Providing skilled graduates to the nuclear industry

M.J.D. Rushton, M.R. Wenman, R. Mella and **P.A. Burr** explain how materials modelling courses at Imperial College's Centre for Nuclear Engineering are creating a pool of talented personnel for academia and industry

The Centre for Nuclear Engineering at Imperial College London was created in 2006 to link the various nuclear research and teaching activities across the university into a coherent hub, and now comprises over 30 academic staff members and more than100 PhD students. Centre members work on topics as diverse as the effects of Chernobyl on thyroid cancer and thermal hydraulic modelling of fuel assemblies. In 2012 the Centre's management took up permanent residence in the Department of Materials, and an official opening is on the agenda for this year. It is directed by Professors Robin Grimes and Bill Lee and focuses on providing industry with the very latest abilities in nuclear engineering research and producing graduates with industrially relevant skills.

The Centre runs three undergraduate courses with a nuclear emphasis: MEng Materials, MEng Mechanical Engineering and MEng Chemical Engineering, all with Nuclear Engineering. Since 2010 a graduate programme providing an MSc in Nuclear Engineering has also been run. Each of these programmes provides about 35–40 MEng graduates and 10–20 MSc per year, with aspirations to grow based on demand.

A strong emphasis is placed on materials modelling, with three postdoctoral researchers and ten PhD students currently working on projects with industrial emphasis and sponsorship. The Centre also provides a course on Modelling for Nuclear Engineers taken by the MSc students. PhD projects range from the atomic scale – using electronic structure calculations by density functional theory (DFT) – to simulating full-size components such as fuel pins, using techniques such as the standard finite element method (FEM) complemented by more state-of-the art methods such as peridynamics.

This research, as well as providing great value to the UK nuclear industry on specific projects, is also providing a pool of talented PhD and postdoctoral personnel for both academia and industry. These people are equipped, not only with prior nuclear knowledge, but also with skills in the most modern techniques of computer programming and materials modelling. They can then take these cutting-edge ideas and embed them into the companies they join. The benefit to industry is someone that can potentially bring a new way of tackling an old problem that can enhance either cost-effectiveness or nuclear safety. Some examples of the materials modelling work we do are described here.

AGR fuel performance modelling

Since the year 2000 there have been several fuel failures potentially attributable to pellet-cladding interaction (PCI) in various advanced gas-cooled reactors (AGRs)[1]. When radioactivity in the coolant gas indicates that fuel in the reactor may have failed, the operators have to follow a procedure mandated by reactor safety cases that may involve reducing reactor power or shutting it down. The potential costs include: replacement for generation loss, non-optimum use of fuel and increased fuel disposal costs, as failed fuel cannot be disposed of by the normal route. Within the Centre efforts are being made to understand these kinds of failure; in particular we have developed a fuel performance code, with a strong focus on mechanistic basis, which uses the FEM[2].

Solving for physical fields in FEM allows the dependence on empirically determined material properties, inherent in traditional fuel performance codes, to slowly be replaced. Furthermore, by leveraging modern modelling techniques, predictions can be made for conditions where no experimental data exist. To this end, the fuel model has been built within the framework of a commercial FE package (ABAQUS)[3]. This allows the creation of a new generation of fuel performance code based on an industrially trusted platform.

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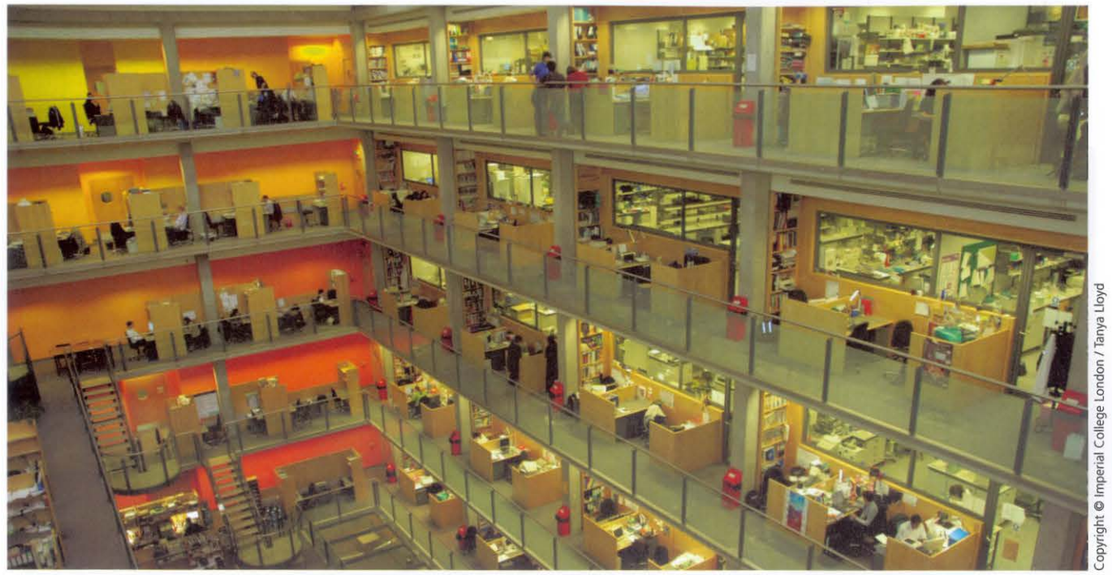
With every new major development in the field of FE modelling being incorporated within ABAQUS, in a stable and verified manner, it is straightforward to incorporate these improvements into the fuel performance code. This attempt at standardisation removes duplicated development effort and its corresponding verification. An example of where this has been of benefit is shown in Figure 1, where the stresses caused by the sharp corners of two fuel fragments impinge on the cladding. By using the error-driven adaptive remeshing, introduced into ABAQUS, this detail was captured, whereas at a lower resolution it would have been lost and in fact an erroneous result would have been obtained.

The fuel performance code includes advanced features such as coupled temperature-displacement-diffusion and highly non-linear fuel cladding properties. Furthermore, fission gas release (parameterised from atomic-scale, first principles simulations), isotope inventory calculation, fission product diffusion and grain growth dynamics are all included in the model.

Development of codes of this kind is time consuming, meaning that it is often prohibitive for industry to pursue such endeavours.



Conversely, a PhD or EngD route is well suited to this kind of work and provides an ideal way for the nuclear industry to work with universities on problems directly relevant to their business. The expectation is that this work will continue to develop and completing students will begin to be embedded into industry.

Peridynamics modelling

The fuel-performance model described above is based on FE methods. Although already extensively deployed in industry, the model has difficulties describing the behaviour of discontinuities such as cracks, bubbles and splinters. By comparison, peridynamics is a relatively recent method that overcomes these issues. We will now go on to give a brief description of the method before continuing to describe some of the work being carried out within the Centre in applying peridynamics to nuclear engineering problems.

Peridynamics is a non-local modelling technique capable of describing a wide range of length scales and material phenomena. It has been developed, primarily over the last decade, to model ballistic impact effects in brittle solids. The non-local approach behind it has been around for many more years, however. The name peridynamics was coined by Silling in 1998[4,5]; it means 'all around force' and is derived from the integral approach to solving the constitutive equations. Rather than assuming a point within a material is influenced by other points that are confined to its immediate locality, or are an infinitesimal distance away (as in classical continuum theories), the point is influenced by points within a finite cut-off radius known as the horizon distance.

Figure 2 illustrates the peridynamics horizon in two dimensions: it shows the bonds between material points and the other points within their horizon. For clarity, the bonds associated with an individual material point have been highlighted in red within the figure. In order to calculate the forces for this central material point, one now only needs to integrate the bond responses within the horizon (the dashed red-line within the figure).

Most of the work published so far has been concerned with the development and extension of the peridynamics theory, with only a few papers written on its application to real engineering problems[6]. While it has mostly been developed for stress, strain and ultimately fracture of brittle solids, it can be used to model many other problems including heat transfer and diffusion[7,8], phase changes[9] and plasticity[10]. Often it can do this without the numerical problems associated with more conventional methods such as FE. Because peridynamics is an integral approach it does not have problems dealing with the formation of discontinuities in the material, such as cracks, that cannot be defined by the partial differential equation approach of classical FE, for surfaces or crack tips. Peridynamics can also accurately describe material behaviour from the nano-scale[11] (where local approaches can fail due to non-local interactions) up to the macro-scale; and unlike many approaches, including FE, it does not force the user to pre-impose a particular damage path. At the micro-scale and larger, the pairwise force function has a direct relationship to the bulk material properties and so is easily defined. Further, for many problems such as brittle fracture, the FE approach is highly mesh-dependent; by comparison, this is not a problem in peridynamics[12].

Even the extended finite element method (XFEM), being developed to combat the shortcomings of the FE approach to damage problems, has disadvantages compared with peridynamics. For instance, in the case of dynamic cracks in brittle solids (e.g. glass) XFEM can have difficulty in describing the speed of crack growth, which is not problematic for peridynamics[13]. The only significant disadvantages of peridynamics in comparison with more established methods such as XFEM, is that it has not been widely deployed in industry and consequently does not have the same kind of support in commercial modelling packages as FE approaches (although this will surely follow as the technique gains acceptance).

A number of discontinuities within nuclear fuel can limit its in-reactor performance. These take the form of bubbles, broken fuel slivers that are bonded to the cladding, and both radial and circumferential fuel cracks. Within the Centre an implicit peridynamics framework has been developed to look at these

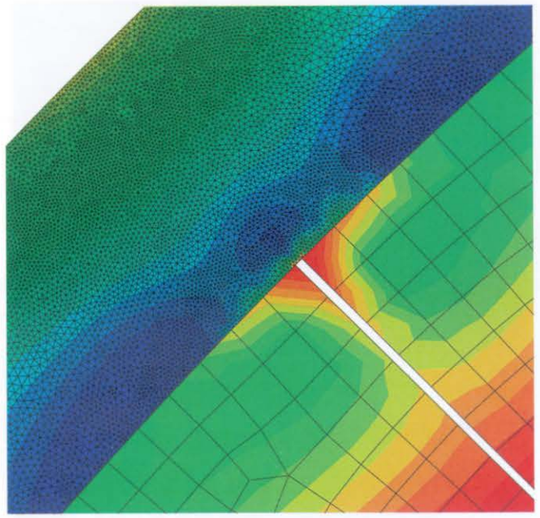


Figure 1: *Stress (von Mises) contour plot of post heat-up contact between the cladding and the fuel in an AGR. Showing the enhancement brought to fuel performance modelling via the use of adaptive remeshing within an industrially verified commercial modelling platform.*

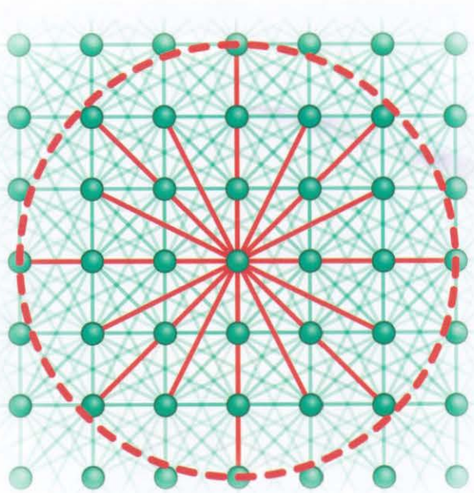


Figure 2: *Two-dimensional representation of point connectivity within peridynamics formalism. Material points that are within a given cut-off of each other (the horizon, here represented by a dashed red line) are linked by bonds. Here the bonds for a single material point are highlighted in red.*

sorts of features. With this we have been able not only to perform convergent calculations for the stress state surrounding a discontinuity, such as a crack, over large time periods, but also to follow their nucleation, growth and propagation. Additionally, we now have the ability to study crack growth and bubble formation in nuclear fuel, which offers huge potential when coupled with a fuel performance code of the kind described earlier.

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Another area in which we are employing peridynamics is to consider PCI. Fuel and cladding can come into contact due to the combined effects of fuel swelling and cladding creep-down. The large stresses induced by this interaction, leading to fuel-cladding bonding, can encourage fuel cracking during power transients. Understanding interfaces between ductile and brittle materials could have benefits in understanding, and possibly help prevent fuel and cladding failures.

Figure 3 shows an example of a peridynamics simulation of the fracture of a bi-material strip where the top layer is a brittle material on a ductile substrate that has been taken through a heating cycle. This acts as an analogue to the behaviour where brittle oxide fuel adheres to ductile cladding. Such simulations can serve as a mechanism for explaining the features found in irradiated fuel micrographs and for integrity testing other reactor components.

Atomic scale modelling

The FE and peridynamic methods described so far are continuum techniques in which the behaviour and interaction of the model elements are generally parameterised from material properties measured at the macroscopic scale. As described above, this means that such methods are relatively straightforward to set up and support a length-scale that allows simulation of entire components and sub-assemblies to be performed. However, the combination of microstructure, defect structure and atomic interactions determine the properties of a material, and although FE and peridynamics have been used to consider microstructural effects, their continuum nature makes them ill-suited to the task of describing atomic-level processes.

By comparison, atomistic simulation techniques include an explicit description of atoms and the forces acting between them. As such, the position of individual atoms under different conditions of composition, temperature and pressure can be probed in response to point and line defects, surfaces, grain-boundaries and interfaces. This makes atomistic techniques particularly well-suited to elucidating property trends and predicting the atomic-level mechanisms that give rise to the sometimes unexpected behaviour of nuclear materials.

Within industry, the kind of information and insight obtained from atomistic simulation could, for example, help add physical basis to fuel performance codes or provide additional data to augment safety cases. Already, data for gas migration, obtained using atomistic simulation, is used in the fuel performance code described earlier. Furthermore, the atomic-level understanding obtained from atomistic methods could be used to help design the next generation of fuel and structural materials for application within future reactor designs. As yet, atomic-level simulation techniques are perhaps not as widely deployed within

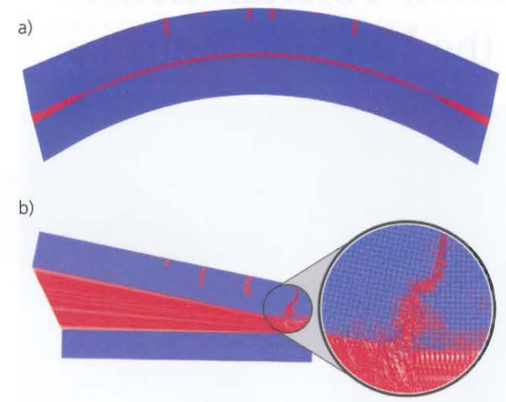

Figure 3: *(a) Whole bi-material strip after heating to 100°C. Failed truss elements are shown in red and no longer carry load. The interface has already almost fully delaminated and the bending has initiated vertical cracks in the brittle top layer; (b) half the strip after heating to 200°C.*

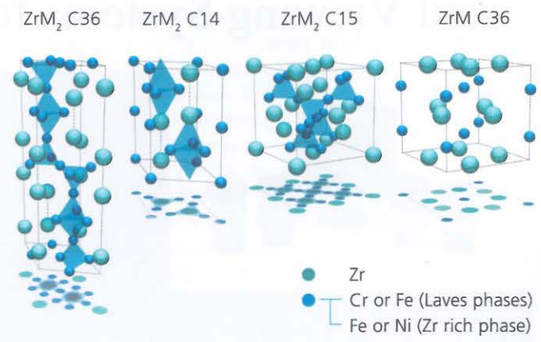

Figure 4: *Unit cells of C36, C14 and C15 Laves and Zr_2M SPP intermetallic structures.*

the industry as their continuum counterparts; however, as the cost of powerful computational resources continues to decrease, their relevance will grow.

In order to facilitate their continued adoption by industry, nuclear engineers with knowledge of these methods are required. Given their widespread use within academia, the university sector is well placed to fill this skills gap. Already, the modelling component of the MSc in Nuclear Engineering at Imperial College contains sessions on atomic-scale simulation techniques using both classical pair potentials and quantum mechanical methods. To highlight potential applications of atomic modelling to nuclear materials some recent research performed within the Centre is presented here.

One of the main concerns for failure in zirconium nuclear fuel cladding is delayed hydride cracking. The mechanism through which hydrogen uptake occurs is not very well understood, but it is suspected that the second phase particles (SPPs) found in the alloys play a critical role. It was proposed by Hatano that $Zr(Cr,Fe)_2$ particles could act as bridges for the migration of H through the oxide layer[14], while, conversely, $Zr_2(Ni,Fe)$-type particles may trap the hydrogen until either dissolved or fully oxidised[15]. Understanding these processes furthers a more fundamental understanding of nuclear fuel cladding and provides useful insight when developing or improving materials and processing routes for cladding materials. To this end, material behaviour can be predicted from the description of atomic interactions provided by quantum mechanics. In particular, Kohn and Sham's Density Functional Theory (DFT) can be used to solve a system's wave-function – and hence probe the local environment of atoms in a system including electronic effects [16]. With relation to SPPs, DFT was employed to investigate the thermodynamic behaviour of H within these SPPs. Burr and co-workers calculated the solution enthalpies of H in various binary intermetallic SPPs and compared these with the solution enthalpy for H in both α- and β-Zr metal phases[17].

Figure 4 shows the four crystal structures of the SPPs considered: Cr forms three intermetallic Laves phases with Zr with the same formula of $ZrCr_2$. These include both cubic (*C15*) and hexagonal forms (*C14* and *C36*) and were all considered. In addition, a tetragonal Zr_2M structure, characteristic of SPPs in the Zr-Fe and Zr-Ni system was simulated. The solution enthalpy for hydrogen in each of these structures is a measure of how favourable hydrogen incorporation is. By comparing enthalpies between SPPs, those phases likely to trap hydrogen become apparent. Furthermore, due to the atomistic nature of Burr's simulations, different crystallographic sites can be compared to give a precise prediction of where hydrogen would sit within each structure. In order to achieve this, the following general procedure was employed. For each crystallographically distinct interstitial site within each crystal structure, a hydrogen atom was introduced. Through the use of the DFT the energy of a system can be calculated from its atomic positions and unit-cell dimensions. Using an iterative procedure, small adjustments to the atomic positions are made in order to lower the system energy until a local minimum is obtained. In this way, the relaxation of atoms around the hydrogen interstitial is obtained. From the energy of this relaxed system, the energy change on introducing the H atom is calculated and used to get an enthalpy of solution.

Using this method, Burr and co-workers found that certain elements, such as V and Ni, form intermetallic phases with Zr that offer very favourable sites for H occupancy, whereas other elements, most notably Cr and Mo, form intermetallic SPPs that do not accommodate H readily when compared with pure Zr.

As a consequence, it is suggested that Cr-containing SPPs may aid the transport of H through zirconium's outer oxide layer, as previously proposed by Hatano[15], but that Ni-containing SPPs will instead trap the H until they are dissolved (by radiation damage) or fully oxidised (by the inward-growing oxide layer).

Conclusion

Within this article, we have attempted to give a flavour of how computer simulation is being applied at the Centre for Nuclear Engineering at Imperial College to industrially relevant nuclear engineering problems. Given the need for young graduate engineers to enter the nuclear industry, it is gratifying to note that a large part of the work presented within this article was produced by PhD students just at the start of their careers. In the coming years, it is likely that many of these young scientists and engineers will choose to make their home within the nuclear industry. We hope that we have demonstrated that they will bring with them new techniques and fresh ideas and become an asset to the industry.

With the correct encouragement, the UK university sector will play a crucial role in filling the skills gap and equipping people with the tools they need to climb the career ladder, and hopefully will provide tomorrow's leaders in both academia and industry. We have given just a highlight of the work done, many more examples could be given of undergraduate and MSc project work that is being carried out both at the university and in industry; however, we have shown that university-based research can continue to provide ideas, solutions and tools that are of direct relevance to industry.

Mark Wenman
Mark Wenman has a BEng in Materials Science and Technology and a PhD in the micromechanics of fracture of BCC metal alloys from the University of Birmingham. He was employed as a lecturer in the nuclear department at HMS Sultan from 2003 to 2008 before moving to Imperial College London to take up a position as EDF Energy Research Fellow and Lecturer. Today Mark has a growing research group focused on metallic systems for nuclear engineering applications. He is also the Director of the MSc in Nuclear Engineering at Imperial College.

Michael Rushton
Michael Rushton works within the atomistic simulation group within the Centre for Nuclear Engineering at Imperial College London. His research considers materials performance and design using atomic-scale simulation. In particular he uses modelling to look at nuclear fuel performance and the design of ceramic and vitreous nuclear waste materials. He also coordinates the modelling component of Imperial College's MSc in Nuclear Engineering.

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