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

Computer Aided Geometric Design (CAGD) Compatible Coarse Mesh Computational Fluid Dynamics (CM-CFD) Models of Natural Circulation (NC) Flow in Pressurized Water Reactors (PWRs)

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The aim of this Rolls-Royce sponsored PhD project is to develop computer aided geometric design (CAGD) compatible spatial discretisation methods for the Navier-Stokes equations (NSE) for use in coarse mesh computational fluid dynamics (CM-CFD) modelling of natural circulation/convection (NC) within the primary nuclear thermal-hydraulic circuit of nuclear reactors. We will term CAGD compatible CM-CFD as CAGD-CFD methods in this PhD project description. More specifically, this PhD project is focussed on NC flow phenomena within pressurised water reactors (PWRs). An example of NC within a closed loop primary nuclear thermal-hydraulic circuit (PNTHC) is presented in **Figure 1** below. The use of CAGD-CFD enables the exact representation, to numerical precision, of the underlying CAGD curvilinear geometry description on coarse computational grids/meshes. The use of high-order basis/shape functions enables solution field variables/unknowns to be represented/interpolated with reasonable numerical accuracy on coarse grids/meshes. Moreover, high-order spatial discretisation methods have certain desirable numerical properties on the latest hybrid multicore (CPU) and manycore (GPU) high performance computing (HPC) hardware architectures. Indeed, such methods are the subject of current research through the United States (US) CEED (Centre for Efficient Exascale Discretisations) programme. The aim is to determine whether CAGD compatible CM-CFD can produce reasonably accurate numerical models of NC phenomena within the primary nuclear thermal-hydraulic circuit (PNTHC) of nuclear reactors. NC is the circulation of a fluid within a pipe system, or open pools, due to the density changes caused by temperature differences, NC does not require any mechanical devices to maintain the fluid flow. NC, also known as free convection (FC), is a phenomenon, or type of mass and heat transport, in which the fluid motion is generated only by density differences in the fluid occurring due to temperature gradients, not by any external source (e.g., recirculation pump, fan, suction devices etc). In NC the fluid surrounding a heat source receives heat, becomes less dense, and rises by thermal expansion. Therefore, thermal expansion of the fluid plays a critical role in NC phenomena (see **Figure 1**). Thus, more dense fluids will fall, whilst less dense fluids will rise, leading to bulk fluid movement or flow. NC is a desirable flow phenomenon as it can provide nuclear reactor core cooling after the loss of reactor coolant pumps (RCPs) power.

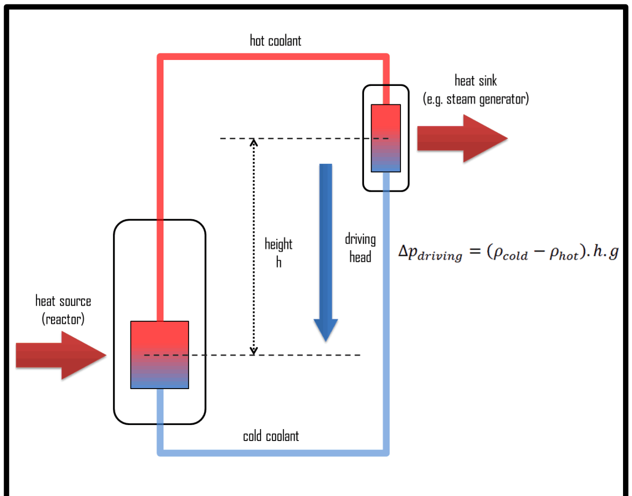

Figure 1: Diagram showing natural circulation (NC) in a closed-loop thermal-hydraulic circuit.

In a civil PWRs, the nuclear power plant (NPP) design provides an elevation difference, h, of approximately 12 metres between the centreline of the steam generator (SG) and the centreline of the nuclear reactor core. The NPP primary nuclear thermal-hydraulic circuit (PNTHC) design must ensure the capability for NC, following a loss of flow, to enable cooldown and removal of residual decay heat without overheating the nuclear reactor core. Moreover, the interconnecting pipe system from the reactor pressure vessel (RPV) to the steam generators (SGs) must be intact, from any obstructions such as non-condensable gasses (e.g., steam pockets within the PNTHC). In this manner, NC phenomena will ensure that the fluid will continue to flow if the reactor is hotter than the heat sink, even when power cannot be supplied to the RCPs. It is important to note that RCPs are not usually "safety systems" due to their function within reactor. After the loss of power to RCPs the nuclear reactor must be shut down immediately, through the insertion of the control rods since RCPs slowly coast down to zero flow rate. Sufficient, and safe, residual decay heat removal is then ensured by a NC flow through the nuclear reactor. If there is no forced flow the coolant in the nuclear reactor core starts to heat up. The increase in coolant temperature causes a reduction in the coolant density which in turn moves the coolant into the SG. It must be noted that NC is not sufficient to remove the heat being generated when the nuclear reactor is operating at power. Modern nuclear reactor designs, such as the AP1000, use NC as a passive safety feature. Many passive safety systems in modern nuclear reactor designs operate without using any reactor coolant pumps (RCPs), which improves the safety, integrity and reliability of these nuclear reactor designs whilst simultaneously reducing their cost. One of the primary drivers for this PhD project is to determine whether coarse mesh CFD models, using CAGD-CFD spatial discretisation methods, can be used to accurately model, and predict, NC phenomena within PWRs.

CAGD-CFD can, in principle, enable fewer numerical cells/elements to be used in modelling curvilinear CAGD computational domains. This is because low-order methods, using straight sided line elements for the surfaces of polygons (2D) or planar facetted faces for the surfaces of polyhedra (3D), would produce very substantial geometrical errors on very coarse computational grids/meshes of curvilinear geometrical domains. Conversely, CAGD-CFD can accurately model curvilinear CAGD geometries even on very coarse computational grids/meshes. However, this is at the expense of potentially reducing the numerical accuracy of the solution field variables/unknowns such as velocity, pressure, and temperature. The use of CM-CFD, using conventional low-order accurate finite difference (FD), finite volume (FV) and finite element (FE) approaches, can lead to several numerical errors. The first numerical error arises through the approximation of the underlying geometry of the spatial domain within the use of straight sided computational cells/elements. The second numerical error arises in the spatial accuracy of the solution if coarse mesh cells/elements are utilised along with low-order spatial discretisation methods. Low-order numerical methods are numerical dissipative (e.g., first-order upwind) whereas high-order numerical methods can be numerical dispersive (centred FD methods, Bubnov-Galerkin FE methods etc). This is embodied in Godunov's theorem that states "linear numerical methods for solving partial differential equations (PDEs), having the property of not generating new extrema (monotone method) are at most first-order accurate". Therefore, numerical analysts developed high-resolution schemes that non-linearly blend low and high-order methods using so-called flux or slope limiters. The idea is to avoid the spurious artefacts (or oscillations) that would otherwise occur with high-order spatial discretization schemes due to shocks, discontinuities or sharp changes in the solution domain but limiting the accuracy of the method at the discontinuity. Numerical simulations employing explicit of time integration schemes are often subject to stability requirements that constrain the size of the timestep depending on the spatial grid/mesh that is used. . It is worth noting that increasing the mesh size enables, in principle, a larger time-step. This might be advantageous for computational efficiency but will also lead to increased temporal discretisation errors. The final error that occurs, using coarse mesh CFD methods, is the model error associated with the modelling of turbulent fluid phenomena. The most accurate numerical model for turbulent fluid phenomena is direct numerical simulation (DNS). A DNS simulation in CFD is one in which the Navier-Stokes are numerically solved without any turbulence model. However, this means that the complete range of spatial and temporal scales associated with the turbulent fluid phenomena must be numerically resolved.

All the spatial scales of the turbulent fluid phenomena must be numerically resolved in the computational mesh, from the smallest dissipative scales (Kolmogorov microscales) to the integral scale, associated with the fluid motions containing most of the kinetic energy. The computational cost of DNS is extremely high even at modest Reynolds numbers and they are typically performed using high-order spectral based methods. For Reynolds numbers encountered in most industrial applications the computational requirements of DNS simulations would exceed the capacity of even tier-0 leadership class, exascale, high performance computing (HPC) systems such as the ORNL Frontier, ANL Aurora, and LLNL El Capitan exascale HPC systems. Alternative approaches for modelling turbulence include Large Eddy Simulation (LES) turbulence models. The LES method is a mathematical model for turbulence that it used in CFD. The central idea behind LES methods is to reduce the computational demands of simulating turbulence phenomena by not resolving the smallest turbulent length scales but modelling their effect on the larger scales. The smallest turbulent length scales are usually the most computationally demanding to resolve and thus LES methods utilise to low-pass mathematical filter operator to the Navier-Stokes equations. Such a low-pass filter can be viewed as a time and spatial-averaging operation which effectively removes small-scale information from the numerical solution. However, even LES methods are often still too demanding for most industrial applications. Therefore, Reynolds Averaged Navier-Stokes (RANS), Unsteady-RANS (URANS) and hybrid RANS/LES methods have been developed which have been used extensively in industrial and research applications. For CM-CFD methods the primary issues will be the inaccuracy of turbulence modelling as well as the spatial discretisation error (not the CAGD geometry error which is negligible even on the coarsest high-order curvilinear computational grid/mesh). Therefore, mathematical, and computational methods to address such issues of model and discretisation error will be an important aspect of this PhD research.

As stated previously, the primary aim of CAGD-CFD is to produce a high-fidelity geometrical representation of the computational/geometrical domain using as few cells/elements as possible. How coarse the computational grid/mesh can be made is a compromise between the computational efficiency and the numerical accuracy with which the solution field variables/unknowns and turbulent fluid phenomena are represented. CAGD software typically utilises Non-Uniform Rational B-splines (or NURBS) to represent curvilinear computational domains within engineering design analysis. Therefore, one way of minimising the number of cells/elements is to develop spatial discretisation methods that utilise the same set of basis/shape functions to represent the geometry of cells/elements that are utilised in the CAGD software (i.e., NURBS basis functions). The use of the same set of basis/shape functions within CAGD and the computer aided analysis (CAE) is termed isogeometric analysis (IGA) methods. The field of IGA spatial discretisation methods has expanded substantially over the last couple of decades from its initial inception and development. They are now a very large family of associated spatial discretisation methods that utilise different spline-based basis functions. These include conventional NURBS, trimmed NURBS, T-splines, locally refinable B-splines (or LR-B-splines), unstructured splines (or U-splines), subdivision surfaces, polyhedral splines, manifold splines, and poly-cube splines. The overall aim of these IGA methods is to streamline the computer aided geometric design (CAGD) to computer aided engineering (CAE) analysis pipeline used in numerical modelling and solution of partial differential equations (PDEs). The term IGA is utilised to indicate that both CAGD and CAE software utilise the same geometrical description of the computational domain. A major benefit of this approach is that it reduces any geometrical error whilst also streamlining the CAGD and CAE modelling pipeline. For IGA based spatial discretisation methods the coarsest computational grid/mesh is geometrically identical to the original CAGD representation of the computational/geometrical domain.

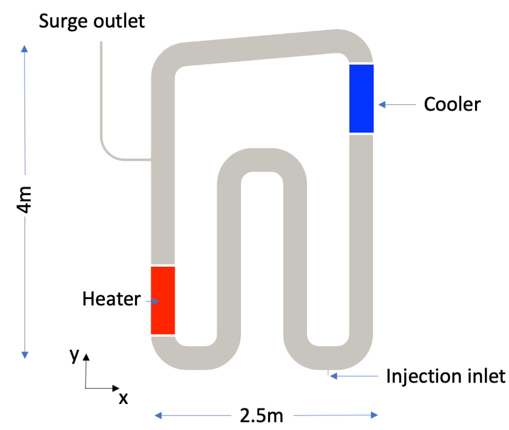

Figure 2: Natural circulation loop geometry with cold flow injection. This is a potential application of the CAGD-CFD methods that will be developed in this proposed PhD project.

As stated previously, there is a very large family of different spline-based geometrical surface representations that are available in the modern computational geometry research literature. However, this PhD will only focus on NURBS representations. The primary reason is that they are ubiquitous within industrial CAGD software and can be utilised directly by Rolls-Royce for industrial nuclear reactor design and safety assessment simulations such as the natural circulation fluid dynamics problems presented in **Figures 2** and **3**. Moreover, most of the literature in IGA spatial discretisation methods utilise NURBS basis/shape functions for the representation of the geometries of the domains. Indeed, these IGA methods can utilise both iso-parametric and super-parametric approaches. In the iso-parametric approach the geometrical shape of cells/elements and the solution field within the cells/elements is represented by the same set of basis/shape functions. In the super-parametric approach, the basis/shape functions used to represent the geometry of the cell/element are of a higher order than the basis/shape functions used to represent the solution field variables. In the conventional iso-parametric IGA method, the basis/shape functions for the geometry of the cell/element and the solution field variables within the cell/element are NURBS basis/shape functions. Conversely, for the recently developed “NURBS-enhanced” finite volume (NE-FV) and “NURBS-enhanced” finite element (NE-FE) methods the geometry and solution field variable basis/shape functions can be different. In these cases, the geometry of the cell/element utilises NURBS basis/shape functions. However, the solution field variables/unknowns are interpolated using different basis/shape functions (e.g., different interpolating high-order polynomials). The PhD would utilize the CAGD and mesh generation capability of the Star-CCM+ CFD software so that development can be made more efficient and applicable to industrial relevant problems for Rolls-Royce which is sponsoring this research. The initial phase of the PhD would provide extensive training to the PhD student in software engineering/programming, numerical analysis, computational geometry, computational grid/mesh generation and CAGD-CFD methods using curvilinear virtual element (VE) methods. The curvilinear VE methods would be developed and implemented using the Nektar++ CFD modelling and simulation (M&S) framework and the NekMesh mesh generator. The department of aeronautics at ICL have developed an application programming interface (API) within NekMesh that enables quadrature points on straight sided (2D) elements and planar surface (3D) elements to be projected onto curvilinear surface patches (i.e., NURBS surface patches). An example of quadrature point projection from a straight sided reference line segment to a curvilinear parametric curve is presented in **Figure 4**. NekMesh can read in a Star-CCM+ CAGD file and a Star-CCM+ polyhedral mesh and project quadrature points on the faces of polyhedral cells onto CAGD surface patches. This is a key functionality that will be developed further during the PhD to enable curvilinear VEM CFD methods to be implemented. One of the major modifications to the Nektar++ M&S framework would be to implement surface and volume integration of curvilinear polyhedral cells/elements, which are required in the CAGD-CFD methods, these will be performed by projecting integration points from cells/elements with faces onto the NURBS surfaces (see **Figures 4** and **5**). In CFD codes, such as Star-CCM+, the computational mesh is

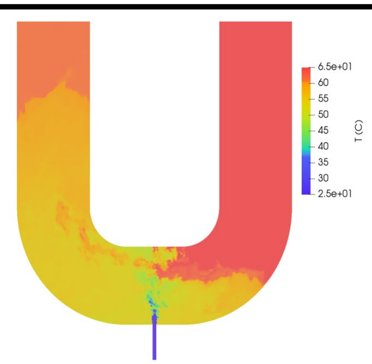

Figure 3: Close up around injection for $\dot{m}_{inj}$ = 0.2 kg/s at t=250 s, showing LES predicted temperature on symmetry plane.

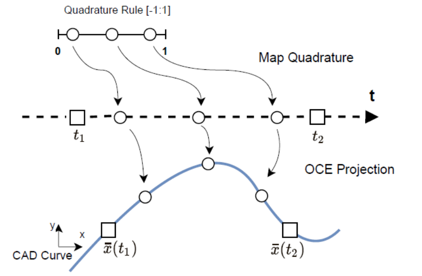

Figure 4: Parametric projection for an edge with a single CAD curve.

formed from planar facetted cells/elements that are circumscribed by the NURBS surfaces i.e., the planar sided faces of surface elements intersect portions of the curvilinear NURBS surfaces. To perform surface integrations of curvilinear cells/elements only planar facetted cells/elements are needed but with quadrature points from the planar cell/element faces projected onto the circumscribing NURBS surfaces (i.e., the planar cell/element faces intersect and are circumscribed by the NURBS surfaces). Therefore, only a conventional 3D mesh generator producing planar facetted cells/elements, along with the CAGD NURBS surface description, is all that is required in this approach. The department of aeronautics at ICL has developed a prototype version of NekMesh that implements this "quadrature point projection algorithm" from planar cells/elements faces onto NURBS surfaces. An example of applying this algorithm to produce a curvilinear high-order polygonal mesh is presented in **Figure 5**. However, this approach needs to be generalised to ensure that it is geometrically robust and linked to both CAGD descriptions and existing commercial mesh generation software such as those implemented within the commercial CFD code Star-CCM+.

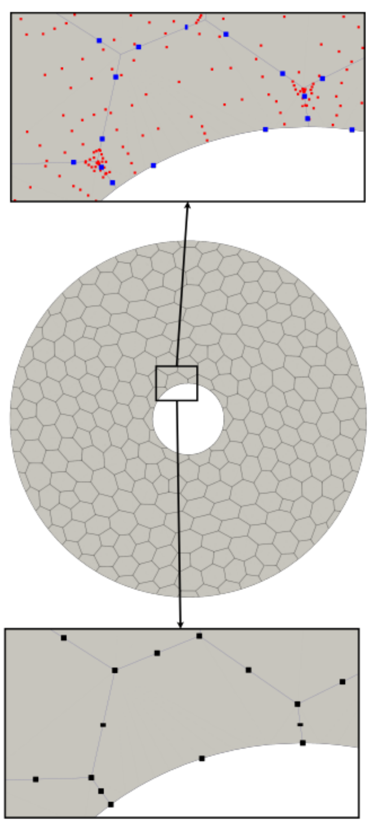

Figure 5: A curvilinear high-order polygonal mesh formed using the NekMesh mesh generator.

The industrial applications of these CAGD-CFD methods will focus on natural circulation/convection (NC) fluid flow phenomena within the primary nuclear thermal-hydraulic circuit of pressurised water reactors (PWRs). An example of such a NC system was recently published by Dr Alex Skillen (MACE – Manchester University) and Dr Ryan Tunstall (Rolls-Royce) at the 17th UK Heat Transfer Conference (UKHTC2021) which was held between the 4th-6th April 2022 in Manchester. Their conference paper was entitled: "Natural Convection within a Loop with Cold-Flow Injection." This paper presented both LES and URANS simulations of the flow within a natural convection (NC) flow loop with cold flow injection, which is presented in **Figure 1**, **2** and **3**. The results of the LES predictions of temperature for this configuration are presented in **Figure 3**. The aim of these applications is to demonstrate the potential of CAGD-CFD to produce more accurate results than phenomenologically based nuclear thermal-hydraulic models but still be more computationally efficient compared to existing finite volume (FV) based CFD methods. The principal benefits of these CAGD-CFD methods will be the ability to produce geometrical models that are compatible, or conform, to the original CAGD representation of the curvilinear computational/geometrical domain (on the coarsest grid/mesh) and the use of high-order basis functions to represent solution field variables. ICL has recently developed curvilinear virtual element (VE) based spatial discretisations that will be used as our prototypical CAGD-CFD methods within this PhD project. They are numerical robust spatial discretisations that can produce high-fidelity solutions even on highly distorted, or even re-entrant, polyhedral meshes. Polyhedral FV methods are the main spatial discretisations within the Star-CCM+ CFD code. Most CFD code use polyhedral FV method due to their ability to mesh geometrically complex domains. However, a key deficiency of CFD codes such as Star-CCM+ is the use of planar facetted polyhedral cells/elements as opposed to polyhedral cells/elements with curvilinear faces that conform to the NURBS surfaces generated by CAGD software. This is the primary challenge that this PhD project will address by developing CAGD-CFD methods. These CAGD-CFD methods will then to be used to them to perform simulations of NC phenomena within pressurized water reactors (PWRs).

PhD project description – The aims of this PhD project are manifold. The **first aim** is to develop CAGD-CFD methods using curvilinear virtual element (VE) methods which would be developed and implemented within the Nektar++ CFD M&S framework. The **second aim** is to apply these CAGD-CFD methods to a series of NC benchmark verification test cases which will be developed during the PhD project in consultation with Rolls-Royce. The **final aim** will be to write any associated conference and journal papers that stem from the research as well as the PhD thesis. The deliverables for the PhD project would be the prototype CAGD-CFD implemented within Nektar++, high-order curvilinear mesh generation API implemented within NekMesh, a suite of NC benchmark verification test cases and the PhD thesis. To summarize, the research and development (R&D) programme for this PhD project will focus on the following:

- Training in numerical methods, software engineering/programming, computer aided geometric design (CAGD), high-order curvilinear mesh generation algorithms using the NekMesh software, commercial and academic CFD software such as Star-CCM+ and Nektar++, advanced CFD discretisation methods, nuclear thermal-hydraulics, and natural circulation (NC) phenomena. The training will be broad based and led by Professor Joaquim Peiro with the support of Dr Matthew Eaton's research group and Rolls-Royce. The training will also encompass high-order curvilinear virtual element (VE) spatial discretisation methods as applied to CFD problems.
- The PhD student will develop CAGD-CFD high-order curvilinear virtual element (VE) spatial discretisation methods within the Nektar++ CFD modelling and simulation (M&S) framework. The Nektar++ CFD M&S framework will be augmented with NURBS basis/shape functions and associated NURBS volume and surface quadrature routines. The primary focus of the PhD project will be ensuring that the implementation is robust and can be utilized for industrial applications by Rolls-Royce. A CAGD API within NekMesh mesh generation software will be used to read both CAGD files and polyhedral meshes from the Star-CCM+ CFD software. The NekMesh API will then be used to project quadrature points from the planar surfaces to the high-order curvilinear NURBS surfaces. These surface and volume quadrature points will be used within the Nektar++ prototype implementation of the high-order curvilinear VE based CFD algorithm.
- The CAGD-CFD curvilinear VE spatial discretisation methods will be verified by utilising simple CFD benchmark verification test cases such as flow within circular pipes to ensure that the methods have implemented correctly and have the correct numerical convergence and stability properties. Further CFD benchmark verification test cases will be performed by comparing against CFD simulations produced by Star-CCM+. A specific NC benchmark verification test case will be developed in tandem with nuclear engineers at Rolls-Royce.
- The final output, or deliverable, from this PhD will be the conference and journal papers as well as the PhD thesis describing the algorithms that have been developed. The papers and PhD thesis will describe to the high-order curvilinear mesh generation algorithms, the high-order curvilinear VE spatial discretisation methods for the Navier-Stokes equations (NSE) and the various NC benchmark verification test cases that will be analysed during the PhD project. This PhD will also lead to the development of a young professional within the field of high-order curvilinear CAGD-CFD and mesh generation as well as nuclear thermal-hydraulics that maybe recruited by Rolls-Royce and continue the development of these novel 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 computational fluid dynamics (CFD) and multiphysics phenomena for both aeronautical and nuclear engineering. During their 3.5 years of study, they will be trained in the latest state-of-the-art numerical methods for simulating turbulent flows, parallel high-performance computing (HPC) techniques, object-oriented programming (OOP), computer aided geometric design (CAGD) algorithms and scalable solvers as well as trained in the use of the industrial CFD 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 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/). This is in addition to courses in numerical analysis, C++, python, MPI and OpenMP programming, nuclear engineering, nuclear thermal-hydraulics and CFD 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 collaborate 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 (Dr Ryan Tunstall) who will assist them in understanding the industrial context of their research as well as helping to mentor them during their PhD studies. There will also be an opportunity for a 3–6-month industrial secondment at Rolls-Royce in Derby. 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 good mathematical skills and the ability to put physical models into a mathematical form.

The successful candidate must be a UK national willing, and able, to achieve security clearance (SC) by the industrial sponsor Rolls-Royce. To apply for this PhD studentship please email Professor Joaquim Peiro (j.peiro@imperial.ac.uk) with a copy of your curriculum vitae (CV).