Modelling
CAD	Computer Aided Design
dpa	displacements per atom
INDE	Integrated Nuclear Digital Environment
NDI	Non-Destructive Inspection
PWR	Pressurized Water Reactor
REA	Rod Ejection Accident
SHM	Structural Health Monitoring
SMR	Small Modular Reactor

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