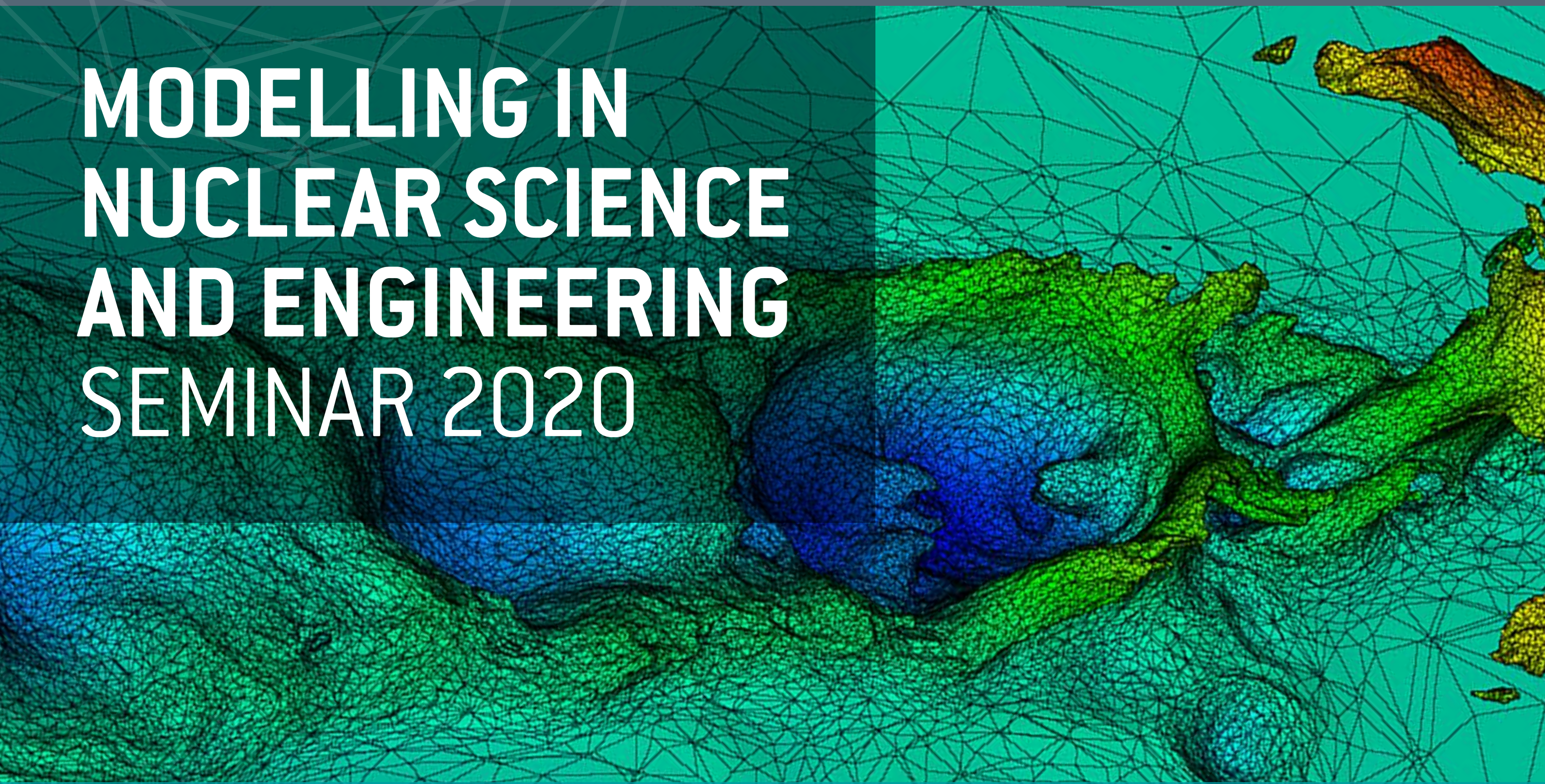
4/5 November 2020

Online Seminar

the nuclear institute



MODELLING IN NUCLEAR SCIENCE AND ENGINEERING SEMINAR 2020

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CHAIR'S WELCOME

Welcome to the Nuclear Institute's Modelling in Nuclear Science and Engineering Seminar 2020, being held on-line for the first time this year. It has been an extremely challenging and unprecedented year. This has brought about innovative and different ways of working very much as the 'new normal'. It has also perhaps brought a new word to the forefront of public attention over recent months; modelling.

The aim of scientific modelling as an activity is to make features and performance of the design easier to understand, quantify, visualize, or simulate by referencing it to existing and usually commonly accepted knowledge, and is applied across all kinds of industries and walks of life. I will return briefly to the pandemic a little later, but in the meantime, I would firstly like to thank all the contributors to and supporters of this year's Seminar. We certainly have a fantastic line-up and a fascinating set of topics and themes to cover.

This year's Seminar aims to provide practical advice, information sharing and a discussion platform to facilitate and improve understanding, problem-solving and cooperation. Massive leaps and scale of opportunities by the introduction of digital technologies have presented the nuclear modelling community with tools that were inaccessible 20 years ago, and whilst the UK nuclear sector alone still expects significant near to mid-term investment, the opportunities for ongoing research across the whole nuclear lifecycle continue to present themselves.

Our contributors are all looking forward to sharing their knowledge, experience and expectations for future modelling demands across decommissioning projects, radioactive waste management and asset support, reactor design and in nuclear new-build.

Our very grateful thanks are extended to our sponsors for this year's event, and we are also thankful to our Seminar partners for their ongoing support.

We are also grateful to all our participating speakers and their associated companies for taking time out of very busy schedules to be here today and sharing their experiences with the modelling community.

The Nuclear Institute aspires to be a home to all Nuclear Professionals; I welcome you all to this Seminar, and hope that you are able to participate and contribute to a successful day.

Prof Ali Tehrani FNucI

Nuclear Institute and Seminar Chair
Office for Nuclear Regulation

the nuclear institute

SESSION SUMMARIES

SESSION 1:
KEYNOTE ADDRESSES: POLICIES AND STRATEGY

Session Chair:
***Ali Tehrani FNucl**, the Nuclear Institute*

with:

***Prof. Robin Grimes CEng FNucl**, Imperial College London*

***Malwina Qvist**, BEIS*

***Mark Salisbury FNucl**, NIRO*

***Andrew Davis**, UKAEA*

The Seminar's first session will provide an overview broadly of Policies and Strategy which underline the importance of nuclear modelling and its place within the Nuclear Innovation Programme; modelling within the Spherical Tokamak for Energy Production – or STEP – Programme; and the place of atomic scale modelling of materials in the overall process of modelling in nuclear, followed by a Q&A session.

SESSION 2:
IMPROVING EFFICIENCY IN THE NUCLEAR MODELLING

Session Chair:
***Dr Simon Middleburgh**, Nuclear Futures Institute, Bangor University*

with:

***Dr Andrew Buchan**, Queen Mary University London, UK*

***Florian Fichot**, IRSN, France*

***Hector Diego Estrada-Lugo**, University of Liverpool, UK*

Session 2 looks in detail at reduced order and multi-physics models for nuclear engineering, computational methods developed to propose a new methodology for IVR efficiency assessment and modelling advanced thermal reactors with confidence using credal networks, followed by a Q&A session.

SESSION 3:
AUTOMATION, VALIDATION AND THE FUTURE

Session Chair:
***Prof. Paul Smith**, Jacobs*

with:

***Dr Steven Dargaville**, Imperial College London, UK*

***Dr Fulvio Mascari**, ENEA, Italy*

***Aniket Joshi**, The Open University, UK*

***Prof John Lillington**, Jacobs, UK*

Session 3 provides an overview of a number of interesting streams related to the session theme, which include robust error metrics for adaptivity with ray-effects; the needs and current activities supporting severe accident and uncertainty estimation; a look at numerical modelling of the LIVE L3 experiment for analysing the melt pool behaviour in transient and quasi steady-state; and a highly interesting overview and status update of modelling with regard to next generation nuclear power – Advanced and Small Modular Reactors. The session closes with a Q&A session chaired by Prof Paul Smith.

SESSION 4:
MATERIALS MODELLING FOR NUCLEAR ENGINEERING, RESILIENCE AND SAFETY

Session Chair:
***Dr Andrew Buchan**, Queen Mary University London*

with:

***Glyn Rossiter**, National Nuclear Laboratory, UK*

***Savneet Kaur**, CEA SACLAY, France*

***TV Santhosh**, University of Liverpool, UK*

***Dr Alex Bond**, Quintessa Ltd, UK*

Day 2 of the Seminar opens with Session 4 and questions whether fuel behaviour can be modelled properly and does it matter? Vacancy elastodiffusion around cavities in aluminium: Fast first passage algorithms based on Krylov subspace projection techniques is examined along with modelling of nuclear systems for resilience assessment; and finally – Safe Cracking: Monte Carlo nonlinear coupled analysis of nuclear reactor bricks. The session closes with a Q&A session chaired by Dr Andrew Buchan.

SESSION 5:
DEVELOPMENT OF NUMERICAL (OR PREDICTIVE) APPLICATIONS

Session Chair:
***Dr Amir Nourian**, University of Salford*

with:

***Robin Dickenson**, Atkins Global, UK*

***Florian Fichot**, IRSN, France*

***Dr Andrew Ian Duff**, STFC, Daresbury Laboratory, UK*

***Simon Middleburgh**, Nuclear Futures Institute, Bangor University*

***Andrew Eustace**, Research Portfolio Manager, EPSRC*

Session 5 – this year's closing session, summarises advances in non-linear seismic analysis techniques; a summary of in-vessel core degradation paradigm myths and reality; perspectives on ATF fuels; an overview of the application of computational methods for modelling of scientific and technological processes at the Science and Technology Facilities Council; perspectives on mechanistic modelling of nuclear fuels for rapid commercial deployment and an interesting update from the Science and Technology Facilities Council on current activities, research and progress related to development of fusion energy. The session closes with a Q&A session and concluding remarks chaired by Professors Ali Tehrani, Nuclear Institute and Christopher Pain, Imperial College London

PROGRAMME – DAY 1

WEDNESDAY 4 NOVEMBER

9:30 SEMINAR OPENS FOR LOG-IN
Nuclear Institute

9:45 **Welcome, safety briefing and IT familiarisation**
*Chair: **Prof. Ali Tehrani**, NI & Office for Nuclear Regulation*

SESSION 1: KEYNOTE ADDRESSES: POLICIES AND STRATEGY

10:00 **The place of atomic scale modelling of materials in the overall process of modelling in nuclear**
***Prof. Robin Grimes** Imperial College London*

10:30 **The importance of modelling within the Nuclear Innovation Programme**
***Malwina Qvist**, BEIS and Mark Salisbury, NIRO and **Mark Salisbury FNucl**, NIRO*

11:00 **Modelling for the STEP programme**
***Andrew Davis**, UKAEA*

11:30 **Q&A Session**
*Chair: **Prof. Ali Tehrani**, NI & Office for Nuclear Registration*

11:45 COMFORT BREAK

12:00 **Poster Presentation – 1st Session**
Please see separate Itinerary

12:40 LUNCH

SESSION 2: IMPROVING EFFICIENCY IN THE NUCLEAR MODELLING

*Chair: **Dr. Simon Middleburgh**, Bangor University*

13:30 **Reduced order and multi-physics models for nuclear engineering**
***Dr. Andrew Buchan**, QMUL, UK*

13:55 **Computational methods developed to propose a new methodology for IVR efficiency assessment**
***Florian Fichot**, IRSN, France*

14:20 **Modelling advanced thermal reactors with confidence using credal networks**
***Hector Diego Estrada-Lugo**, University of Liverpool, UK*

SESSION 3: AUTOMATION, VALIDATION AND THE FUTURE

*Chair: **Prof. Paul Smith**, Jacobs*

14:55 **Robust error metrics for adaptivity with ray-effects**
***Dr. Steven Dargaville**, Imperial College London, UK*

15:20 **Severe accident and uncertainty estimation, needs and current activities**
***Dr. Fulvia Mascari**, ENEA, Italy*

15:45 **Numerical modelling of the LIVE L3 experiment for analysing the melt pool behaviour in transient and quasi steady-state**
***Aniket Joshi** et al, The Open University, UK*

16:10 **Next generation nuclear power Advanced and small modular reactors – an overview of current UK activities and present status**
***Prof. John Lillington**, Jacobs, UK*

17:00 **Q&A session**
*Chair: **Prof. Paul Smith**, Jacobs*

17:25 **Poster Presentations -2nd Session**
Please see separate Itinerary

17:55 SEMINAR DAY 1 CLOSES

PROGRAMME – DAY 2 THURSDAY 5 NOVEMBER

08:10 **SEMINAR OPENS FOR LOG-IN**
Nuclear Institute

08:25 **Welcome back, safety briefing and IT familiarisation**
Chair: ***Prof. Ali Tehrani****, NI & Office for Nuclear Regulation*

SESSION 4: MATERIALS MODELLING FOR NUCLEAR ENGINEERING, RESILIENCE AND SAFETY

08:30 **Fuel behaviour: can we model it properly and does it matter?**
Glyn Rossiter*, NNL, UK*

08:55 **Vacancy elastodiffusion around cavities in aluminium: Fast first passage algorithms based on Krylov subspace projection techniques**
Savneet Kaur*, CEA France*

09:20 **Modelling of nuclear systems for resilience assessment**
T V Santhosh et al*, University of Liverpool, UK*

09:45 **Safe Cracking: Monte Carlo nonlinear coupled analysis of nuclear reactor bricks**
Dr Alex Bond*, Quintessa Ltd, UK*

SESSION 5: DEVELOPMENT OF NUMERICAL (OR PREDICTIVE) APPLICATIONS

Chair: ***Dr. Amir Nourian****, University of Salford*

10:30 **Advances in non-linear seismic analysis techniques**
Robin Dickenson*, Atkins Global, UK*

10:55 **In-vessel core degradation paradigm... Myths and reality, perspectives on ATF fuels**
Florian Fichot*, IRSN, France*

11:25 **Application of computational methods for modelling of scientific and technological processes at STFC**
Dr. Andrew Ian Duff*, STFC, Daresbury Laboratory, UK*

11:50 **Mechanistic modelling of nuclear fuels for rapid commercial deployment**
Simon Middleburgh*, Bangor University, UK*

12:15 **EPSRC nuclear fission update**
Andrew Eustace*, Research Portfolio Manager, EPSRC*

12:45 **Concluding remarks and thanks**
Prof. Ali Tehrani*, NI & Officer for Nuclear Regulation and* ***Prof. Christopher Pain****, Imperial College London*

13:00 **SEMINAR DAY 2 CLOSES**

14:00 **COVID-19 MODELLING, SPECIAL INTEREST GROUP**

The organising committee for the Modelling in Nuclear Science and Engineering Seminar includes leading experts in the field from across the UK and internationally.

There is considerable interest in how application of the nuclear science and engineering modelling approach can be applied to support the Covid-19 Pandemic modelling effort.

This session is separate to the Seminar, and will be the initial meeting to establish a formal **Nuclear Institute Special Interest Group** (SIG) to bring together the Modelling community from across the nuclear sector to share their expertise and knowledge.

To register for this session or for any enquiries related to this session, please email **nuclear@bangor.ac.uk**. We are very grateful to the Nuclear Futures Institute at Bangor University for hosting this session on their web-based conferencing platform.

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POSTER PRESENTATIONS

WEDNESDAY 4 NOVEMBER

SESSION 1:
THEME: FUEL MODELLING

12:00 **Impact of dopants on diffusion in crystalline and amorphous zirconia**
Megan Owen, *Bangor University, UK*

12:05 **Modelling the phonon and electron transport through nuclear fuels Dr.**
Lee Evitts, *Bangor University, UK*

12:10 **Developing an understanding of Li incorporation into ZrO^2 :a fuel performance study**
Gareth Stephens, *Bangor University, UK*

12:15 **Bayesian model updating of fatigue crack growth prediction parameters using adapted likelihood functions**
Adolphus Lye *et al, University of Liverpool, UK*

12:20 **Multi-objective Optimization of Heterogeneous Light Water Reactor Fuel Assemblies**
Alan Charles, *Jacobs, UK*

12:25 **Modelling and experimentation of different small specimen tensile testing (SSTT) techniques in efforts of test standardisation**
Aniket Joshi, *The Open University, UK*

SESSION 1:
THEME: REDUCED ORDER MODELLING

12:30 **A hierarchical projection based-reduced order model applied to neutron transport**
Toby Phillips, *Imperial College London, UK*

12:35 **Reduced Order angular discretisation for neutron transport simulation**
Alexander Hughes, *Queen Mary College London, UK*

SESSION 2:
THEME: ACCIDENT ANALYSIS

17:25 **Modelling and risk analysis in French PSA level 2**
Nicolas Duflot, *IRSN, France*

17:30 **Utilisation of Spill Return Atomiser (SRA) in Decontamination, Coating and Fire Suppression**
A. Nourian & ***G.G Nasr***, *University of Salford, UK*

SESSION 2:
THEME: THERMAL-HYDRAULICS

17:35 **THOR – the new thermal-hydraulics rig at M-Sparc**
Dr. Marcus Dahlfors, *Bangor University, UK*

17:40 **Flow Modelling of Injection Orientation of Supercritical CO2 In Porous Media for Enhanced Gas Recovery (EGR)**
M. K. Abba, A. J.Abbas & ***A. Nourian*** *University of Salford, UK*

17:45 **Fluid Flow Solver for Nuclear Reactors using Automatic Code Generation**
Kene Nwegbu, *Imperial College London, UK*

17:50 **Track Record: Flexible Mesh Multiphysics Coupling for Nuclear Engineering (reFINE)**
Liang Yang, *Cranfield University*

17:55 **Vacancy elastodiffusion around cavities in aluminium: Fast first passage algorithms based on Krylov subspace projection techniques**
Savneet Kaur, *CEA France*

ABSTRACTS

Impact of dopants on diffusion in crystalline and amorphous zirconia

Megan Owen, Nuclear Futures Institute, Bangor University

Grain boundaries in ZrO2 may act as favourable pathways for corrosion species in comparison to diffusion of species through the bulk material. Impurity and alloying element segregation to grain boundaries has been observed experimentally (high Fe contents for example). These highly doped grain boundaries may become amorphous in nature [1] and the impact of this structural change is investigated here and compared to the crystalline doped material.

Atomic scale modelling methods have been conducted to analyse diffusion of all components in trivalent doped and un-doped crystalline and amorphous zirconia, ZrO2, at a range of concentrations between 2.6-11 at. % and temperatures. Diffusion coefficients, pre-exponential factors and activation energies have been calculated for all structures at all concentrations and a comparison has been made – clear differences were observed indicating the potential benefits of amorphous grain boundary formation in retarding diffusion compared to the bulk at reactor operating temperatures.

Relating these coefficients gives a description of crystalline and amorphous structures and their differences in diffusive behaviour. These values can be exploited by mechanistic higher-level fuel performance codes and models to better predict the corrosion rate of Zr-alloys.

[1] P.R. Cantwell et al. "Grain boundary complexion", Acta Materialia, 62 (2014) 1-48.

Modelling the phonon and electron transport through nuclear fuels

Lee Evitts, Nuclear Futures Institute, Bangor University

Ab-initio calculations of the phonon and electron transport can lead to the determination of fundamental properties of a material. These properties may include the electrical and thermal conductivities, heat capacities and emissivities amongst others. Moreover, it is possible to investigate how such properties may be affected through the inclusion of crystalline defects, such as the introduction of fission gas products.

In this work, the properties of advanced fuels UB2 and U3Si2 are calculated with Quantum Espresso, coupled with the Electron-Phonon Wannierization code. In doing so, it is shown how the electron-phonon scattering term significantly affects the thermal conductivity of UB2.

Developing an understanding of Li incorporation into ZrO2: a fuel performance study

Gareth Stephens, Nuclear Futures Institute, Bangor University

More effort is being given to investigating the impact of water coolant chemistry on zirconium alloy corrosion in the primary circuit of a pressurised water reactor. Lithium is observed to accelerate corrosion, although the mechanism is not certain.

Atomic scale simulation using density functional theory have been used to identify the most stable accommodation mechanism for Li in both monoclinic and tetragonal ZrO2. The results have been used to predict the defect concentrations in the form of a Brouwer diagram.

The results have been used to predict the defect concentrations in the form of a Brouwer diagram.

These results will be combined with experimental data to corroborate the most stable accommodation mechanism of Li in ZrO2 and the impact that other species may have in aiding or limiting its accelerating effect within a nuclear reactor.

Bayesian Model Updating of Fatigue Crack Growth Prediction Parameters using adapted Likelihood Functions

Adolphus Lye, University of Liverpool
Edoardo Patelli, Strathclyde

With the growing prominence of nuclear energy as a viable option of alternative energy in the face of climate change, comes with the need to monitor the structural health status of the technology employed to generate such energy.

One significant structural component worth looking into would be the carbon-steel piping used to transport fast-flowing water and wet steam in light and heavy water reactor. Subjected to cyclic loading during the service period of the reactor, the pipes are susceptible to fatigue which leads to the development of fatigue cracks. This brings the importance to studying the fracture mechanics of the carbon-steel piping, especially in predicting the fatigue crack growth which is essential so as to perform timely predictive maintenance. One commonly used model used to predict the rate of fatigue crack growth would be the Paris' Law model.

In this research, Bayesian model updating technique will be used to obtain estimates of the material-dependent constants in the Paris' Law model via the use of two proposed likelihood functions: the adapted inverse error likelihood and adapted inverse square error likelihood functions. From there, the results of the estimates will be compared in terms of its degree of precision.

Multi-objective Optimization of Heterogeneous Light Water Reactor Fuel Assemblies

Alan Charles, Jacobs

This work applies formal mathematical optimisation methods to fuel assembly design problems and investigates their effectiveness in tackling realistic fuel assembly design problems, incorporating both multi-physics and 3D modelling of MOX type fuel assemblies.

Two novel Differential Evolution algorithms are created and used to optimize PWR and BWR fuel assemblies through varying individual pin compositions, sizes and placement of burnable absorbers. Objectives include maximizing plutonium content whilst simultaneously maximizing safety performance criteria such as PPF and DNBR. Results showed that the multi-objective DE algorithms could outperform other algorithms from the literature as well as improve on expert designs, offering engineers a flexible and robust tool to aid in nuclear assembly design.

This work was completed as part of the author's PhD in nuclear engineering at the University of Cambridge, utilising the latest advancements in the WIMS reactor physics software package, along with the support of the ANSWERS team.

Numerical modelling of the LIVE L3 experiment for analysing the melt pool behaviour in transient and quasi steady-state

Aniket Joshi, The Open University

This study aims to model numerically the L3 test of the LIVE (Late In-Vessel Phase Experiments) framework. To model the L3 test, the IC-FERST, a finite element, control- volume code with the ability to adapt the mesh resolution as the simulation evolves is utilised.

The objective of this study is twofold. Primarily, it is intended to be the first step in establishing high-fidelity modelling capabilities for severe accident scenarios within the code's framework. Secondly, it intends to highlight the benefits of using mesh adaptivity to capture the key phenomena in accident modelling. Some of the experimental data available from the L3 test has been used as input for this study and some has been used for comparison.

For modelling purposes, the experiment can be divided into three phases– air cooling, water cooling at 10 kW heating, and water cooling at 7 kW heating [1]. Both 2D and 3D simulations of the first phase of the test have been performed, with the mesh adapting to the velocity and temperature fields.

Overall, the melt pool temperatures have been compared with the first phase of the experiment, and this remains the focal point of the study. The melt pool temperatures of the simulations show a maximum error of 14.5% when compared with the L3 experiment.

[1] Fluhrer B, Miassoedov A, Cron T, Foit J, Gaus-Liu X, Schmidt-Stiefel S, Wenz T, Ivanov I, Popov D. The LIVE-L1 and LIVE-L3 experiments on melt behaviour in RPV lower head. FZKA. 2008 Sep 15;7419:3-13.

A hierarchical projection based-reduced order model applied to neutron transport

Toby Phillips, Imperial College London

Reduced order modelling (ROM) is a method of approximating a discretised model (the high fidelity model) by a model with fewer degrees of freedom (reduced model) than the original one. Such reduced models have been proven to reduce the computational cost by several orders of magnitude in the field of nuclear modelling [1, 2].

A typical ROM framework consists of two stages: a computationally expensive offline stage and a rapid online stage. In the offline stage, many solutions of the high fidelity model are computed. The information in these so-called snapshots is compressed often by using Singular Value Decomposition (SVD), however autoencoders [3] are an alternative. The resulting basis functions can either be used to project the discretised governing equations onto the reduced space, (projection-based ROM [4]) or they can be used to project the snapshots onto the reduced space, and these variables can train a neural network to approximate the discretised governing equations (a non-intrusive ROM). In the online stage, the reduced order model is solved for previously unseen parameter values.

Within the nuclear field these reduced order models have typically been applied to the whole system. However, due to the complexity of reactors and the need for a high resolution in certain

dimensions, the amount of data required to describe the system is extremely large which makes constructing a reduced order model intractable. Instead, one method of reducing the amount of data is to split the spatial domain into a number of sub-domains. A reduced order model is then created for each sub-domain and the resulting models can then be combined to solve for the whole system. One such example of this is the so-called reduced-basis element method [5]. The offline stage for this process will typically be less time consuming because the ROMs for each sub-domain can be trained simultaneously.

This poster demonstrates the effectiveness of the hierarchical reduced order modelling approach for a problem of interest to nuclear engineers.

Reduced Order angular discretisation for neutron transport simulation

Alex Hughes, Queen Mary University London

Alex Hughes is a 2nd year PhD student at the School of Engineering and Materials Science at Queen Mary, University of London.

His work is focused on the development of reduced order models (ROM) for neutron transport simulation.

For his PhD he has developed a novel ROM method for the angular discretisation of the Boltzmann transport equation using new adaptive angular basis functions.

RModelling and risk analysis in French PSA level 2

Nicolas Duflot, IRSN, France

Utilisation of Spill Return Atomiser (SRA) in Decontamination, Coating and Fire Suppression

A. Nourian & G. G. Nasr, Petroleum and Spray Research Group, Salford Innovation Research Centre (SIRC), School of Science, Engineering and Environment (SEE)

This poster presents the effect of utilising a novel design of Spill Return Atomiser (SRA) to generate very fine spray particle sizes which can be applied in different sections such as:

(i) healthcare environment in which this type of atomisers generates uniform spray and 'mist like' coverage onto a given surface without having streaking issue;

(ii) industries with risk of exposure to hazardous materials such as Chemical, Biological, Radiological or Nuclear (CBRN) in which fine spray particles can be used ,with considering standard safety shower, on human body during decontamination;

(iii) Fire suppression and explosion mitigation in industries (i.e. nuclear and/or oil and gas) to mitigate fire with low velocity deflagration in which the very fine particle sizes are extracting heat in the short finite moments that the flame and droplets interact.

The Sauter Mean Diameter (SMD) of spray particle sizes from the developed SRA are within the range 15 microns to 30 microns at different supply pressure of up to 120 bar. The discharge rate of SRA varies between 0.1 l/min to about 2 l/min, depending on different application.

The researchers are exploring the applicability of the techniques developed in this programme to other applications, particularly the broader energy industry.

THOR – the new thermal-hydraulics rig at M-Sparc

Marcus Dahlfors, Nuclear Futures Institute, Bangor University

The Nuclear Futures Institute at Bangor University is developing the first phase of a Thermal-Hydraulics Open-access Research facility – THOR at Menai Science Park (M-SParc) on Anglesey.

THOR will be instrumental within a stepwise approach to develop relevant competence, research capability and techniques to pave the way for an eventual establishment of the National Thermal-Hydraulics Facility (NTHF) at the site. The initial configuration is foreseen to be an atmospheric to intermediate pressure capable prototype for water T/H testing in advance of a subsequent high-pressure loop to be based on techniques and experience thus developed.

The presentation reports on THOR design developments, installation progress and future plans.

Fluid Flow Solver for Nuclear Reactors using Automatic Code Generation

Kene Nwegbu, Imperial College London

Thermal hydraulic analysis of nuclear reactor systems is performed using different codes to model the thermal hydraulic safety margins at different scales: System codes intend to predict the behaviour of the whole primary system, subchannel codes for core behaviour predictions and CFD codes to simulate the thermal-hydraulics in a fixed part of the core. Even still, one approach that could aid this field even further is a code developed using automatic code generation. The high-level code used in code-generation has the advantages of being quicker to implement, more consistency and being more readable.

In this project, a fluid flow solver will be developed on Devito - a DSL and automatic code-generation framework for finite difference equations. Devito allows symbolic equations written using SymPy to be converted to highly optimized C++ code [1]. The fluid modelling for this solver will be developed using a porous media model, which has been applied in other examples of nuclear reactor core analysis [2]. Then, to introduce internal structures to the geometry, the immersed body method will be used [3].

Validating this solver and assessing its feasibility will be done continuously with the project's progression using benchmarks of thermal hydraulic analysis from existing technologies

[1] Fabio Luporini, Michael Lange, Mathias Louboutin, Navjot Kukreja, Jan Hückelheim, Charles Yount, Philipp Witte, Paul HJ Kelly, Gerard J Gorman, and Felix J Herrmann. Architecture and performance of Devito, a system for automated stencil computation. arXiv preprint - arXiv:1807.03032, 2018.

[2] Ronghua Chen, Maolin Tian, Sen Chen, Wenxi Tian, GH Su, and Suizheng Qiu. Three dimensional thermal hydraulic characteristic analysis of reactor core based on porous media method. Annals of Nuclear Energy, 104:178{190, 2017.

[3] S Jewer, AG Buchan, CC Pain, and DG Cacuci. An immersed body method for coupled neutron transport and thermal hydraulic simulations of PWR assemblies. Annals of Nuclear Energy, 68:124{135, 2014.

Track Record: Flexible Mesh Multiphysics Coupling for Nuclear Engineering (reFINE)”

Lian Yang, Cranfield University

We propose to develop a multi-scale and multiphysics modelling framework with intelligent adaptive spatial resolution, within the world-leading nuclear modelling code framework FETCH2. The focus of this work will be on the development of high fidelity multi-physics models for simulating some of the most important and exciting application areas in nuclear engineering, spanning nuclear reactor design (current generation for validation reasons), core accident analysis and spent fuel reprocessing operations (involving fissile liquids).

For power generation the existing PWR reactor designs will be investigated but the intention is that the technology will be applicable for all reactor types. The model will analyse damage mitigation operations that follow severe accidents, it will determine whether there is sufficient cooling of debris-beds and the potential risk of re-criticality. In re-processing facilities involving fissile liquids, this modelling technology will help to avoid (or mitigate consequences of) criticality accidents through improved design.

The project outcomes include facilitating major breakthroughs in important and new reactor application areas and the most accurate modelling framework currently possible that can be used for design and safety cases.

Flow Modelling of Injection Orientation of Supercritical CO2 in Porous Media for Enhanced Gas Recovery (EGR)"

M. K. Abba, A. J. Abbas & A. Nourian, Petroleum and Spray Research Group, Salford Innovation Research Centre (SIRC), School of Science, Engineering and Environment (SEE), University of Salford

Injection orientation of supercritical CO2 (S-CO2) during Enhanced Gas Recovery (EGR) and sequestration is one of the key factors to the overall technique in terms of displacement efficiency and extent of gas mixing. Injection orientation plays a vital role in the behaviour of S-CO2 as it traverses the pore spaces of the porous medium during CH4 displacement at reservoir conditions under gravity. However, the rate of mixing between the injected CO2 and the displaced CH4 appeared more rapid in the horizontal injection orientation compared to that of vertical injection from previous laboratory tests. This study aims to investigate the flow behaviour of S-CO2 in a rock core under gravity using a numerical method. The modelling was used to evaluate the gravity effect on the efficiency of CH4 displacement by mimicking a laboratory experimental approach.

COMSOL Multiphysics® was used to perform the simulation using two different interfaces to model the gas-gas displacement in porous media. Brinkman equation was used to model the fluid flow in porous media and the Transport of Concentrated Species (TCS) was used to model the species transport. These models were coupled with the in-built reacting flow. The results show that gravity contributes significantly to the mixing between CO2 and CH4 during the displacement process in the horizonal orientation as it moves to the bottom of the porous media along the longitudinal axis of the porous medium. This is attributed to the density of the S-CO2 in relation to that of CH4 at those conditions. The numerical results demonstrate a reasonable representation of the laboratory experimental trend obtained for the concentration profiles of CO2 as it displaced the CH4. This study explains the reason behind the trend of early emergence of CO2 observed in the horizontal orientation and subsequent higher mixing between CO2 and CH4 compared to the vertical orientation injection.

The researchers are exploring the applicability of the techniques developed for these analyses in other applications, particularly the energy industry.

Vacancy elastodiffusion around cavities in aluminium: Fast first passage algorithms based on Krylov subspace projection techniques

Savneet Kaur, Manuel Athènes, CEA SACLAY, France

The Kinetic Monte Carlo (KMC) method is widely used in material science to simulate the microstructural evolution of alloys, specifically under irradiation. This simulation approach is based on a master equation and a transition rate matrix that together govern the jumps of defects between substitutional sites of a crystalline lattice.

The KMC method becomes cumbersome when the transition rate matrix exhibits a broad spectrum of frequencies. Defects such as vacancies perform a huge number of transitions between atomic configurations which are connected by small energy barriers. These connected configurations form trapping basins from which the typical escape time of a defect is much higher than its typical time to cross the small barriers inside the basins. Hence, the system remains trapped in metastable thermodynamic states.

To overcome this recurrent issue in KMC simulations several acceleration techniques are available. These techniques are based on the theory of absorbing Markov Chains1. The escaping events are characterized by their first passage and no passage distributions to distant locations. These two distributions can be extracted through the eigenvalue decomposition or direct factorisation of the transition rate matrix. Assuming the diffusion processes are reversible, a property satisfied by the dynamics of defects in metals and alloys, we show that the involved linear and eigenvalue problems to be solved can be symmetrised. Moreover, the slowest mode (associated with the smallest eigenvalue) is observed to contribute the most to the first-passage and no-passage distributions. As a result, Krylov subspace projection techniques implementing reverse iterations provide us with an efficient tool for extracting the slowest modes at a relatively low cost2. We discuss the convergence, scalability and range of applicability of the approach.

However, the cost increases with the number of eigenmodes significantly contributing to the first passage distribution. Here, we provide a more efficient way to compute the probability vector at times shorter than the mean first passage time. We present several Krylov subspace projection methods, discuss their efficiencies and illustrate their performance by computing sink strengths and transition currents for the emission and absorption of vacancies from and to cavities in aluminium3. We eventually discuss the effect of elastic interactions between the cavity and the jumping vacancy at its saddle positions, which introduces anisotropy in both transition rates and transition currents to the sinks.

[1] An energy basing finding algorithm of Kinetic Monte Carlo acceleration, B.Puchala, M.L.Falk, and K.Garikipati, J. Chem. Phys. 132,134104 (2010)

[2] Elastodiffusion and cluster mobilities using kinetic Monte Carlo simulations: Fast first-passage algorithms for reversible diffusion processes, Manuel Athènes, Savneet Kaur, Gilles Adjanor, Thomas Vanacker, and Thomas Jourdan, Phys. Rev. Materials 3, 103802 (2019)

[3] Effect of saddle point anisotropy of point defects on their absorption by dislocations and cavities, D.Carpentier, T.Jourdan, Y.Le Bouar, M.C.Marinica, Acta Mater. 136 323-334 (2017)

SPEAKER PROFILES

DR ALEX BOND

Principal Consultant, Quintessa Ltd

Alex is a geologist by training, and has an academic background covering physical natural sciences and hydrogeology, leading into a PhD in complex non-linear numerical analysis of groundwater flow in fractured rocks.

He works for Quintessa Ltd., an employee-owned scientific and mathematical consultancy that provides leading-edge scientific, mathematical and strategic consultancy, scientific software development and research to public and private science-based organisations to facilitate a low carbon energy future.

Through his work for BNFL and Quintessa, Alex has gained considerable practical experience of modelling at all scales of interest required for understanding environmental systems, ranging from highly detailed coupled analysis to whole-system analysis techniques.

Currently he specialises in coupled numerical analysis of thermal-hydraulic mechanical systems primarily focussed on radioactive waste management, the geological storage of carbon dioxide and support to nuclear reactor safety cases. Alex is also responsible for developing Quintessa's in-house multiphysics software and is leading a growing company capability in the application of COMSOL Multiphysics®. He also participates, on behalf of a range of clients, in international research projects addressing issues around coupled modelling in radioactive waste and carbon dioxide storage, and is currently the Technical Secretary for DECOVALEX-2023.

In addition to his consultancy work Alex also provides international training on the use and application of software for environmental impact assessment.

DR ANDREW BUCHAN

Queen Mary University London

Andrew is a Lecturer in Engineering at Queen Mary University of London. He has 18 years' research experience in developing computational methods and models for radiation, heat transfer and multi-phase flows.

He obtained his PhD from Imperial College in 2006 and holds an EPSRC early career research fellowship for developing computational models for simulating multi-physics processes in nuclear engineering applications.

His modelling research interests include finite elements, wavelets, reduced order models, self-adaptive methods, sensitivity and uncertainty quantification techniques. He has around 50 publications in leading journals/conferences for nuclear and computational physics.

ALAN CHARLES

Jacobs

Alan is a professional nuclear engineer with over six years of experience in the nuclear industry, working in the areas of reactor physics and thermal-hydraulics.

He has worked on projects at concept and detailed design level as well as support for currently operating reactors, with particular experience in the areas of development and validation of analysis methods for nuclear reactors, mathematical optimisation and international collaboration.

DR MARCUS DAHLFOR

Bangor University

Marcus joined the NFI as Reader in Nuclear Engineering in January 2020, to head a research group in Reactor Design and Thermal-Hydraulics. He has worked with nuclear applications within both academic and industrial contexts since 1994.

During the past 15 years, Marcus has worked with LWR analysis and safety including various R&D aspects. Specialisms also include reactor new build and its permissioning with regulatory interaction especially in the UK regime; development, testing and verification of nuclear reactor simulation software; BWR nuclear fuel & core design; core monitoring; reactor physics, thermal-hydraulics related measurements and in-core fuel management.

Outside of LWR technology, Marcus has pursued academic research and industrial R&D focused on systems operating with fast neutrons. Within this context, he has worked with the physics simulations of molten-salt and sub-critical lead-cooled reactors. In 2006, Marcus defended his PhD thesis in nuclear physics on the subject of Accelerator-Driven Systems for Transmutation of Nuclear Waste.

STEVEN DARGAVILLE

Imperial College London

Steven is a postdoctoral researcher in the Applied Modelling and Computation Group (AMCG) at Imperial College London. Currently he is the head developer of FETCH2 at Imperial College, a highly parallel, deterministic adaptive code for simulating coupled multi-physics problems involving Boltzmann transport. These problems are found in fields such as civil nuclear, spectral wave, lattice Boltzmann and more.

His research involves the development of numerical methods for Boltzmann problems which feature scalable angular adaptivity and large-scale sweep-free parallelism. This adaptivity can be performed in a goal-based fashion and is robust in the presence of ray-effects common in Boltzmann problems, through the use of novel angular discretisations. This technology has been deployed across a number of EPSRC grants, along with a number of industrial and academic partners.

He also supervises MSc and PhD students in radiation transport methods and teaches several courses at Imperial College, in both the Nuclear Engineering MSc and the Applied Computational Science and Engineering (ACSE) MSc.

Steven completed his PhD in applied/computational mathematics in 2013, which was based on modelling the discharge of LiFePO4 batteries, and involved building coupled multi-physics models which match observed discharge behaviour. More broadly, his research interests are centred on modelling and numerical methods in the energy sector.

ROBIN DICKENSON

Atkins

Robin currently works for the Nuclear and Power business of Atkins, a member of the SNC-Lavalin Group. He has 20 years of experience in the static, dynamic and thermal assessments of safety critical structures across the aerospace, rail and nuclear industries.

Robin started at Atkins in 2000 after graduating from the University of Bristol with a master's degree in Aeronautical Engineering. One of his first roles at Atkins was the development of a finite element model, known as GCORE, for the seismic assessment of the graphite core of the Hinkley Point B reactors.

He then moved into the Aerospace business at Atkins, where he was involved in the thermal analysis of the Airbus A380 wing systems, the structural certification of the A400M composite wing and the dynamic analysis of the A350 landing gear separation to demonstrate crashworthiness.

In 2017 Robin returned to the GCORE project and the Nuclear business at Atkins. Here he has been developing user subroutines for the Abaqus/Explicit finite element solver to create a bespoke simulation capability for the seismic assessment of the graphite cores of the UK AGR stations.

HECTOR DIEGO ESTRADA-LUGO

University of Liverpool

Hector is a PhD student at the Institute for Risk and Uncertainty of the University of Liverpool, and has been there since 2017. Originally from Mexico City, he studied a BSc degree in Physics at the Autonomous National University of Mexico and participated as assistant researcher at the project "Multi-wired muons detector at the Teotihuacan pyramid" from 2012 to 2015.

He was awarded a scholarship from the National Council of Science and Technology and the Energy Secretary of Mexico to study his MSc in Radiometrics: Instrumentation and Modelling in 2016 at the School of Physics of the University of Liverpool.

Hector's current PhD project is about modelling critical safety systems in thermal reactors, to perform resilience assessments under different accident scenarios. Bayesian networks are used to capture the complexity of component's dependency within such engineered installations.

In their most recent work, developed on the uncertainty quantification software "OpenCossan", Bayesian networks are combined with imprecise probabilities to consider the epistemic uncertainty that can arise from the lack of information.

With such an approach, they can produce a resilience assessment that not only informs of the resilience profiles during different accident scenarios, but also the level of ignorance in cases of incomplete or unreliable data.

ANDREW DUFF

Science & Technology Facilities Council

Andrew is a Senior Computational Scientist at STFC Daresbury Laboratory (DL), where he collaborates with academia and industry on materials science projects based on his expertise in density functional theory (DFT), atomistic simulation and potential optimization.

His background is in the development and implementation of ab initio methods, including the TU-TILD approach— in collaboration with Prof. Mike Finnis from Imperial College and Prof. Blazej Grabowski from the University of Stuttgart –for computing free energies at ab initio accuracy up to the melting point [Phys. Rev. B, 91, 214311].

His developments improved the efficiency of such calculations by an order of magnitude, rendering accessible accurate high temperature properties of refractory alloys. The approach was demonstrated by computing, up to the melting point, the properties of the exemplar ultra-high temperature ceramic zirconium carbide, with results in improved agreement with experiment (where available) and CALPHAD assessment.

He is developer of the MEAMfit potential optimization code [Comp. Phys. Comm. 196, 439], and has recently made progress in the challenging area of multi-component potentials, fitting potentials for quaternary high entropy alloys (HEAs) [npj Comp. Mat. 5 80].

He is a co-I on EP/S032835/1 which will apply DFT methods (inc. TU-TILD) and atomistic simulations to model HEAs for nuclear applications.

PROFESSOR ROBIN GRIMES FREng FNucl

Imperial College London

Robin is Professor of Materials Physics at Imperial College and was Founding Director of the Centre for Nuclear Engineering.

In his research, he uses computer simulation techniques to predict the behaviour of materials for energy applications including nuclear fission and fusion, fuel cells, batteries and solar cells.

He is the current UK Ministry of Defence, Chief Scientific Adviser (Nuclear), a Fellow of the Royal Society and the Royal Academy of Engineering.

LEE EVITTS

Bangor University

Lee obtained his Ph.D. in experimental nuclear physics from the University of Surrey, in collaboration with TRIUMF, Canada. At TRIUMF, Lee commissioned a spectrometer that is now being successfully used in experimental campaigns to probe the underlying nuclear structure of radioactive isotopes.

Currently, Lee is a Sêr Cymru Research Fellow at Nuclear Futures Bangor, specialising in modelling the electron and phonon transport through nuclear materials under extreme environments. Lee is also interested in other nuclear related fields such as scintillator development and cogeneration.

FLORIAN FICHOT

IRSN, France

Florian is a research engineer and expert at the Institute of Radioprotection and Nuclear Safety (IRSN, France). His expertise covers several areas related to the physical processes occurring in case of a severe accident in a nuclear power plant (core damage, safety injection of water, in-vessel corium retention).

He graduated from Ecole Centrale Paris (1989), with a specialty in Mechanical Engineering, Heat Transfers and Combustion, and obtained a Ph.D. in Mechanical Engineering at Ecole Centrale Paris (1994) on the topic of “Modelling of the ignition of a turbulent diffusion flame: Application to cryogenic rocket engines”. He was a visiting scientist at the Jet Propulsion Laboratory of NASA, Pasadena (California).

Florian has been working at IRSN for 25 years, mostly developing physical models for codes used to predict the behaviour of core materials, thermalhydraulics and the evaluation of corium cooling strategies in case of severe accident in a nuclear reactor. He supervises Ph.D. and post-doctoral students, as well as visiting foreign scientists (India, Russia, China, USA).

He has coordinated several international projects sponsored by OECD or EURATOM, in particular the recent H2020 project IVMR, dealing with in-vessel corium retention strategy. He was coordinator and writer of the chapter ‘In-vessel phenomena’ of the book ‘Nuclear Safety in Light Water Reactors’ (published by Academic Press in 2012) and gives lectures organised by international organisations (European Network of Excellence SARNET, IAEA).

ALEXANDER HUGHES

Queen Mary University London

Alex is a PhD student in the School of Engineering and Materials Science at Queen Mary University London.

His work is focused on reduced order modelling of neutron transport, particularly in the context of reactor physics.

Alex obtained a BSc in Physics from the University of Nottingham in 2018, and began his research at Queen Mary the same year.

He is currently developing new models for discretising the angular dimension of the Boltzmann Transport Equation.

ANIKET JOSHI

The Open University, UK

Aniket Joshi is a PhD student with The Open University, pursuing his research in creep of steels used in nuclear reactors.

He obtained his MSc degree with Distinction in Advanced Nuclear Engineering from Imperial College London. He is currently involved with modelling severe accidents in nuclear reactors with Imperial College's Applied Modelling & Computation Group (AMCG).

His research interests include numerical methods for engineering fluids, shock physics, and creep damage in materials.

SAVNEET KAUR

CEA France

Savneet is a PhD researcher in Materials Science at the Department of Nuclear Materials, French Alternative Energies and Atomic Energy Commission (Saclay) in France. Her research involves the study of the interstitial defects and vacancies for the materials (alloys) of a nuclear pressure vessel.

In nuclear material science, the Kinetic Monte Carlo (KMC) technique is used for monitoring irradiation defects such as displacement of vacancies and interstitials, and observe the recombination processes.

The objective of her thesis mainly concerns the improvement of KMC algorithms in order to simulate vacancies in multi-solute clusters in the presence of irradiation defects with the help of parallel computation (MPI) and the numerical libraries of linear algebra (PETSc, SLEPc, ScaLAPACK, LAPACK, BLAS).

Savneet graduated with a bachelor's degree in Physics from University of Delhi (2013), and has five years of curriculum experience (Double master's degree) in Nuclear Engineering from the University of Delhi (2016) and University of Paris Saclay (2018). She gained hands-on experience in the field of Nuclear Reactor Physics and Fluid dynamics during her internship projects at CEA Cadarache & IGCAR Chennai (India) and has also worked as a Student Research Assistant for 6 months in a reactor design group at KIT, Germany.

PROFESSOR JOHN LILLINGTON

Jacobs

Professor Lillington has worked for 45 years within the UK Nuclear Industry with the UKAEA, AEA Technology, Serco, Amec Foster Wheeler, Wood and Jacobs. Originally graduating in mathematics from the University of London (BSc, PhD) he is a Fellow of the Institutes of Physics and Mathematics (FInstP, FIMA) and a Chartered Engineer (CEng).

John has worked on all the major reactor systems (water, gas and fast reactor) as a thermal-hydraulics specialist, theoretical physicist, safety analyst, technical programme, resource and project manager. He is currently Chief Technologist, Nuclear Reactors within Jacobs.

He is a part-time lecturer/ external examiner at several UK Universities (Cambridge, Imperial, Birmingham & Surrey) and an Honorary Professor at Bangor University. He has published two books (Elsevier 1995 & 2004) and numerous articles on nuclear power related subjects.

John was appointed as a member of the first UK Government Nuclear Innovation and Research Advisory Board (NIRAB) to advise on R&D for future nuclear energy. He is an UK delegate to the International Generation IV Forum and the European FORATOM R&D Task Group. He is also a member of the WNA CORDEL SMR Task Force currently assessing different countries' licensing approaches applicable to SMRs.

ADOLPHUS LYE

University of Liverpool

Adolphus graduated from the National University of Singapore in 2018 with a major in Physics and a minor in Mathematics. His final year dissertation looks into the use of the Accident Source Term Evaluation Code (ASTEC), developed by IRSN, in simulating loss of coolant accidents, performing parametric studies and observing the effects on the accident sequence in a pressurised water reactor.

He commenced his PhD candidature in the University of Liverpool's Institute for Risk and Uncertainty in the autumn of 2018 under the joint-supervision of Professor Edoardo Patelli and Associate Professor Alice Cicirello.

His current research looks into the topic of Bayesian Model Updating and he is currently looking into advanced sampling techniques used in such areas with the aim of applying such techniques in probabilistic safety assessment of nuclear power plants. His PhD study is being funded by the Singapore Nuclear Research and Safety Initiatives (SNRSI), the organisation under which he did his final-year project with as an undergraduate.

To date, Adolphus has written 3 conference papers and a journal paper which is currently under review. Work aside, he enjoys travelling to different countries around the globe, photography, networking with people, and long-distance running, the latter of which he is currently partaking in actively as a member of the University's Cross-country team.

FULVIO MASCARI

ENEA, Italy

Fulvio has a Master's Degree in Nuclear Engineering (2006) and the doctorate PhD in "Nuclear, Chemical and Safety Technology" (2010) at the University of Palermo.

Since September 2013 he has worked as a researcher at the ENEA. His technical field is the nuclear reactor thermal-hydraulics in reactor coolant systems/containment, and their coupling and the analyses of severe accident phenomena. In relation to that, he is an expert on the use of best estimate thermal-hydraulic system code (RELAP5 and TRACE) and severe accident code (ASTEC and MELCOR).

Currently Fulvio is investigating severe accident issues in PWR and BWR reactor types, the aerosol behaviour in the containment of Sodium-Cooled Fast Neutron Reactor by using severe accident code, the application of the probabilistic method to propagate input uncertainty in deterministic safety analyses, the capability of best estimate thermal-hydraulic system code to simulate the main phenomena typical of advanced light water SMR in DBA and BDBA conditions, and the analyses of the scaling issues.

He is involved in several international activities (e.g. H2020-EURATOM Projects, OECD/NEA/CSNI/WGAMA activities, IAEA activities, etc). He represents ENEA in CSARP and CAMP USNRC Research Program.

DR SIMON MIDDLEBURGH

Bangor University

Simon Middleburgh is a Reader in Nuclear Materials at Bangor University and was appointed to the Nuclear Futures Institute in March 2018. His research is focused on developing new nuclear materials, investigating material behaviour in extreme environments (including nuclear and aerospace) and combining materials modelling techniques with experimental methods.

Simon has over 60 peer reviewed journal articles and 13 patents. He is building a suite of software and hardware capabilities at Bangor University in order to support industrially relevant research in order to produce research required by the nuclear industry in a timely manner.

Simon has held positions at the Australian Nuclear Science and Technology Organisation (ANSTO), Australia as a Research Leader, and at Westinghouse Electric Sweden AB as a Senior Engineer where he used his methods to advance fuel development and fuel performance modelling methods.

Simon brings experience from the nuclear industry to Bangor University and has taken part in a number of expert panel groups including within the IAEA. Simon is part of a number of international research collaborations and has been on the nuclear advisory committee at the Centre of Nuclear Engineering at Imperial College London, consulted for the UK Foreign and Commonwealth Office and the UK National Nuclear Laboratory.

DR AMIR NOURIAN

Salford University

Amir has been a lecturer in Mechanical and Petroleum Engineering since 2013, and has been actively involved in teaching and research during this time.

He is currently an associate head of the internationally recognised Spray Research Group (SRG) at the University of Salford, which has both national and international-scale collaboration working arrangements with large and SME companies and educational establishments.

Amir completed his PhD at the University of Salford on an Eco-friendly valving arrangement for domestic aerosol sprays (i.e. hair spray) utilising ‘clean air’ propellant such as compressed air, as opposed to harmful Liquefied Petroleum Gas (LPG). The outcome of this research formed part of a ‘Technology Transfer’ by the University of Salford and in 2014, SRG won the Times Higher Education Award for ‘Outstanding Contribution to Innovation and Technology’.

KENE NWEGBU

Kene is a 1st year PhD student in the Applied Modelling and Computation Group at Imperial College London.

He previously completed an MEng in Chemical Engineering at the University of Sheffield before working for a year as a graduate engineer at Honeywell. Despite this, he was drawn to computational modelling and its applications in nuclear engineering.

This led to him joining ESPRC Centre for Doctoral Training in Nuclear Energy Futures in October 2019 where began his PhD under the supervision of Professor Christopher Pain, Professor Paul Smith and Dr Gerard Gorman.

MEGAN OWEN

Bangor University

Megan completed her degree in Electronic Engineering B.Eng at Bangor before joining the Materials in Extreme Environments research group at Bangor University's Nuclear Futures Institute in 2019 as a Ph.D. student.

Her Ph.D. project focuses on the corrosion of zirconium alloys used within the nuclear industry and the possible role of alloying elements on grain boundary complexions.

The project is supported by Westinghouse Sweden AB and KESS 2 and is part of the MUZIC-3 project (Mechanistic Understanding of Zirconium Corrosion). Through participation of this project, a further understanding of zirconium corrosion can be obtained to try and develop materials for improved performance.

Alongside her studies, Megan is a keen STEM ambassador for the University, for both the Electronic Engineering department and the Nuclear Futures group. She is an active member of the University, organising events that aim to encourage and enthuse students into STEM subjects by showing them the vast opportunities within the STEM subject fields.

Megan is also a part of the Athena SWAN Self-Assessment Team for the Electronic Engineering and Computer Science department to try and promote gender equality among the subject areas.

PROFESSOR CHRIS PAIN

Imperial College London

Christopher is head of the Applied Computation and Modelling Group (AMCG) consisting of approximately 50 scientists and engineers at Imperial College London. He was the original developer of the group's main modelling framework Fluidity (http://fluidityproject.github.io) that he conceived in the first year of his PhD.

He has attracted considerable research funding for the group's modelling development and application from UK research councils, the EU and industry. Fluidity has been released as open source software and has a rapidly growing user/developer community across North America, Europe and Asia. In 2010 the AMCG won the Imperial College Research Excellence Award, an award from the College in recognition of world leading research

Christopher's main academic interests are in general Computational Fluid Dynamics (including multiphase flow, air flows and geophysical fluid dynamics); nuclear engineering (neutron and photon transport, nuclear criticality, nuclear reactor dynamics, nuclear waste repositories); Optimisation, Data Assimilation; sensitivity analysis; reduced order modelling; Numerical Research, including parallel solution techniques; recurrent and feed- forward neural networks; a priori error measures and mesh adaptivity; discretisation techniques; resolution of linear and non-linear equations; non-linear dynamics; numerical shape description and differential geometry.

Professor Pain has supervised 50 successful PhDs and published 240 journal papers.

TOBY PHILLIPS

Imperial College London

During an MEng in Mechanical Engineering at the University of Nottingham Toby developed a strong interest in energy production. Subsequently, this led to him joining Imperial College's ESPRC Centre for Doctoral Training in Nuclear Energy where he completed an MRes and is now studying for a PhD. Within

Imperial, he is a member of the Applied Modelling and Computation Group where his work focuses on reduced order modelling and machine learning applied to nuclear engineering under the supervision of Professor Christopher Pain, Dr Claire Heaney and Professor Paul Smith.

MALWINA QVIST

Senior Engineer, Low-carbon Energy Technologies BEIS

Malwina joined BEIS in 2016 to advise policy makers and ministers on a variety of innovative low carbon energy sources in the Science and Innovation for Climate and Energy Directorate.

She has been working with nuclear innovation and research for the past 4 years, supporting the department in a variety of ways. She is the UK delegate to two NEA boards, MBDAV and NDC, and supports the nuclear research collaboration with the US, leading on reactor design and modelling themes.

Before working for BEIS, Malwina worked with variety of research programmes, supporting deployment of non-electric applications of nuclear power. Her background is in nuclear engineering, specialising in computational fluid dynamics design of advanced reactor technologies. She completed her PhD at Oregon State University, followed by a postdoctoral researcher appointment at the University of California Berkeley.

MARK SALISBURY FNucI

Nuclear Innovation and Research Office (NIRO)

Mark is currently a senior technical advisor to the UK Government at NIRO. He graduated with a degree in Chemistry from the University of Warwick in 2002 and is a Fellow of the World Nuclear University, the Royal Society of Chemistry and Institute of Innovation and Knowledge Exchange. He is a Chartered Chemist and Scientist and sits on the Board of Trustees at the Nuclear Institute, of which he is also a Fellow.

Prior to his current role, Mark worked for Horizon Nuclear Power Ltd in numerous positions, latterly as the Operations Department Manager; responsible for developing plans for the operational utility intending to operate Horizon's plants. This included Horizon's Technical Apprenticeship Programme and its Training Support Partner.

Whilst he was at Horizon, he was one of seven members of staff to successfully complete the initial operator training on Hitachi-GE Ltd's Advanced Boiling Water Reactor in Japan through consecutive translation!

Prior to this, Mark has worked for British Energy at Sizewell B and for PowerGen on nuclear, coal and gas-fuelled power stations in both Chemistry and Operations Departments.

DR T V SANTHOSH

University of Liverpool, UK

Dr Santhosh is a senior scientific officer at the Bhabha Atomic Research Centre (BARC), Mumbai, India, and currently postdoctoral research associate at the Institute for Risk and Uncertainty, University of Liverpool in the UK. He joined BARC in 2001 after obtaining a Post Graduate Diploma in Nuclear Science and Engineering. He received his Bachelor's degree in Electrical and Electronics from Bangalore University; Masters in Reliability Engineering from IIT Bombay; and PhD in Engineering from Homi Bhabha National Institute, Mumbai. Additionally, he is a faculty of BARC Training School and has delivered several short-term courses on risk and reliability.

Dr. Santhosh has been Guide and Technology Advisor for several bachelor and master theses on risk, reliability, operator support systems, virtual simulation, artificial intelligence and accelerated life testing, and is a permanent member of several committees of the Atomic Energy Regulatory Board for nuclear power plant safety.

He has published over 80 publications in refereed journals and conferences, and was a key contributor for several nuclear and non-nuclear projects for obtaining clearance from the ministry of environment, and has been a Co-collaborator for national and international projects, including one EPSRC project.

Dr Santhosh is a recipient of the DAE Group Achievement Award in 2015 for his outstanding research contributions, and is currently working on the EPSRC project: "A Resilience Modelling Framework for Improved Nuclear Safety".

PROFESSOR PAUL SMITH

Jacobs

Paul is a mathematical modeller with over 40 years' experience of mathematical modelling including 35 years of experience in nuclear reactor safety and performance. His particular technical expertise is in radiation transport, severe accidents and atmospheric dispersal.

For the last 14 years he has managed the ANSWERS® Software Service which develops and supplies nuclear modelling codes worldwide for reactor physics, criticality, radiation shielding and dosimetry etc. Prior to that he worked on the atmospheric dispersal of radioactive materials resulting from events such as severe accidents in nuclear power plants.

This was a natural progression from Paul's first decade in the nuclear industry, which was spent supporting the severe accident safety case for the Sizewell B reactor.

This was followed with modelling of severe accidents in gas reactors to assist with the production of Severe Accident Management Guidelines for the UK's Magnox and AGR fleets of nuclear power plants.

Paul is a visiting professor in the Applied Modelling and Computation Group (AMCG) in Imperial College London and also in Bangor University, where he helps direct research into next generation methods for radiation transport, multi-phase fluids and severe accident analysis.

GLYN ROSSITER

National Nuclear Laboratory

In his role as Laboratory Fellow for Fuel Performance at National Nuclear Laboratory (NNL), Glyn is NNL's technical lead on the thermo-mechanical behaviour of nuclear fuel.

Glyn has 25 years' experience working in the nuclear industry, first for the (now defunct) UK nuclear fuel vendor British Nuclear Fuels plc (BNFL), and later for NNL and its predecessor organisations.

His primary expertise is in nuclear fuel performance and reactor core thermal-hydraulics, and the design, licensing, experimental testing and computational modelling of nuclear fuel that is associated with this.

Glyn is chair of the Nuclear Energy Agency (NEA) Expert Group on Reactor Fuel Performance (EGRFP) and the UK representative on the International Atomic Energy Agency (IAEA) Technical Working Group on Fuel Performance and Technology (TWGFPT).

GARETH STEPHENS

Bangor University

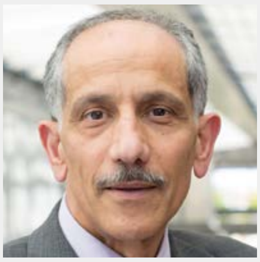
Gareth completed a Masters of Physics degree in material physics at Aberystwyth University. He is now a PhD student studying the complex grain boundary behaviour of zircaloy and the impact of coolant chemistry at Bangor University's Nuclear Futures Institute, with Dr Simon Middleburgh.

The project, which began in 2019, is funded by Jacobs and the Nuclear Energy Futures EPSRC Centre for Doctoral Training. The focus of Gareth's project is to study the mechanism of zircaloy corrosion whilst subject to a lithiated water environment.

Primarily, computational simulation and analysis will be adopted to gain an understanding of possible mechanisms including oxygen, hydrogen and lithium transport through the material which will then be verified by traditional experimental methods including characterisation.

PROFESSOR ALI TEHRANI FNucI

Office for Nuclear Regulation



Professor Tehrani is a Chartered Engineer, a Fellow of the Institution of Mechanical Engineers, and Fellow of the Nuclear Institute. He has considerable experience of the nuclear industry in a wide range of roles, many at a senior level, developing safety enhancements, codes and methods supporting many operating facilities.

Ali is a Principal Nuclear Safety Inspector at the Office for Nuclear Regulation (ONR) and has led the assessment of UK-EPR and AP1000 designs in the areas of Fault Studies, Severe Accident and containment thermal hydraulics performance within the UK's Generic Design Assessment (GDA) and construction.

He works closely with international regulators to enhance plant safety features at the design stage by focusing on regulatory concerns and safety standards, and supports the development of strategic research activities by OECD NEA, and also played a leading role in ONR's response to the events at Fukushima Daiichi.

Ali is a Visiting Professor at Imperial College London and leads a number of challenging and complex research activities developing CFD and multi-physics codes to improve understanding of the plant performance in accident conditions.

LIANG YANG

Cranfield University

Liang's areas of expertise encompass thermal hydraulics, porous media flow, computational mechanics, and high-performance computing.

His interests lie in numerical methods for solving multiphysics, multiscale problems, with the application to energy systems.

He received his PhD in Computational Mechanics at Swansea University along with a dual MSc in Computational Mechanics from Swansea University and Universitat Politècnica de Catalunya.

Liang has worked on EP/P013198/1, 'Investigation of the safe removal of fuel debris: multi-physics simulation' with Prof. Chris Pain, Imperial College London and Dr. Andrew Buchan, Queen Mary University London.

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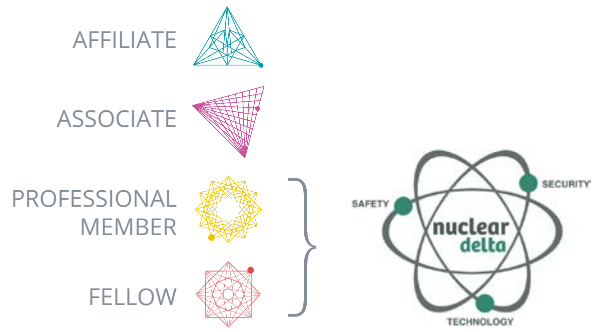

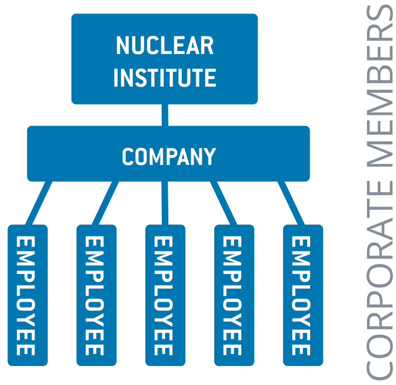

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