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

Computational Methods for Radiation Transport within Multiphase Materials with Application to Nuclear Reactor Physics and Reactor Shielding Modelling and Simulation (M&S)

The aim of this PhD project is to develop high-fidelity computational methods for modelling and simulating (M&S) radiation transport within multiphase media and materials. These methods will be applied to both nuclear reactor physics and reactor shielding modelling and simulation (M&S). A multiphase material is one that has more than one distinct compound in it and the compounds form distinct regions in the substance with different properties. A typical example is the use of particulate nuclear fuels such as TRISO (TRI-Structural ISOtopic) particles within high temperature gas reactors (HTGRs) or the use of TRISO particulate pebbles within pebble bed modular reactors (PBMRs). The geometry, and configuration, of particulate nuclear fuel forms, such as the nuclear fuel used within the Japanese Atomic Energy Agency (JAEA) High Temperature Test Reactor (HTTR), is presented in Figure 1. One can clearly see the complex nature of the nuclear fuel forms, and this presents substantial challenges when performing nuclear reactor physics simulations. Such particulate fuel forms are utilized within advanced modular nuclear reactor (AMR) designs such as the Rolls-Royce microscale nuclear reactor. The Rolls-Royce microscale reactor is being developed for both space and terrestrial nuclear power applications. The primary aim is to improve the safety, performance, and reliability of the nuclear power plants (NPPs) by using these types of advanced technology nuclear fuels (ATFs).

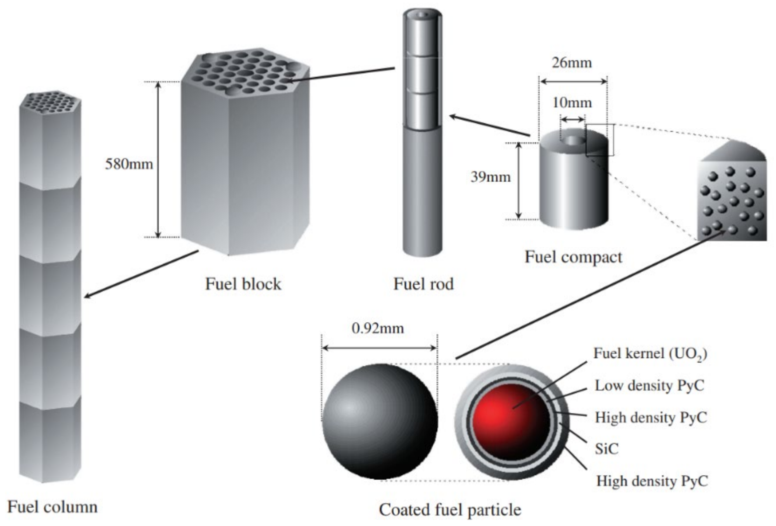

Figure 1: Japanese Atomic Energy Agency (JAEA) High Temperature Test Reactor (HTTR) nuclear fuel form (i.e., TRISO particles, nuclear fuel pin and hexagonal nuclear fuel assembly). This image is from Minoru Goto, Naoki Nojiri and Satoshi Shimakawa, Neutronics Calculations of HTTR with Several Nuclear Data Libraries, Journal of Nuclear Science and Technology, Volume 43, Number 10, Pages 1237–1244 (2006).

More recently, some innovative small modular reactor (SMR) designs have proposed utilizing particulate nuclear fuels with Mixed OXide (MOX) TRISO particles. The aim of this novel nuclear fuel form was to improve nuclear waste management, safety, reliability, and performance. Another example is the use of composite metals foams with absorbing inclusions for use in reactor shielding. This can produce a new generation of advanced reactor shielding materials that can reduce the weight and size of nuclear reactor shields for nuclear power plants (NPPs). The introduction of significant heterogeneities within nuclear fuel pins and assemblies represents significant challenges to deterministic and Monte Carlo neutron transport methods. The primary issue is the double heterogeneity spatial self-shielding phenomena due to the random absorbing inclusions within the multiphase nuclear materials which can significantly distort the spatial and angular of neutrons and reaction rates (e.g., neutron fission and capture rates) within nuclear reactor cores and shields. This can also have a significant impact upon energy resonance self-shielding phenomena within nuclear fuel assembly neutron transport simulations. For deterministic neutron transport methods, the approach usually taken in modelling such systems is to utilize spatially homogenization methods. The aim of spatial homogenization is to produce equivalent homogenized materials that reproduce the reaction rates predicted within the heterogeneous materials. However, this can lead to significant modelling errors in the reaction rates within the nuclear fuel pins and fuel assemblies (e.g., neutron fission and capture rates).

For Monte Carlo methods typical modelling approaches involve simulating the particles explicitly and then using efficient methodologies such as woodcock, or delta tracking, algorithms. This is because for such problems standard Monte Carlo ray-tracing algorithms are computationally demanding as they must perform particle tracking through billions of potential surfaces and cells. However, such Monte Carlo methods provide reference solutions against which deterministic methods can be verified. For reactor shielding the use of multiphase materials can potentially reduce the weight and size of reactor shields. However, the large-scale nature of most reactor shields, the highly anisotropic nature of the angular neutron flux and the highly anisotropic nature of the neutron and gamma-ray photon scattering makes modelling radiation transport in reactor shields composed of multiphase materials mathematical and computationally challenging. Therefore, the aim of this PhD is to develop high-fidelity mathematical methods and computational radiation transport algorithms that can model radiation transport in such multiphase materials.

Typically, the NTE is used for nuclear fuel pin-cell and fuel assembly simulations whereas the NDE is used for whole nuclear reactor core simulations. However, the use of the NDE can introduce significant modelling errors if not performed carefully using spatial homogenisation methods. The NTE is a linearised form of the full non-linear Boltzmann transport equation that describes the migration of neutral particles within a host medium. 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)**.** Its application to nuclear reactor analysis is also made increasingly complex by the multiscale nature of the typical 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 2 which shows a typical pressurized water reactor (PWR) nuclear reactor core geometry. This multiscale structure is further complicated when modelling nuclear fuel pins and fuel assemblies that are composed of particulates, TRISO particles or other multiphase nuclear fuel materials. When numerically discretising the NTE numerical errors can incur in the space (x, y, z), energy (E), angular (θ, χ), and temporal (t) variables. The latest high-fidelity numerical models aim to substantially reduce these numerical discretisation and modelling errors.

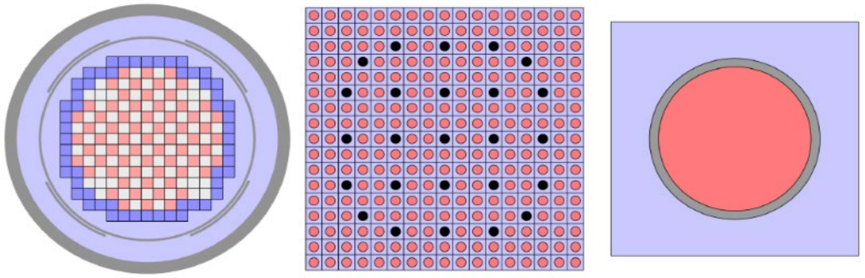

Figure 2: Water Reactor Nuclear Reactor Core, Fuel Assembly and Pin-cell.

The conventional approach to nuclear reactor modelling is a multistage simulation process. The first stage involves solving the NTE over a 2D/3D 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. These spatially homogenized, resonance self-shielded and energy group condensed material data, along with discontinuity factors us 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 the nuclear fuel assembly (or node) to be determined. If the fine scale scalar neutron flux (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.

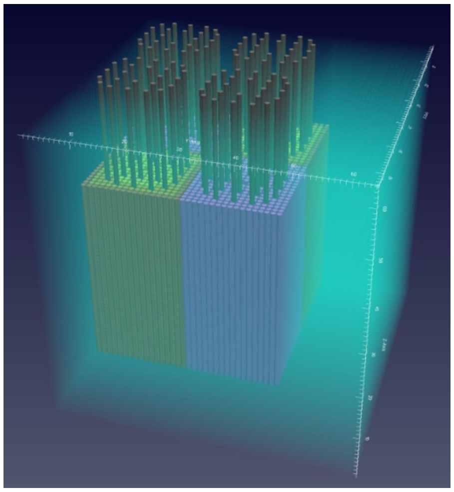

Figure 3: Four Pressurized Water Reactor (PWR) nuclear fuel assemblies within a surrounding water reflector region.

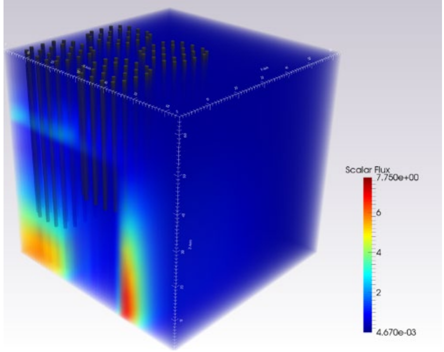

Figure 4: Scalar neutron flux distribution (related to the density of neutrons and the spatial power distribution in the nuclear reactor core) within the OECD/NEA C5G7 international nuclear reactor physics benchmark verification test case. The scalar neutron flux distribution was computed using an isogeometric 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 pressurized water reactor (PWR) technology. 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. This HTGR would utilize advanced multiphase nuclear materials such as TRISO particulate fuel compacts. The UK has extensive experience with such nuclear fuels through the European High Temperature Reactor (HTR) programme which explored the use of TRISO nuclear fuel and high temperature Helium gas cooling for future high thermodynamic efficiency reactor designs. This led to the development of the DRAGON reactor which was an experimental high temperature Helium gas-cooled reactor built at Winfrith in Dorset, England which was operated by the United Kingdom Atomic Energy Authority (UKAEA). The aim of the DRAGON reactor programme was to test HTGR fuel and materials. The project was built and managed as Organization for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA) international project. In total thirteen countries were involved in its design and operation during the project lifetime (1965 to 1976).

Other examples of innovative nuclear reactor design include the Rolls-Royce microscale advanced modular (AMR) 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 AMR 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 due to the use of advanced technology fuels (ATFs). Moreover, it will also support the regulatory approval of these innovative AMR 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 the latest massively parallel high-performance computing (HPC) algorithms as well as multiscale and multiphysics modelling methods to producer the next generation of high-fidelity nuclear M&S software. This is the background and context for this PhD project which focussed on the development of advanced multiscale M&S methods for simulating innovative nuclear reactors that utilize advanced multiphase nuclear materials within their nuclear reactor cores and shields. Examples of such advanced multiphase nuclear materials include particulate nuclear reactor fuels and composite metal foams reactor shielding materials. The nuclear engineering group (NEG) within the mechanical engineering department (MED) at Imperial College London (ICL) has been pioneering advanced multiscale M&S methods within nuclear reactor physics and reactor shielding. Such methods include multiscale spatial and energy discretisation approaches and advanced spatial uncertainty quantification (UQ) algorithms such as high-dimensional model representation adaptive sparse grid collocation generalized polynomial chaos (HDMR-ASGC-gPC) algorithms combined with Kosambi–Karhunen–Loève expansions (KKL), Nataf and Rosenblatt transform (NRT) methods. These methods can model the complex, multiscale, non-Gaussian, spatial statistics associated with random particulates or inclusions within multiphase nuclear materials such as TRISO particulate nuclear fuel and composite metal form reactor shielding materials. The aim would be to combine these advanced mathematical and computational multiscale IGA and spatial UQ methodologies with the very latest hybrid multicore CPU and manycore Graphics Processing Unit (GPU) algorithms as well as cutting-edge spatial and energy resonance self-shielding algorithms. Such an approach would produce high-fidelity nuclear reactor physics and reactor shielding methods capable of modelling the very latest advanced multiphase nuclear materials within nuclear reactor cores and shields.

PhD project description – The aims of this PhD project are manifold. The **first aim** is to conduct a comprehensive survey of the latest heterogeneous multiphase nuclear materials used in both nuclear fuels (e.g., TRISO fuel compacts etc.) as well as in reactor shields (e.g., composite metal foams etc.). This will investigate the latest technologies for both conventional light water reactor (LWR), small modular reactors (SMRs) and advanced modular reactors (AMRs). In addition, a comprehensive survey of deterministic radiation transport and resonance self-shielding methods for multiphase materials will be conducted. This will also encompass methods developed within the materials modelling research literature. Such methods will encompass multiscale spatial and energy discretisation methods, high-dimensional model representation adaptive sparse grid collocation generalized polynomial chaos (HDMR-ASGC-gPC), Kosambi–Karhunen–Loève expansions (KKL), Nataf and Rosenblatt transform (NRT) methods to deal with the non-Gaussian statistics of the spatial distribution of nuclear fuel particulates and absorbing inclusions within multiphase nuclear materials.

The **second aim** of the PhD is training in the basic spatial discretization methods associated with the neutron diffusion equation (NDE) and the neutron transport equation (NTE). This initial phase of training will encompass finite difference (FD), finite volume, (FV), finite element (FE) and virtual element (VE) spatial discretization methods. It will also encompass training in nuclear reactor physics and reactor shielding methods and software (e.g., Serpent, MCNP6.3 and OpenMC), software engineering and version control systems (VCS such as Git), modern Fortran and python programming, formalized verification (e.g., method of manufactured solutions or MMS methods) and validation (using the IRPhE reactor physics and SINBAD reactor shielding international integral data benchmarks) methods. and the use of visualization (e.g., Paraview and Mayavi2) and mesh generation software (e.g., Gmsh). In addition, the training will also encompass multicore CPU shared (OpenMP) and distributed memory (MPI) parallelization algorithms and the use of advanced hierarchical one-level (e.g., preconditioned conjugate gradient or PCG, Bi-Conjugate Gradient or BCG and General Minimal Residual or GMRES algorithms) and multi-level or multigrid matrix solution algorithms using the Portable, Extensible Toolkit for Scientific Computation (PETSc) libraries. This training phase of the PhD will also encompass multiscale modelling and simulation (M&S) methods. Finally, the training will encompass advanced spatial uncertainty quantification (UQ) algorithms such as high-dimensional model representation adaptive sparse grid collocation generalized polynomial chaos (HDMR-ASGC-gPC), Kosambi–Karhunen–Loève expansions (KKL), Nataf and Rosenblatt transform (NRT) methods that are able to model the non-Gaussian statistics of the spatial distribution of nuclear fuel particulates and absorbing inclusions within multiphase nuclear materials. Potentially, if time permits, the PhD training phase will encompass hybrid multicore central processing unit (CPU and manycore core Graphical Processing Unit (GPU) HPC acceleration algorithms as well. The approach would be to utilize the Intel OneAPI HPC software framework that incorporates libraries for multicore CPU shared (OpenMP) and distributed memory (MPI) parallelization as well manycore GPU HPC acceleration algorithms.

The **third aim** of the PhD is the development of multiscale NURBS enhanced spatial discretization methods. The multiscale spatial discretization methods will be able to model the complex three-dimensional (3D) Voronoi cells which are typically found at the microstructural grain and mesoscale level in materials. The multiscale approaches will then be used to couple the microscale, mesoscale and macroscale spatial scales together using appropriate scale resolving spatial functions. Such an approach will be able to model random heterogeneities at all the three spatial scales depending upon the size of the random inclusions within the multiphase nuclear materials. The multiscale spatial discretization methods will be combined with high-dimensional model representation adaptive sparse grid collocation generalized polynomial chaos (HDMR-ASGC-gPC), Kosambi–Karhunen–Loève expansions (KKL), Nataf and Rosenblatt transform (NRT) methods to model the stochastic variation in space of random absorbing inclusions within the host media (e.g., TRISO particles, burnable absorbers or other neutron absorbing grains). A key aspect of this PhD project will be to model the spatial resonance self-shielding effects of these random inclusions within the multiphase nuclear materials. This is especially important for particulate nuclear fuels such as TRISO fuel compacts. Therefore, cutting-edge multiscale or embedded energy resonance self-shielding methods will be integrated within the multiscale and spatial UQ models. Finally, if time permits the combined multiscale and spatial UQ resonance self-shielding models will be parallelized using hybrid multicore CPU and manycore GPU algorithms to ensure that the algorithms are computationally efficient and scalable on the latest massively parallel leadership class (Tier 0), Tier 1 and Tier 2 HPC hardware architectures.

The **fourth aim** will be to verify these multiscale and spatial UQ algorithms by analysing various international Nuclear Energy Agency (OECD/NEA) nuclear reactor physics benchmark verification test cases. Inter-code comparison and benchmarking will include comparison against conventional Monte Carlo methods implemented with the codes MCNP6.3, Serpent and OpenMC. The **final aim** will be to write any associated conference and journal papers that stem from the research as well as the PhD thesis. To summarize, the research and development (R&D) programme for this PhD will focus on the following:

- A comprehensive survey of latest heterogeneous multiphase nuclear materials for nuclear reactor physics and reactor shielding, multiscale M&S methods, advanced resonance self-shielding methods, hybrid multicore CPU and manycore GPU algorithms and spatial UQ methods.

- Training in the spatial discretization methods, energy resonance self-shielding methods, spatial UQ methods, modern Fortran programming, multicore CPU and manycore GPU programming (using the MPI and OpenMP shared and distributed memory parallel programming software libraries within the Intel OneAPI software framework), python programming for data processing and manipulation, mesh generation (e.g., Gmsh) and visualization software (Paraview and Mayavi2), uncertainty quantification methods (e.g., generalized polynomial chaos or gPC methods and Monte Carlo algorithms), software engineering and revision control systems (RCS such as Git), formalized verification (MMS or method of manufactured solutions) and validation methods (e.g., IRPhE reactor physics and SINBAD reactor shielding international integral benchmarks). Training will also be provided on transferable skills such as the writing of journal and conference papers, industrial reports, and presentations. Aspects of this training programme will be conducted within the nuclear engineering group (NEG) within the mechanical engineering department (MED) at Imperial College London (ICL). However, aspects of this training programme will involve attending the ICL high performance computing (HPC) courses (https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/rcs/get-support/training/), the Cambridge 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/).

- Development of multiscale NURBS enhanced spatial discretization methods. The multiscale spatial discretization methods will be able to model the complex three-dimensional (3D) Voronoi cells which are typically found at the microstructural grain and mesoscale level in materials. The multiscale approaches will then be used to couple the microscale, mesoscale and macroscale spatial scales together using appropriate scale resolving spatial functions. Such an approach will be able to model random heterogeneities at all the three spatial scales depending upon the size of the random inclusions within the multiphase nuclear materials. The multiscale spatial discretization methods will be combined with high-dimensional model representation adaptive sparse grid collocation generalized polynomial chaos (HDMR-ASGC-gPC), Kosambi–Karhunen–Loève expansions (KKL), Nataf and Rosenblatt transform (NRT) methods to model the stochastic variation in space of random absorbing inclusions within the host media (e.g., TRISO particles, burnable absorbers or other neutron absorbing grains). A key aspect of this PhD project will be to model the spatial resonance self-shielding effects of these random inclusions within the multiphase nuclear materials. This is especially important for particulate nuclear fuels such as TRISO fuel compacts. Therefore, cutting-edge multiscale or embedded energy resonance self-shielding methods will be integrated within the multiscale and spatial UQ models. Finally, if time permits the combined multiscale and spatial UQ resonance self-shielding models will be parallelized using hybrid multicore CPU and manycore GPU algorithms to ensure that the algorithms are computational efficient.

- The final output from this PhD will the conference journal papers and PhD thesis describing the multiscale nuclear reactor physics and reactor shielding methods, a prototype multiscale M&S framework, and a suite of nuclear reactor physics and reactor shielding benchmark verification test cases for nuclear reactor cores and shields containing multiphase nuclear materials. This PhD will also lead to the development of a young professional, within the field of multiscale nuclear reactor physics and reactor shielding M&S, by Rolls-Royce who can continue the development of these multiscale M&S methods within an industrial context.

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 overemphasized 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).