Rolls-Royce Sponsored PhD in Nuclear Engineering at Imperial College London

Nuclear Reactor Physics Burn-up/Depletion Algorithms on Shared and Distributed Memory High Performance Computing (HPC) Multicore (CPU) and Manycore (GPU) Hardware Architectures

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The aim of this PhD project is to develop nuclear reactor physics burn-up/depletion algorithms on shared (OpenMP) and distributed memory (MPI) multicore and manycore (Graphics Processing Units – GPU) high performance computing (HPC) hardware architectures. The advent of digital twin models in engineering is revolutionising the design of modern nuclear reactors. This is leading to multiscale and multiphysics models within digital reactor design (DRD). In addition, innovations in advanced manufacturing such as additive manufacturing (AM) or 3D printing technologies is providing greater flexibility in the design of nuclear reactor cores and components. Also, modern high-performance computing (HPC) hardware architectures are rapidly evolving with the advent of exascale (capable of performing 10^{18} IEEE 754 Double Precision (64-bit) operations) computing technologies. These exascale HPC systems involve greater integration of multicore (CPU) and manycore (GPU) technologies. This is leading to innovations in multiscale and multiphysics nuclear reactor modelling and simulation (M&S) methods that utilise massively parallel algorithms on the latest multicore (CPU) processor and manycore (GPU) co-processor and accelerator technology based HPC systems.

The high-fidelity M&S of nuclear reactors requires the computation of the power distribution as well as burn-up/depletion of fissile isotopes such as U^{235}. The computation of the power distribution within a nuclear reactor is determined using the neutron transport equation (NTE). The NTE is a linearized form of the full non-linear Boltzmann transport equation (BTE). It models the migration of neutrons through a host medium and enables nuclear reactor physicists and nuclear engineers to determine the power distribution in nuclear reactor fuel pins and assemblies as well as the radiation damage in reactor shields or the radiation dose to nuclear workers. However, many challenges are posed in obtaining numerical solutions due to the seven-dimensional phase space of solution variables – position, energy, angle, and time (x, y, z, E, θ, χ, t). The NTE is a hyperbolic partial-integral differential equation (PIDE) which requires specialised numerical discretisation methods, pre-conditioned matrix iterative solution algorithms and parallelisation strategies.

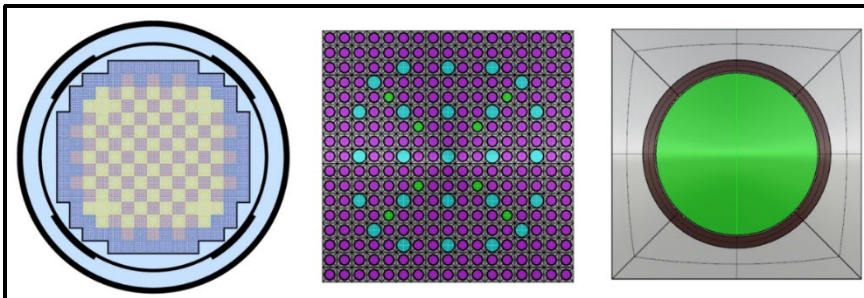

Figure 1: Schematic of a typical Pressurized Water Reactor (PWR) core, nuclear fuel assembly and nuclear fuel pin.

In addition, to compute the burn-up/depletion chains within a nuclear reactor a coupled system of ordinary differential systems (ODEs) needs to be solved called the Bateman equation (BE). The BE is a mathematical model describing abundances and activities in a decay chain as a function of time (t), based upon decay rates (λ_i) and initial abundances (N_i) for isotope (i). The Bateman equation (BE) requires the scalar neutron flux (which is determined by solving the NTE) to compute the atomic number densities of nuclides within a nuclear reactor during depletion. However, the application of the NTE and BE to nuclear reactor analysis is challenging due to the multiscale nature of the nuclear reactor geometries that range from the nuclear fuel pin-cell level (~ 1.26 cm) to the nuclear fuel assembly level (~ 21.42 cm) and the whole nuclear reactor core level (~ 3.0 to 4.0 m) as shown in Figure 1. The conventional approach to nuclear reactor modelling is a multistage process. The first stage involves solving the NTE over a 2D nuclear fuel assembly with periodic boundary conditions using a couple of hundred neutron energy groups. The single fuel assembly calculations are performed using lattice physics codes that solve the NTE. These lattice physics codes also perform spatial and energy resonance self-shielding to account for the effects of neutron resonances (or significant spikes) within the neutron cross-section data which occur within the neutron resonance region (epi-thermal neutron energy region). These resonances (or spikes in the neutron cross-sections) complicate the calculations. They arise due to neutrons having the same energy as one of the underlying quantum energy levels of the nucleons of atomic nuclei within the host material through which the neutrons are migrating. The geometry and material data are then homogenized over a single nuclear fuel assembly (often called a node) using the solution of the NTE. In addition, the number of neutron energy groups (used to discretize the energy variable of the NTE) is reduced to between 2-4 using energy group condensation or averaging methods. The spatially homogenized, resonance self-shielded and energy group condensed material data, along with assembly discontinuity factors, is then utilized within whole core nuclear reactor physics simulation software called nodal codes using an approximation to the NTE called the neutron diffusion equation (NDE). The whole core nodal neutron diffusion codes are like finite volume (FV) methods and enable the averaged scalar neutron flux (related to the average power and neutron density) within in nuclear fuel assembly (or node) to be determined. If the fine scale scalar neutron flux (or power) or power is required, then the lattice physics and whole core nuclear reactor physics solutions are combined to perform so called pin-power reconstruction to compute the fully heterogeneous pin-by-pin scalar neutron flux (or power). However, this leads to substantial approximations within the whole core nuclear reactor physics simulations due to the spatial homogenization and energy group condensation.

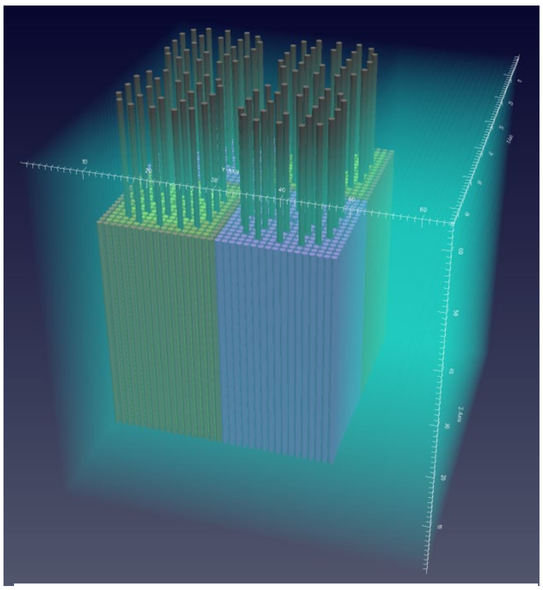

Figure 2: Four Pressurized Water Reactor (PWR) nuclear fuel assemblies within a surrounding water reflector region.

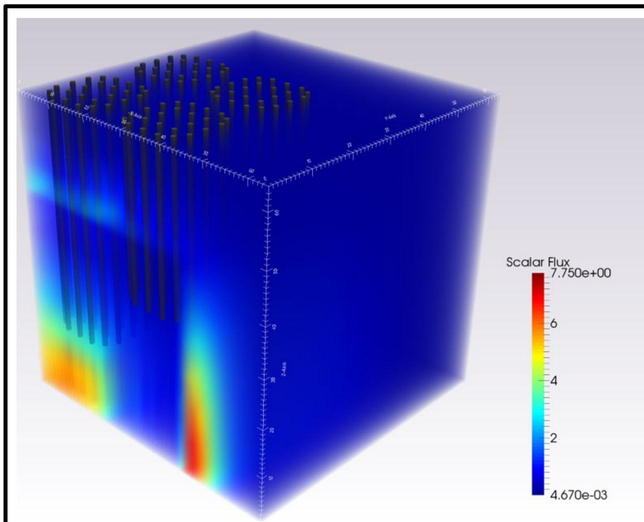

Figure 3: Scalar neutron flux distribution (related to the density of neutrons and the power distribution) within the OECD/NEA C5G7 international nuclear reactor physics benchmark verification test case. The scalar neutron flux distribution was computed using an isogeometric analysis (IGA) based neutron transport method.

Therefore, modern approaches to nuclear reactor physics simulations attempt to eliminate many of these approximations by performing high-fidelity, massively parallel, neutron transport (NT) simulations over the full 3D heterogeneous geometry of the nuclear reactor core. Typical 3D whole core nuclear reactor physics PWR problems consist of between 200-300 nuclear fuel assemblies with between 57,800 to 86,700 nuclear fuel pins. This represents a substantial computational challenge even for high-fidelity, massively parallel neutron transport codes to accurately compute the pin-by-pin power distribution and the isotopic nuclide distribution within the nuclear reactor core. An example of a 3D high-fidelity neutron transport simulation in Figure 2 which represents four Pressurized Water Reactor (PWR) nuclear fuel assemblies with a surrounding water reflector region and with the control rods (CR) partially inserted. Two of these PWR nuclear fuel assemblies are conventional uranium dioxide (UOX) nuclear fuel and the other two are mixed oxide (MOX) nuclear fuel assemblies that utilise zonal enrichment to flatten the power peaking within the MOX nuclear fuel assemblies. Each UOX and MOX nuclear fuel assembly is around 21.42 cm in width and breadth and with a height of around 400 cm. Each UOX and MOX nuclear fuel assembly comprises a 17×17 array of nuclear fuel pins of approximate width and breadth of 1.26 cm. This example nuclear reactor physics problem is called the 3D OECD/NEA C5G7 international nuclear reactor physics benchmark verification test case and is used primarily to verify the numerical implementation and results from deterministic neutron transport software. The scalar neutron flux (related to the density of neutrons and the power distribution), computed by solving the OECD/NEA 3D C5G7 nuclear reactor physics benchmark test case using an isogeometric analysis (IGA) based deterministic neutron transport method, is presented in Figure 3.

Developments and innovations in nuclear reactor design are one of the main drivers behind improvements in numerical M&S methods. The recent renaissance in the UK nuclear industry has provided renewed impetus behind developing improved high-fidelity digital reactor design (DRD) methods. In this regard, the UK is embarking on a nuclear new build programme that is being led by EDF with their evolutionary power reactor (EPR) which is under construction at Hinkley Point C in Sommerset. A second EDF EPR is planned to be constructed at the Sizewell C site in Suffolk. In addition, the UK government, through the department for energy security and net zero (DESNEZ) is supporting the development of both small (SMR) and advanced modular reactor (AMR) technologies. These novel nuclear reactor designs aim to reduce the cost and improve the safety, reliability, performance of nuclear power plants (NPPs). Examples include the UK SMR programme which is based upon a close coupled pressurized water reactor (PWR) design. DESNEZ is also considering support for a UK demonstration high temperature gas cooled reactor (HTGR) programme for use in power generation and within the UK's emerging hydrogen economy. Other examples of innovative nuclear reactor design include the Rolls-Royce microscale nuclear reactor programme for use in space and terrestrial power applications. These innovative nuclear reactor designs will require the latest high-fidelity, massively parallel, multiscale and multiphysics modelling and simulation (M&S) methods. The use of such high-fidelity models will not only streamline and speed-up the development of these innovative nuclear reactors but also lead to improved nuclear reactor designs with reduced cost (due to reduced pessimisms within the designs) as well as improved safety, reliability, and performance. Moreover, it will also support the regulatory approval of these innovative nuclear reactor designs as high-fidelity models can also quantify the model, discretisation, and parametric uncertainties within the simulations. Therefore, it is critically important that companies, such as Rolls-Royce, invest in massively parallel algorithm development on the latest multicore (CPU) and manycore (GPU) HPC hardware architectures to produce the next generation of high-fidelity nuclear M&S software. This is the background and context for this PhD project which focusses on the development of nuclear reactor physics burn-up/depletion algorithms on shared (OpenMP) and distributed memory (MPI) multicore and manycore (Graphics Processing Units – GPU) high performance computing (HPC) hardware architectures. Such methods will enable high-fidelity simulations of SMR, AMR and advance microscale nuclear reactors to be performed.

A second driver behind improvements in DRD methods are developments in massively parallel HPC hardware architectures. The latest generation exascale, tier-0, leadership class high performance computing (HPC) systems such as the Oak Ridge National Laboratory (ORNL) Frontier system (8.73 million compute cores), the Lawrence Livermore National Laboratory (LLNL) El Capitan system and the Argonne National Laboratory (ANL) Aurora system involve paradigm shifts and innovations in hardware architecture and software stack technologies. These innovations in HPC hardware architecture and software stack technologies will permeate throughout the whole of the HPC pyramid from the Tier-0 leadership class systems down to high performance multicore workstations with co-processor and accelerator card (Graphics Processing Units - GPU) technologies. Exascale HPC hardware architectures are based upon both multicore and manycore (GPUs) within each node with high bandwidth, low latency, infiniband for the internal connection technology within the HPC system. The ORNL Frontier exascale HPC system utilizes AMD EPYC 7A53s 64 core CPUs and Radeon instinct MI250X GPUs. Frontier has coherent interconnects between the CPUs and GPUs allowing GPU memory to be accessed coherently by code running on the EPYC CPUs. The LLNL El Capitan HPC system uses a similar hardware architecture but with the latest generation of AMD CPUs and GPUs. The key aspect to both exascale HPC systems is the close integration of both the CPU cores and the GPUs which will be a feature of all large scale HPC systems in the immediate future. This means that it is vitally important for companies, such as Rolls-Royce, to initiate research and development (R&D) into computationally efficient, massively parallel, deterministic neutron transport algorithms. These massively parallel algorithms must also be scalable and computationally efficient on hybrid CPU and GPU HPC systems. This will mean that companies, such as Rolls-Royce, will then be well positioned to take advantage of future HPC hardware architectures that integrate both multicore CPU processors and manycore (GPU) co-processor and accelerator technologies.

One of the many challenges of high-fidelity nuclear reactor physics M&S, aside from solving large systems of coupled PIDEs and ODEs, is storing and manipulating the associated large data sets. In addition, nuclear data, within high-fidelity nuclear reactor physics simulations, also involves large data sets. The storage and manipulation of large data sets becomes one of the primary challenges when using spatially highly resolved computational meshes. Therefore, computationally efficient, scalable, parallel algorithms for data reading, data transfer, data compression and data manipulation are critically important. To obtain scalability of the resulting parallel algorithms it is important to carefully analyse them for data reading, data transfer, data compression and data manipulation. When solving the NTE in parallel the computational mesh is often spatially domain decomposed using graph partitioning algorithms implemented in software such as ParMETIS. Information is passed between each of the sub-domains in the mesh to enable parallel solution of the resulting matrix system of linear equations. Each sub-domain must also solve the BE as well so that the depletion and spatial distribution of nuclides and fission products can be computed. The computationally efficient resolution of the coupled NTE and BE, as well as the parallel data management issues, are the main challenges and focus of this PhD project.

It is often challenging to develop and implement algorithms that are scalable, as well as memory efficient, on shared and distributed memory multicore (CPU) and manycore (GPU) HPC systems. Moreover, the challenge of dealing with the large data sets that arise from performing 3D high-fidelity, parallel nuclear reactor physics burn-up/depletion calculations is substantial. This is one of the major challenges for both massively parallel Monte Carlo and deterministic nuclear reactor physics simulations performed on the latest multicore (CPU) and manycore (GPU) HPC hardware architectures. In terms of the resolution of the stiff sets of ODEs associated with the Bateman equations of nuclear reactor physics, the most computationally efficient parallel backward differentiation ODE algorithms have been implemented within the massively parallel SUNDIALS (SUite of Nonlinear and Differential/ALgebraic Equation Solvers) numerical library. This massively parallel numerical ODE algorithm library enables systems of stiff ODEs to be solved on shared and distributed memory HPC systems. However, this needs to be integrated within a domain decomposition/graph partitioning of the computational mesh used to resolve the NTE. A high-fidelity numerical model of a typical civilian nuclear reactor, using small burn-up/depletion time steps, represents a formidable computational challenge even for the latest massively parallel nuclear reactor physics software. Therefore, this provides the motivation for the development of improved shared and distributed memory parallel burn-up/depletion algorithms within this PhD project.

PhD project description – The advent of shared and distributed memory high performance computing (HPC) hardware architectures is driving innovations in nuclear reactor physics modelling and simulation software. In the research literature improvements in parallel nuclear reactor physics algorithms have primarily focussed on the parallelisation of the NTE. However, less attention has been devoted to how the coupled NTE and the nuclear fuel burn-up/depletion computations are performed on shared and distributed memory HPC systems. As discussed in the introduction this presents a significant computational challenge in terms of parallel data reading, data transfer, data compression and data manipulation associated with the resolution of the scalar neutron flux field (related to density of neutrons and power distribution) within domain decomposed/graph partitioned computational meshes, nuclear data and the resolution of large stiff sets ODEs. The aim of this PhD is to evaluate the main challenges, develop appropriate shared and distributed memory parallel solution algorithms that are computational efficient for extremely large data sets and that can resolve each nuclear fuel burn-up/depletion time-step using a highly scalable approach that can resolve in space and time the fissile nuclides and fission products throughout highly complex, 3D, geometry conforming meshes. The research and development (R&D) programme for this PhD will focus on the following:

- Training in nuclear reactor physics, shared and distributed memory parallel algorithms using OpenMP and MPI (as well as potential introduction to GPUs algorithms), parallel backward differentiation ordinary ODE solution algorithms (as implemented in the SUNDIALS library), domain decomposition/graph partitioning methods (as implemented within ParMETIS) and parallel neutron transport methods, nuclear data, and resonance self-shielding methods. This ensures that the PhD student has a focussed yet detailed knowledge base in which to perform the R&D associated with their PhD. This will also mean that Rolls-Royce have a young professional with focussed training within the field who can integrate within their current software development team if they are recruited after their PhD is complete.

- The approach taken will be to utilise the AVARIS shared and distributed memory parallel neutron transport M&S framework. A protype version of AVARIS with a parallel nuclear fuel burn-up/depletion module will be implemented. From R&D conducted by two PhDs on resonance self-shielding AVARIS will be coupled to a HDF5 and/or XML based nuclear data library that will be extensible and able to be read in parallel. The AVARIS M&S software already utilises domain decomposition/graph partitioning algorithms to decompose large scale, 3D, computational meshes of the problem domain into a series of contiguous computational mesh sub-domains. The Bateman ODE equations of nuclear fuel burn-up/depletion will be solved for each burn-up/depletion step on each of the computational mesh sub-domains with parallel information/data transfer within each sub-domain. An analysis of the parallel solution of the Bateman ODE equations on each computational mesh sub-domain will be performed in terms of computational scalability and memory efficiency. The parallel data reading, data transfer, data compression, data manipulation will also be analysed carefully to produce scalable and memory efficient approaches to the spatial and temporal resolution of fissile nuclides and products throughout the lifetime of a nuclear reactor core. Algorithms within AVARIS will be implemented to represent the continual movement of the control rods within the nuclear reactor core and the associated power variations that will affect the nuclear fuel burn-up/depletion simulations.

- A suite of nuclear reactor burn-up/depletion verification and validation (V&V) benchmark test cases from the OECD/NEA will be utilised to validate and verify (V&V) the implementation of these shared and distributed memory parallel nuclear fuel burn-up and depletion algorithms within the AVARIS nuclear reactor physics modelling and simulation (M&S) framework. The feasibility of further V&V benchmark test cases will be discussed with Rolls-Royce.

- The final output from this PhD will the PhD thesis, journal papers and industrial reports describing the shared and distributed memory HPC algorithms used to produce 3D high-fidelity numerical models of spatially large-scale nuclear reactor burn-up/depletion problems. In addition, this PhD will result in a prototype nuclear fuel burn-up/depletion version of AVARIS that implements these shared and distributed memory algorithms. This PhD will also lead to the development of a young professional within the field of nuclear reactor physics that can be recruited to Rolls-Royce submarines after the successful completion of their PhD project.

The successful candidate will join, and be supported by, a vibrant and dynamic group with world class expertise in the numerical modelling of radiation transport and multiphysics phenomena for nuclear engineering. During their four years of study, they will be trained in the latest state-of-the-art numerical methods for simulating radiation transport in nuclear reactor cores and shields, parallel high-performance computing (HPC) techniques, object-oriented programming (OOP), and scalable solvers as well as trained in the use of the industrial nuclear reactor physics and reactor shielding software for verification and validation (V&V) purposes. The successful candidate will be sent on a wide variety of national, and international, training courses such as: the ICL high performance computing (HPC) courses (https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/rcs/get-support/training/), the University of Cambridge's high performance computing (HPC) autumn academy (https://www.csc.cam.ac.uk/academic/cpd/hpcacademy), the INSTN/CEA international school in nuclear engineering held in Paris (https://instn.cea.fr/en/), the Frederic Joliot/Otto Hahn Summer School in reactor physics (FJOH) which are held in France and Germany (http://www.fjohss.eu) and also the GRE@T-PIONEeR European Union Nuclear Engineering courses (https://great-pioneer.eu/courses/). In addition, the successful candidate will be sent on an experimental nuclear reactor physics course that is held annually in Europe. This is in addition to courses in numerical analysis, MPI and OpenMP programming, nuclear reactor physics and radiation shielding at Imperial College London (ICL).

The successful candidate will have the opportunity to develop their career, transferable skills, and profile by presenting at international conferences and publishing in high impact nuclear engineering and numerical analysis journals. ICL also has a wide variety of professional development (PD) courses that PhD students must undertake as part of their studies in addition to all the technical training. The professional development courses that the successful candidate will undertake will help develop their non-technical transferable skills. This will help widen their recruitment appeal to both engineering/science and non-science/engineering-based companies. The successful candidate will have the opportunity to work with engineers and scientists from the industrial sponsor, Rolls-Royce, during their PhD studentship to help broaden their industrial experience. They will be assigned at least one Rolls-Royce industrial co-supervisor who will assist them in understanding the industrial context of their research as well as helping to mentor them during their PhD studies. Candidates for this PhD studentship should have a good mathematical background and a good degree (First Class or Upper Second-Class honours) in an appropriate field such as physics, mathematics, computer science or engineering. Applications from candidates with an MSc in scientific computing or numerical modelling are particularly welcome. It cannot be over-emphasized that the candidate must have very good mathematical skills and the ability to put physical models into a mathematical form. The successful candidate must be willing, and able, to achieve security clearance (SC) by the industrial sponsor Rolls-Royce. To apply for this PhD studentship please email Dr Matthew Eaton (m.eaton@imperial.ac.uk) with a copy of your curriculum vitae (CV).