

7–8 April 2022 • Imperial College London

NUCLEAR MODELLING 2022

5th Annual Modelling in Nuclear Science and Engineering Seminar

Room G41, Department of Earth Science and Engineering, Royal School of Mines, Imperial College London, Prince Consort Road, London SW7 2BP

ABSTRACTS

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5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

WELCOME

The 5th Modelling in Nuclear Science and Engineering Seminar is to bring together the nuclear community to share innovative and different ways of adopting modelling to help improve design and protect the society by improving of safety of plants.

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. The Seminar this year offers a fantastic line-up and a fascinating set of topics and themes to offer scientist and engineers a view on future developments.

The 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 2 decades 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.

Professor Ali Tehrani, CEng, FINucE, FIMechE





5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

SESSION 1: FUEL & PROCESS MODELLING AND STRUCTURAL INTEGRITY

09:45 Validation of modelling and simulation: Linking Data, Methods and Needs

The programme of work of the Nuclear Energy Agency's (NEA) Nuclear Science Committee (NSC) covers various aspects of methods, tools and data for validation of modern modelling and simulation. Much of the work organised into development of benchmarks, where participants perform either code to code verification, or code to experiment exercises. These benchmarks attract a wide variety of participants, ranging from reactor designers to graduate students, testing the latest developments in modelling and simulation. To provide experimental evidence for validation, the NEA collects, preserves and disseminates experimental data in different domains, including reactor physics, shielding, criticality safety, fuel performance, spent fuel isotopic composition, and thermal-hydraulics. The data are widely used for international activities involving validation of current and new calculational schemes, including computer codes and nuclear data libraries, for assessing uncertainties, confidence bounds and safety margins, and to record measurement methods and techniques.

With new demands from various nuclear stakeholders and recent advances in theory, methods, and computing power all the pieces are in place for the paradigm to shift in validation, which requires tight integration between the nuclear data, modelling and benchmark disciplines. The NEA has been at the forefront of organising peer-reviewed benchmarks and developing relational databases that contain metadata and physics sensitivities, which allow experts to identify experiments to support validation for their applications. Linking these databases directly with the nuclear data development community offers a testing pipeline that can inform both users and data evaluators of biases and the impact of change in real time. The Nuclear Science Committee and Data Bank are working together to establish a central international reference for sensitivity data that will be directly linked to the Joint Evaluated Fission and Fusion (JEFF) library and will be available to other projects through the Working Party on International Nuclear Data Evaluation Co-operation (WPEC). All communities are invited to contribute, with or without detailed models and proprietary information, to ensure that their needs are addressed in the development of the next generation of modelling and simulation systems that employ nuclear data.

Keywords

Benchmark, Integral experiments, Modelling, Nuclear data, Validation

Dr Tatiana Ivanova, Organisation of Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA) *Michael Fleming*, OECD NEA Data Bank

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

10:10 Safe Cracking: Monte Carlo Nonlinear Coupled Analysis of Nuclear Reactor Bricks

Keyway root cracking of reactor bricks is an important consideration for the continued operation of the UK Advanced Gas-Cooled Reactor (AGR) fleet. Quintessa is supporting EDF Energy using a combination of statistical methods and finite element analyses to give a diverse prediction of keyway root cracking rates. COMSOL Multiphysics® is used as the core component in the finite element analysis; it is used to calculate stresses and graphite brick deformation to inform predictions of future reactor state and increase the robustness of conceptual understanding of prior reactor observations.

Monte Carlo simulation is used to account for variability in brick behaviour. Data from AGR measurements are used to construct statistical models of graphite properties. A response surface (surrogate) model has been developed to calculate bore shapes and cracking times, which can be used to optimise the fit of bore shapes and primary keyway root cracking rates against observations, and hence calibrate the parameter distributions to provide more accurate and rapid model predictions.

The method provides a straight-forward means of calibrating parameter distributions against inspection data, building transparency and confidence in the modelling process. It also provides a means to estimate confidence bounds for comparing model predictions with measurement data using limited samples and estimating the probability of keyway root cracking for a wide range of bore shapes and burnup times.

Keywords

Multiphysics, Finite element, Monte Carlo, AGRs, Uncertainty

Dr Alex E Bond, Quintessa Ltd

Louise Bruffell, Quintessa Ltd, Henley-on-Thames, Town, UK

Rebecca K Newson, Quintessa Ltd.

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

10:50 Stress Analysis Modelling of Cracked AGR Graphite Moderator Bricks

In the UK ~17% of our electricity is provided by Advanced Gas-cooled Reactors (AGR's), many of which have been in service for over 30 years. These reactors consist of a central graphite core made of a large array of interlinked graphite bricks, in order to provide structural integrity to the core, channels for fuel and coolant and fundamentally neutron moderation. During operation the bricks are subjected to fast neutron irradiation and radiolytic oxidation, resulting in changes to the material properties of the graphite and dimensional change. The last two reactors stations, Heysham B and Torness, introduced sealing rings between vertical graphite bricks to improve coolant heat transfer and flow. These graphite sealing rings sit in grooves cut into the top of the graphite brick as shown in Figure 1.

In this study, a finite element analysis of a two-brick model with sealing ring addition has been developed and an induced cracked has been incorporated. The sensitivity of several variables to the build-up of stresses in the seal ring groove (SRG) has been analysed to interrogate the affect and the build-up of stresses.

The FE analyses has shown that the dose and irradiation temperature field variables have a significant effect on the predicted stresses. Analyses indicated restrictions to the opening of the crack through the addition of radial keys also resulted in lower stresses, making failure of the brick at the seal ring groove less likely.



Figure 1: AGR brick showing location of seal ring and the seal ring groove wall.

Keywords

Finite Element Analysis, Stress Analysis, AGR, Nuclear Graphite

Dr Ahmadreza Farrokhnia, Nuclear Graphite Research Group, Department of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK

email: ahmadreza.farrokhnia@manchester.ac.uk

Dr. G.N. Hall, Prof A.N. Jones

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

11:30 A monolithic fluid-structure interaction solver towards fullspectrum simulation of flow-induced vibration

In nuclear engineering components, multiple excitation mechanisms exist for flow-induced vibration (FIV), presenting a vibration spectrum consisting of a wide range of frequencies and amplitudes. Existing FIV simulations often use partitioned coupling methods with simplified solid mechanics model. Such methods fail when coupling is strong, e.g., the magnitude of structure response is large.

In this study, a monolithic fluid-structure interaction solver is developed to solve this problem. Governing equations are discretised in the current domain of an ALE configuration for both fluid and solid fields, allowing accurate interface modelling due to alignment of interface and mesh facets. Solid structures are modelled using nonlinear finite strain theory. Moving mesh and adaptive mesh techniques are combined to describe solid geometry and movement in the fluid domain. A projection-based monolithic solver is used to solve the fluid-solid system which is efficient and robust even in strong coupled cases. Results for validation cases are presented to show the robustness and accuracy of the solver. Compared to partitioned methods, this monolithic solver leverages load balancing and parallelisation designed for fluid solver and shows good promise in engineering application.

Keywords

Fluid-structure interaction; monolithic solver; finite element method; flow-induced vibration

Linfeng Li, Jiansheng Xiang, Christopher Pain, Department of Earth Science and Engineering, Imperial College London SW7 2AZ email: I.li20@imperial.ac.uk*

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

11:50 Peridynamic Modelling of Cracking in TRISO Particles for High Temperature Nuclear Reactors

A linear-elastic model for a single particle of TRISO fuel has been built using a bond-based peridynamic technique implemented in the finite element code 'Abaqus'. The model is able to consider the elastic and thermal strains in each layer of the particle and to simulate potential fracture both within and between layers. The 2D cylindrical model makes use of a plane stress approximation perpendicular to the plane modelled. The choice of plane stress was made by comparison of 2D and 3D finite element models.

During an idealised raise to normal operating power for a kernel to 0.3 W and a bulk fuel temperature of 1300 K, cracks initiate in the buffer near to the kernel-buffer interface and propagate towards the buffer-iPyC coating interface, but do not penetrate the iPyC and containment of the fission products is maintained. In extreme accident conditions, at around 600% power during a power ramp at 100% power per second, cracks were predicted to form on the kernel side of the kernel-buffer interface, opposite existing cracks in the buffer. These were predicted to then propagate slowly. The SiC coating was predicted to subsequently fail at a power of 940%, with cracks formed rapidly at the iPyC-SiC interface and propagating in both directions. These would overcome the containment to fission gas release offered by the SiC 'pressure vessel'. The extremely high power at which failure was predicted indicates the potential safety benefits of the proposed HTR design.

Keywords

Peridynamics, TRISO, HTR

Thomas A. Haynes, School of Engineering, University of East Anglia, Norwich, UK email: t.haynes@uea.ac.uk

Angelo Battistini, Mark R. Wenman, Department of Materials, Imperial College London, London, UK

Daniel Shepherd, National Nuclear Laboratory (NNL), NNL Preston Laboratory, Preston, UK

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

SESSION 2: PLANT PERFORMANCE AND NUCLEAR SAFETY

13:15 An Overview of UK Programmes and the Requirements for Modelling and Model Development

We are at a pivotal time for nuclear. Be that clean energy, environmental restoration, medicine, or space. This is the decisive decade in tackling climate change, and it is also a decisive decade for nuclear. To deliver on the ambitions across the range of UK programmes will need research, development, and innovation – with modelling and model development a key pillar and enabler.

What role will nuclear play in delivering net zero in the UK by 2050? Increasing demand for electricity as we electrify where we can, but achieving net zero is about more than electricity – so what about nuclear beyond electricity? A UK programme with nuclear playing a key role as part of a low cost, low carbon integrated energy system could include large, small, advanced, and fusion reactor technologies. This provides significant opportunities and challenges when we consider modelling and model development; from system level assessment of integration of energy technologies to modelling the latest technologies for nuclear co-generation – including new fuels and fuel cycle - that define the experimental and verification programmes to fulfil regulatory requirements for implementation. Including, as set out in the recent nuclear innovation theme of the Department for Business, Energy, and Industrial Strategy (BEIS) Energy Innovation Programme (IP) – now Net Zero Innovation Programme (NZIP) - and the UKAEA Spherical Tokamak for Energy Production or STEP fusion programme, the ambition to develop digital twins.

This talk will consider the future UK programmes around energy but also the Nuclear Decommissioning Authority (NDA) programmes, nuclear medicine and UK space strategy. Setting a picture of how modelling and model development will be the backbone of the UK achieving its nuclear and 'science superpower' ambitions.

Keywords

Nuclear, Net Zero, Integrated Energy Systems.

Paul Nevitt, 1 National Nuclear Laboratory, Chadwick House, Birchwood, UK email: paul.nevitt@uknnl.com

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

13:40 Performance of Cr-coated cladding in LOCA

The conventional design of Pressurised Water Reactors (PWR) consists of a reactor pressure vessel and a number of steam generators; connected by pipework. The vessel inlet nozzle weld has a history of cracking, so the detachment of the cold-leg pipe, leading to loss of primary circuit water, is generally a design-basis fault.

Fuel performance in such loss-of-coolant accidents (LOCA) is complicated by the gas pressure within the cladding of the fuel pins.

The ductility of zirconium cladding is high and the pitch of the fuel bundle sufficiently small that, should the cladding balloon, maintenance of a coolable geometry comes into question.

Once a threshold temperature of approximately 1200°C is reached, zirconium cladding can achieve ignition in steam and preventing this is a design criteria for the primary-coolant safety injection system.

The addition of a thin coating of chromium to the outside of the cladding, helps prevent cladding creep, or at least reduces the cladding ductility to levels where ballooning is not a concern. Furthermore, the coating substantially reduces cladding oxidation and therefore inhibits ignition.

This presentation discusses the licensing issues associated with clad ballooning from a historical perspective and illustrates the effect of preventing clad oxidation on the progression of a postulated large-break loss-of-coolant accident in a Generation Three PWR; with a vessel and external steam generators.

Analysis indicates that the adoption of accident-tolerant cladding could relax some safety injection system design requirements.

Keywords

LOCA PWR ballooning chromium oxidation

John Jones, 1 Fairlie Associates, Station Road, Churchdown, UK email: info@fairlie-associates.co.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7–8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

14:20 Usage of Numerical Simulations in the Field of Severe Accident by Framatome

Modern nuclear reactors are nowadays expected to be prepared to mitigate a severe accident with core damage, and safely contain the fission products possibly released by the reactor core during such an event.

However, severe accidents with core damage are a rare occurrence. Further, it is not feasible to perform real sized experiments. Thus, the knowledge about severe accidents is based on observations made during the few occurred accidents, scale experiments, and to a large degree on numerical simulations.

In this presentation, a general overview of the severe accident simulation tools employed by Framatome will be given. The fields of application thereby reach from the lisencing process of a GENIII+ EPR-reactor, over support for back-fittings of severe accident mitigation hardware, to operator guidance and training.

These different fields of applications also have different requirements on numerical simulations concerning run-time, model complexity, robustness, quality assurance, and conservativeness. The requirements will be discussed at the specific example for the treatment of combustible gases released during a severe accident. An outcome of these simulations is for example the H2-cloud in a reactor containment during a severe accident, as predicted by CFD code, shown in the picture below.



Keywords

Severe Accident, EPR, Hydrogen, V&V, conservative, best-estimate

Matthias Braun, Framatome GmbH, 91052 Erlangen, Germany email: matthias.braun@framatome.com

5th Annual Modelling in Nuclear Science and Engineering Seminar

7–8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

14:40 Integrated Risk Management and Visualisation Software for a Nuclear Reactor

CRA and Assystem are developing a digital tool that is an end-to-end tool for measuring and managing the risk associated with the design of a fusion power plant.

The tool connects to engineering software such as Model-Based Systems Engineering (MBSE) and risk models as shown in the figure below. It will extract data from MBSE software and convert it into risk information that can be read by risk modelling software to automatically build a model to assess the risk of the plant's design and operation.

The tool will capture the inter-dependencies between each system component, their functions and interfaces, already defined from engineering models, and convert the output data into Object-Orientated Programming (OOP) language-based class objects. This is needed to understand how component failures can propagate which can impact the operation of your plant. It will then convert this information to be readily accepted by risk modelling software and automatically build risk models, such as Reliability Block Diagrams, Fault Trees, or Markov Models. Component failure data and maintenance data can then be assigned to the model to quantify the risk associated with the proposed configuration.

The tool will provide a platform that let users visualise and manage risk. It will also create logical and easy to understand visualisations from the models empowering entire organisations to see the whole picture; instantly gaining insights from once fragmented data and help with the decision-making process for the design and operation of nuclear fusion companies.



Keywords

Risk Management, MBSE, Visualisation, Nuclear, Fusion.

Marinos Panayiotou*, Peter Williams, Victor Richet, Ajit Rai

*email: mpanayiotou@crarisk.com

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

ABSTRACTS

DAY 1 THURSDAY 7 APRIL

15:00 **Development of a gamma ray dose rate calculation and mapping tool for Lagrangian marine nuclear emergency response models.**

This paper presents the development and testing of a gamma radiation dose rate calculation model for the marine environment, and evaluates the potential use for such a model in both short term nuclear emergency response management and emergency response planning.

This is believed to be the first implementation of a full field gamma radiation mapping model (including air attenuation and buildup) to be incorporated within a Lagrangian marine dispersion model.

Calculated surface gamma ray dose rates for nine generic release scenarios are presented and used to undertake an emergency countermeasure optioneering assessment.

This paper has been submitted for publication in Marine Pollution Bulletin special edition "Impact of Nuclear Wastewater Discharge on Oceans and Countermeasures".

Keywords

Nuclear emergency response , Gamma ray dose rate , Air attenuation , Buildup, Radionuclide impact assessment , Marine release, Lagrangian model

Andrew Little, Ministry of Defence, HMS Sultan, Military Road, Gosport, PO12 3BY, UK email: A.Little14@imperial.ac.uk

Matthew Piggott, Department of Earth Science and Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK

Andrew Buchan, School of Engineering and Materials Science, Queen Mary University of London, London E1 4NS, UK

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

SESSION 3: REACTOR PHYSICS, RADIATION TRANSPORT AND THERMAL HYDRAULICS: PART 1

15:55 Sustainability of Reactor Modelling and Analysis in the UK

UK has a glorious legacy of pioneering many nuclear technologies. These include advanced reactor design ideas, such as high temperature gas- and heavy water-cooled reactors, fast reactors, advanced fuels and fuel cycles, such as coated particles, mixed-oxide and others with full recycling of plutonium, and, finally, more recently, advanced technologies in decommissioning, clean-up and robotics. This magnificent heritage is arguably at a danger of being lost. The majority of fast reactor program facilities have been decommissioned, documentation – largely forgotten, and experts – long retired. A similar faith awaits AGR technology which are due to retire within less than a decade. This includes unique high-temperature fuel manufacturing capability, as well as engineering and modelling expertise. This talk will explore some of the current challenges and opportunities to build on the existing knowledge and strengths within the UK reactor design and modelling methods community in order to achieve its carbon emissions and energy independence goals.

Keywords

Advanced reactors, Reactor modelling methods, Monte Carlo.

Eugene Shwageraus, 1 Department of Engineering, University of Cambridge, Cambridge, UK email: es607@cam.ac.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

16:20 Adaptivity and iterative methods for Boltzmann transport

Simulating the distribution of radiation (neutrons/photons) in nuclear reactors is very challenging. One of the main difficulties is due to the dimensionality of the (linear) Boltzmann transport equation (BTE) that must be solved; this equation has three spatial, two angular, one time and one energy dimension (7D). Different material properties also mean the problem has both strongly hyperbolic and diffusive regions.

Traditionally, deterministic solver technology and the space/angle discretisations are intimately linked; sweep-based (wavefront) methods are typically used with DG FEM in space and Sn in angle to solve the BTE. These parallelise well (scaling to >100,000 cores) on structured grids, however achieving good scaling on unstructured grids is still an open problem.

This talk will focus on alternate space/angle discretisations and solver technology we have been developing within the Applied Modelling and Computation Group (AMCG) at Imperial College. These approaches enables the use of traditional angular discretisations like Pn, Sn, along with new approaches based on wavelets. We can use these angular discretisations to perform regular and goal-based anisotropic adaptivity in angle, focusing resolution in important directions.

We have also been developing multigrid solver technology which does not require sweep-based methods, allowing the possibility of excellent scaling on unstructured grids on large supercomputers.

Keywords

multigrid, iterative methods, adaptivity, wavelets

S. Dargaville*, R. Smedley-Stevenson, P.N. Smith, C.C. Pain, Applied Modelling and Computation Group, Imperial College London, UK

*s.dargaville@ic.ac.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

16:40 Framatome toolkit for radiation transport applications Efficient multi-purpose digital workflow for radiation transport

Monte Carlo codes, such as MCNP or TRIPOLI, are recognized as reference codes to deal with a large range of radiation transport problems. However, the inherent drawbacks of theses codes - laboring input file creation and long computation time - contrast with the maturity of the treatment of the physical phenomena. Complex modeling of nuclear facilities is out of reach unless strong approximations are made. That's why over the past decade Framatome has developed a toolkit to cope with multiple radiation transport challenges and application.

A major development was on a software based on Computer Assisted Design (CAD) to create complete and precise Monte Carlo datasets. It is a data entry platform that allows via automation to feed multiple workflows toward different fields. The developed features of the 3D software address both legacy solvers inputs and new hybrid geometrical syntaxes to obtain higher fidelity in the geometrical model and to reduce the preparation times for engineers. This software can be used for a wide range of analyzes (neutron / gamma DER evaluation, shielding, neutron activation, radiological inventory), for different technologies (nuclear reactors: PWR, BWR, SMR... and nuclear facilities (hot cells...)) and be applied for all the phases (design, production, dismantling).

This toolkit makes it possible to answer more effectively to the different project needs. One can anticipate requests by promptly performing sensitivity analyses to respond to emerging issues. This solution no longer fits into traditional sequences. Indeed, the parallelization of calculations allows faster design loops (sensitivities, propagation of uncertainties...).

Keywords

CAD, MCNP, 3D Meshes, Radiological Inventory Mock-Up, 3D Neutron Activation Analyses

Louis Sgandurra*, Nicolas Chapoutier, Matthieu Culioli, 1 Framatome, 2 Rue Professeur Jean Bernard 69007 Lyon France *email: louis.sgandurra@framatome.com

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

17:00 Multiple gas-liquid flow regime computational modelling for nuclear reactor thermal hydraulics

In multiphase gas-liquid flows multiple flow regimes exist, each with a different arrangement of the phases and morphology of the interfaces separating them. Many of these flow regimes, as well as mixed and transition conditions, can be found in nuclear thermal hydraulics, often in scenarios of major safety relevance. The talk will introduce the generalized multifluid modelling approach (GEMMA), developed to predict multiple regimes and complex mixed and transition conditions, where dispersed and large scale interfaces co-exist. GEMMA aims at overcoming current limitations of computational fluid dynamics (CFD) modelling to selected regimes and is based on the implementation of a resolving-like large interface model in an Eulerian-Eulerian multifluid solver. The talk will focus on development and application of GEMMA to cocurrent stratified flows and flow regime transition in horizontal pipes. Co-current stratified flows can occur during loss of coolant accidents and lead to pressurized thermal shock and counter-current flow limitation conditions. With turbulence suppression modelled at the large horizontal interface, the model predicts the stratified regime with accuracy. Further application to the detection of slugs, a common issue in the transport of multiphase mixtures, will be shown. Flow regime transition in a horizontal pipe, fundamental in phenomena such as boiling, is also predicted. The model, starting from a bubbly flow, detects the formation of large plugs and slugs and the transition to stratified conditions (Figure 1). Future developments, such as extension to heat and mass transfer processes and transition from continuous to dispersed regimes, are also discussed.



Figure 1. Air volume fraction distribution from the top of a horizontal pipe in the (from left to right) bubbly, plug, slug and stratified flow regime.

Keywords

Nuclear thermal hydraulics; multiphase flows; computational fluid dynamics; flow regime transition; multifluid modelling.

Marco Colombo, Department of Mechanical Engineering, University of Sheffield, Sheffield S10 2TN, UK m.colombo@sheffield.ac.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 1 THURSDAY 7 APRIL

17:40 **Localised reduced order modelling of the angular dimension of the Boltzmann transport equation using proper orthogonal decomposition**

Computational modelling of the neutron distribution within nuclear reactors involves solving the Boltzmann transport equation (BTE). Due to the dimensionality of the equation, high-resolution models can become too computationally expensive to run in a reasonable time. Reduced order modelling (ROM) allows this issue to be counteracted by reducing the dimensionality of the discretised equations.

One such method is Proper Orthogonal Decomposition (POD), which projects the governing equation onto an optimised set of basis functions generated from existing solutions, reducing the computational cost of further solutions. This presentation focuses on the application of POD to the angular dimension of the BTE. It describes modifications to the standard angular POD method, which are intended to improve the accuracy and solver stability of the method.

Previous implementations of POD in angle used continuous, global functions to describe the angular flux distribution. Here, we propose a localised angular ROM, constructed by partitioning the space-angle phasespace and generating independent, optimised angular basis function sets for each partition. These sets are each optimised to represent the neutron flux distribution in a particular partition of space and angle, rather than the entire domain. Thus, fewer basis functions are required to achieve a given level of accuracy.

Two numerical examples are presented to demonstrate the efficacy of these methods - a duct problem involving advection only, and the Watanabe-Maynard problem, which also includes significant scattering. In both cases, it is shown that the method reduces the angular flux error significantly for a given computation time.

Keywords

Boltzmann Transport Equation, Reduced Order Modelling, Proper Orthogonal Decomposition

*Alex Hughes**, *Andrew Buchan*, 1 School of Engineering and Materials Science, Queen Mary University of London, London, England *email: a.c.hughes@qmul.ac.uk



Angular flux distribution at a point in the Watanabe-Maynard problem.

Top to bottom: S30 full order solution, standard angular POD, discontinuous adaptive angular POD.

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

ABSTRACTS

DAY 2 FRIDAY 8 APRIL

SESSION 4: REACTOR PHYSICS, RADIATION TRANSPORT AND THERMAL HYDRAULICS: PART 2

09:35 Thermal hydraulics research relevant to current and next generation nuclear reactors

The purpose of the talk is to discuss thermal hydraulics modelling challenges associated with a number of reactor designs while summarising recent research carried out in our research group at the University of Sheffield. We first discuss modelling and simulation tool developments addressing both high-fidelity simulations and multi-scaling modelling. We then provide an overview of studies of liquid metal heat transfer relevant to sodium- and lead-cooled fast reactors, and mixed convection heat transfer encountered in passive cooling of all reactor types in general and supercritical water-cooled reactor in particular. Finally, we discuss some recent work carried out in supporting the safe operation of the Advanced Gas-cooled Reactors (AGRs) unique to and currently in operation in the UK.

Keywords

Thermal Hydraulics, DNS, Advanced Reactors.

Shuisheng He, Department of Mechanical Engineering, University of Sheffield, Sheffield, UK s.he@sheffield.ac.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

10:00 An Autoencoder-based Reduced-Order Model with Domain Decomposition applied to Neutronics in Reactor Physics

Modelling Neutron behaviour within a real reactor can be computationally expensive due to the large number of degrees of freedom that can be required to model them accurately. Reduced-Order Modelling (ROM) is a technique that has been proven to reduce this cost for modelling nuclear reactors, using the traditional Proper Orthogonal Decomposition method (POD) and the more recently developed autoencoders. ROM achieves this computational reduction by splitting the process into offline/online stages where the computationally demanding parts are performed in the offline stage, which can be very expensive depending on the system being solved.

Domain Decomposition is a method by which a large problem can be split into multiple problems where the smaller problems are iterated over until convergence. The standard structure of a reactor forms a natural hierarchy that can be used as sub-domains within domain decomposition; The reactor core can be decomposed into fuel assemblies, and these can be further decomposed into fuel rods. This method has been utilised with POD on a 1D reactor where it was proven that a similar accuracy can be established, with the potential of a less computationally demanding offline stage and online stage. Presented here is a method of utilising Domain Decomposition with autoencoder-based ROM applied to a 2D multi-group neutron transport problem. This method is compared with the standard global methods and the POD-based method previously utilised.

Keywords

Reduced-Order Modelling, Autoencoder, Domain Decomposition, Neutron Transport

Toby R.F. Phillips*, **Claire E. Heaney**, **Christopher C. Pain**, Applied Modelling and Computation Group, Department of Earth Science and Engineering, Imperial College London, London, SW7 2AZ, United Kingdom *email: t.phillips18@imperial.ac.uk

Brendan S. Tollit, Paul N. Smith, Jacobs, King's Point House, Queen Mother Square, Poundbury, DT1 3BW, United Kingdom

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

10:20 WIMS and MONK Modelling of the NuScale SMR on the MCSAFER Project

One aim of the MCSAFER project is to compare traditional and advanced reactor physics methods for analysing SMR designs. Four SMR designs are considered on the project: CAREM (CNEA), SMART (KAERI), Nuward (CEA) and NuSCALE (NuScale). Jacobs is one of thirteen organisations participating in the project and will provide analysis of the NuScale design using ANSWERS software. This will provide a comparison of the deterministic, 3D whole core capability in the WIMS code with the Monte Carlo approach adopted in the MONK code.

A new depletion solver is being developed for use with the WIMS and MONK codes to provide improved burnup capability. The solver includes advanced numerical methods, including the Chebyshev rational approximation method (CRAM). The new solver will provide improved accuracy and time-stepping for burnup calculations.

Coupled neutronic and thermal-hydraulic analysis will be used to perform the burnup calculations. The ARTHUR module has been developed to provide sub-channel thermal-hydraulic analysis for the WIMS and MONK codes. ARTHUR is already implemented in the WIMS code and will be integrated into the MONK code for the MCSAFER analysis.

Coupling to system thermal-hydraulic behaviour is required for accident analysis. The FCP (Fortran-C-Python) method has been developed to couple ANSWERS software to third-party software for multi-physics analysis. The FCP methodology is described and will be used to couple WIMS to the TRACE system thermal-hydraulics code for transient analysis on the MCSAFER project.

Keywords

MCSAFER, SMR, NuScale, WIMS, MONK

Magda Stefanowska*, Paul Smith, Brendan Tollit, Will Ferguson, Alan Charles, Andy Smethurst, Peter Smith, Simon Richards, Jacobs, Clean Energy Ltd, Dorchester, United Kingdom *email: Magda.Stefanowska@jacobs.com

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

10:40 Modelling flows in nuclear fuel rod bundles using automatic code generation

Within the AMCG, there is the development of a finite-difference fluid solver for pressurized water reactor thermal hydraulics analysis. This uses a pressure-based method to solve the incompressible Navier-Stokes equations for single phase flow. This solver is being developed on Devito - a Python package for code generation of finite difference stencils.

Devito generates highly optimized parallel C++ code for several computing platforms including GPUs, CPUs and clusters. These features support the project's aim, which is perform large scale simulations with fast execution times on different architectures.

Additionally, the high-level language which integrates with SymPy allows the partial differential equations to be expressed in a readable format. In this work, we present the validation of this fluid solver against PWR rod bundle tests: the 7 x 7 PNL tests and the Weiss et al. two 14 x 14 assembly tests. The rod bundles are represented as a porous medium which simplifies the geometry and reduces the computing time. Other models used include a turbulence model and a pressure drop model. Alongside this, numerical test cases will be presented to verify the fluid solver's numerical methods. These will demonstrate the solvers accuracy as a general-purpose fluid solver.

Keywords

Code-generation, Thermal hydraulics, Porous-medium

Kenechukwu M. Nwegbu*, Claire E. Heaney, Alan V. Jones, Gerard J. Gorman, Christopher C. Pain and Paul N. Smith, Applied Modelling and Computation Group, Imperial College London, UK *email: k.nwegbu19@imperial.ac.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

ABSTRACTS

DAY 2 FRIDAY 8 APRIL

SESSION 5: APPLICATION OF MULTIPHYSICS, THERMAL HYDRAULICS AND WASTE

11:15 Data Learning: Integrating Data Assimilation and Machine Learning for reliable AI models

This work fits into the context of digital twins, which are usually made of two components: a model and some data. When developing a digital twin, many fundamental questions exist, some connected with the data and its reliability and uncertainty, and some to do with dynamic model updating. To combine model and data, we use Data Assimilation (DA). DA is the approximation of the true state of some physical system by combining real-world observations with a dynamic model. DA models have increased in sophistication to better fit application requirements and circumvent implementation issues. Nevertheless, these approaches are incapable of fully overcoming their unrealistic assumptions. Machine Learning (ML) shows great capability in approximating nonlinear systems and extracting meaningful features from high-dimensional data. ML algorithms can assist or replace traditional forecasting methods. However, the data used during training in any ML algorithm include numerical, approximation and round off errors, which are trained into the forecasting model. Integration of ML with DA increases the reliability of prediction by including information in real time and with a physical meaning. This talk introduces Data Learning, a field that integrates Data Assimilation and Machine Learning to overcome limitations in applying these fields to real-world data. We present several Data Learning methods and results for some test cases, though the equations are general and can easily be applied elsewhere.

Keywords

Al, Digital twins, Data Assimilation, Machine Learning, Data Learning

Rossella Arcucci

Department of Earth Science and Engineering, Imperial College London, UK / Data Science Institute, Imperial College London, UK email: r.arcucci@imperial.ac.uk

Abstract

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

11:40 **Progress with the THOR rig – Installation and Commissioning**

The Nuclear Futures Institute of Bangor University is in the process of commissioning the Thermal-Hydraulics Open-access Research Facility (THOR) at Menai Science Park (M-SParc) on Anglesey, North Wales during the spring/summer 2022. THOR was conceived to provide a fundamental platform to serve the region's aspirations within the nuclear engineering research field and is sponsored by the Sêr Cymru programme through the Welsh European Funding Office (WEFO) under the European Development Fund (ERDF). Through a step-wise, flexibly upgradeable approach, THOR deploys water-steam Thermal-Hydraulics (TH) experimentation capability that can be exploited to the ends of local up-skilling, cutting-edge TH research as well as rig and instrumentation development in support of large-scale loop projects, e.g., the National Thermal Hydraulics Facility as led by NNL and CHIMERA by the UKAEA.

THOR commissioning is also conducted in a step-wise manner, initially at lower system temperatures and pressures, to successively approach operation at full system parameters of about 205 °C and 16 bar. The talk will relate the basics of THOR design together with a report of experiences from loop installation and early commissioning.

Keywords

Thermal-hydraulics, experimentation loop, commissioning

Marcus Dahlfors, Nuclear Futures Institute, Bangor University, Bangor, Gwynedd, UK email: m.dahlfors@bangor.ac.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

12:00 Modelling of intensified extraction separations for spent nuclear fuel reprocessing

Reprocessing of spent nuclear fuel reduces the volume and toxicity of radioactive waste and can improve the sustainability of nuclear power generation. A common process for the separation of actinides and lanthanides is solvent extraction,. Recent developments have shown that solvent extractions in smallscale channels can intensify the separation process and enhance the mass transport rates. In addition, they enable the use of non-organic solvents for the extractions, which further improves the safety and sustainability of the process.

Results will be shown on the extraction of uranium, lanthanides and their mixtures in small-scale channels using both organic solvents and ionic liquids. Numerical models have been developed to predict the mass transfer and extraction, which take into account the details of the two-phase flow patterns in the channels. The findings can be used to design and optimise spent fuel reprocessing flowsheets based on intensified channel extractors, which demonstrate reduced solvent usage and improved safety compared to conventional contactors.

Keywords

Solvent extractions; separations; reprocessing; intensification; CFD modelling

Panagiota Angeli*, **Eric Fraga**, **Dimitrios Tsaoulidis**, Department of Chemical Engineering, UCL, London, UK *email: p.angeli@ucl.ac.uk

Dimitrios Tsaoulidis, Department of Chemical and Process Engineering, University of Surrey, UK

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

12:20 Design of micro-analytic detector system for nuclear waste

Decommissioning nuclear power plants is a complex and expensive process. In the case of unexpected scenarios, such as the decommissioning of the Fukushima Dai-chi Nuclear Power Plants, significant amounts of waste, such as fuel debris, structural materials, rubble, soil, and adsorbents for treating contaminated water, may need to be analysed. Detecting the presence of radionuclides is essential for the efficient and safe treatment and disposal of this waste. This motivates the development of fast and sensitive sensor systems for detection, monitoring, and assessment.

Such systems are based on specific detector technology. In this work, thermal lens microscopy (TLM) is considered. TLM can detect the presence of radionuclides and may discriminate between different radionuclides. The detector measurements are subject to uncertainty and there are limits to the detection. Designing an analytic system must take uncertainty and limits into account. The resulting problem is one of design under uncertainty.

A nature inspired optimization method, mimicking the propagation of strawberry plants, is used to solve the design problem. The aim of the design procedure is to generate a design for a micro total analytic system that can be implemented as part of a lab on a chip for portability and minimal cost. The objectives for the optimization procedure are minimisation of the number of false readings while maximising the detection capabilities. Results illustrate the trade-offs between these two conflicting criteria and the effectiveness of the optimization procedure in obtaining good designs

Keywords

Microdevices; Radionuclides; Solvent extraction; Detection system design; Stochastic optimization; Design under uncertainty, Thermal lens microscopy.

Miguel Pineda, Eric Fraga, Panagiota Angeli, Dimitrios Tsaoulidis, Department of Chemical Engineering, UCL, London, UK *email: m.pineda@ucl.ac.uk*

Dimitrios Tsaoulidis, Department of Chemical and Process Engineering, University of Surrey, UK

Takehiko Tsukahara, Laboratory for Advanced Nuclear Energy, Tokyo Tech, Japan

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

12:40 **Project FAITH Fuel Assembly Incorporating Thermal Hydraulics** - off-site modular manufacture digital twin for fast reactor experiments

Project FAITH was an activity funded under the UK Department for Business, Energy & Industrial Strategy (BEIS) nuclear Innovation programme that ran from June 2019 through to December 2021. Its aim was to begin to address the shortage of UK facilities and the loss of sodium expertise in the UK while building upon the existing UK fuel R&D capability. During the project we explored the following four themes:

- 1. Off-site modular manufacturing
- 2. Design, and manufacture and deliver modular experimental test rigs
- 3. Develop R&D expertise in thermal hydraulics covering modelling and experimentation and finally,
- 4. Leverage state of the art digital technologies to assure the operation of the integrated experimental and modelling capability throughout its lifetime

The digital stream of project FAITH brought together the R&D and modular manufacture to create a capability that works together as a whole. Our goal was to develop new ways to manage the asset(s), both the physical asset and the data they generate across the lifecycle. Project FAITH provided an ideal test bed for digital technologies in that it represents a small, self-contained project but anyway requires most of the same considerations as a much larger project where it would be much more challenging to be implemented and thus to understand and quantify the benefits.



Keywords

Digital Twin, fast reactors, Internet of Things,

Mark Bankhead, National Nuclear Laboratory, Warrington, Cheshire, United Kingdom email: mark.bankhead@uknnl.com

Jamie Willgress, Cammell Laird Birkenhead, Merseyside, United Kingdom

Bruno Merk, University of Liverpool Liverpool, Merseyside, United Kingdom

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

SESSION 6: APPLICATION OF NUCLEAR MODELLING TO SIMULATION OF COVID-19 TRANSMISSION

14:00 Validation of modelling and simulation: linking data, methods and needs

The programme of work of the Nuclear Energy Agency's (NEA) Nuclear Science Committee (NSC) covers various aspects of methods, tools and data for validation of modern modelling and simulation. Much of the work organised into development of benchmarks, where participants perform either code to code verification, or code to experiment exercises. These benchmarks attract a wide variety of participants, ranging from reactor designers to graduate students, testing the latest developments in modelling and simulation. To provide experimental evidence for validation, the NEA collects, preserves and disseminates experimental data in different domains, including reactor physics, shielding, criticality safety, fuel performance, spent fuel isotopic composition, and thermal-hydraulics. The data are widely used for international activities involving validation of current and new calculational schemes, including computer codes and nuclear data libraries, for assessing uncertainties, confidence bounds and safety margins, and to record measurement methods and techniques.

With new demands from various nuclear stakeholders and recent advances in theory, methods, and computing power all the pieces are in place for the paradigm to shift in validation, which requires tight integration between the nuclear data, modelling and benchmark disciplines. The NEA has been at the forefront of organising peer-reviewed benchmarks and developing relational databases that contain metadata and physics sensitivities, which allow experts to identify experiments to support validation for their applications. Linking these databases directly with the nuclear data development community offers a testing pipeline that can inform both users and data evaluators of biases and the impact of change in real time. The Nuclear Science Committee and Data Bank are working together to establish a central international reference for sensitivity data that will be directly linked to the Joint Evaluated Fission and Fusion (JEFF) library and will be available to other projects through the Working Party on International Nuclear Data Evaluation Co-operation (WPEC). All communities are invited to contribute, with or without detailed models and proprietary information, to ensure that their needs are addressed in the development of the next generation of modelling and simulation systems that employ nuclear data.

Keywords

Benchmark, Integral experiments, Modelling, Nuclear data, Validation

Tatiana Ivanova, Organisation of Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA) email: Tatiana.ivanova@oecd-nea.org

Michael Fleming, OECD NEA Data Bank

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

14:40 Data-driven Modelling of Covid-19 Transmission Risk in Schools

Air pollution and airborne virus transmission are ubiquitous concerns in environmental scenarios, which is particularly important after the outbreak of the coronavirus disease 2019 (Covid-19). Ventilation is an effective strategy to improve air quality and mitigate virus infection risk by introducing outdoor air into buildings. At ventilated spaces, it is a challenging task to obtain a theoretical understanding of the airborne spread of diseases through droplets and aerosols since such phenomenon commonly exhibits turbulent or pseudo-turbulent behavior at a wide range of scales. An accurate prediction is critical to assess the performance of ventilation and provide the transformative applications to enhance the air quality at indoor and outdoor spaces.

Large-eddy simulation is applied to investigate the ventilation in primary school by using the open-source computational fluid dynamics (CFD) code Fluidity, where individual classrooms in the school are modelled and the air exchange with outdoor spaces is reproduced. The model solves the Navier-Stokes equation for unsteady, incompressible and viscous flow with an advanced adaptive mesh capability. The simulation results are used to explore the mechanisms of Covid-19 infection and ventilation in thermally stratified environment by monitoring the components in air, such as carbon oxide (CO2), particle matters (PM) and virus. Based on the CFD dataset obtained, AI modelling is performed to establish a data-driven model that is adopted to predict the air quality in the school by Generative Adversarial Networks (GAN). Furthermore, the integration of CFD and AI modelling will address the optimalization of combined ventilation and energy use in buildings.

Keywords

Covid-19 infection; Ventilation; Large-eddy simulation; AI modelling, Energy use

Boyang Chen*, Christopher Pain, Pablo Salinas,

Claire Heaney, Department of Earth Science and Engineering, Imperial College London, London, UK *email: boyang.chen16@imperial.ac.uk

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

DAY 2 FRIDAY 8 APRIL

15:00 A Multi-Physics Model for the Prediction of Coronavirus Inactivation in Populated Rooms using 222 nm Far-UVC

Transmission of SARS-CoV-2 by aerosols has played a significant role in the rapid spread of COVID-19. Indoor environments pose a particular risk and, consequently, many efforts have focused on ways to disinfect air. Recently it was realised that 222 nm UVC light (far-UVC) can be employed to disinfect air of populated rooms. Unlike standard 254 nm UVC, far-UVC is minimally hazardous to the skin and eyes, and therefore is safe to use around humans while still being an effective antimicrobial. This is potentially significant in the fight against all airborne diseases as it requires no movement or stiring of air. It can therefore be used effectively in poorly ventilated buildings, and mitigates the potential to spread the virus by forcibly agitating the air to transport it to other removal mechanisms.

Quantifying the efficacy of far-UVC inactivation of SARS-CoV-2 within a room is complicated. Each room is unique, with its own atmospheric conditions with spatially varying UVC intensities. Assessing the transport and inactivation of virus is therefore a multi-physics (radiation-fluids) problem, perhaps best suited to computational modelling. We present the first high-fidelity model for simulating coupled radiation transport and CFD for such a purpose. The framework (WYVERN) has demonstrated far-UVC to provide effective removal of virus when used with ventilation of simplified rooms (up to 85%), and we present its use in complex scenarios of rooms used for hospitality. Again it demonstrates high efficacy in virus removal but also it advises on the placement of lamps for improved air disinfection.

Keywords

Multiphysics Simulaton, Computational Modelling, Far-UVC, COVID-19

A. G. Buchan*, Queen Mary University of London, London, UK email: a.buchan@qmul.ac.uk

L. Yang, Cranfield University, Bedford, UK

K. D. Atkinson, Ontario Tech, Ontario, Canada

D. Welch, D. J. Brenner, Columbia University, New York, USA

NUCLEAR MODELLING 2022

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

BIOGRAPHIES

Professor Ali Tehrani, CEng, FINucE, FIMechE

Office for Nuclear Regulation

Professor Tehrani 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 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.

Dr Rossella Arcucci

Dr Rossella Arcucci (https://www.imperial.ac.uk/people/r.arcucci) is a Lecturer in Data Science and Machine Learning at the Department of Earth Science and Engineering, Imperial College London. Rossella has been with the Data Science Institute at Imperial College since 2017, where she has created the Data Assimilation and Machine Learning (DataLearning) Working Group. She is the elected speaker of the Artificial Intelligence Network of Excellence at Imperial College London - https://www.imperial.ac.uk/artificial-intelligence/people/ where she represents >240 academic working on AI. She collaborates with the Leonardo Centre at Imperial College Business School,

where she contributes to the development of integrative, just and sustainable models of economic and social development by discovering, testing and diffusing new logics of business enterprise.

During the past two years, she has worked as volunteer for the RAMP Task 7: From exhalation to inhalation, COVID-19 infection risk indoors.

The models Rossella has developed have produced impact in many applications such as finance (to estimate optimal parameters of economic models), social science (to merge twitter and pooling data to better estimate the sentiment of people), engineering (to optimise the placement of sensors and reduce the costs), geoscience (to improve accuracy of forecasting), climate changes and others. She has developed accurate and efficient models with data analysis, fusion and data assimilation for incomplete, noisy or Big Data problems, always including uncertainty quantifications and minimizations.

She works on numerical and parallel techniques for accurate and efficient Data Assimilation and Machine Learning models. Efficiency is achieved by virtue of designing models specifically to take full advantage of massively parallel computers.

Degree and master's degree in mathematics. She finished her PhD in Computational and Computer Science in February 2012. She received the acknowledgement of Marie Sklodowska-Curie fellow from European Commission Research Executive Agency in Brussels the 27th of November 2017.





BIOGRAPHIES

NUCLEAR MODELLING 2022

5th Annual Modelling in Nuclear Science and Engineering Seminar

7–8 April 2022 • Imperial College London

Dr Mark Bankhead

Dr Mark Bankhead is a scientist with over 19-years of experience working in the nuclear industry. My work involves the development of complex mathematical models of chemical behaviour. I'm a technical lead with experience of leading several multi-disciplinary research projects. This ranges from modelling the behaviour of atoms, through to understanding the impact of chemistry on process behaviour. Since 2006 I've led projects developing of scientific computing for NNL and this for example has led me to play an active in digital for Nuclear Industry Association and the UK's Nuclear Innovation Programme helping the nuclear industry adopt digital twin technology. Outside

of digital, I'm a chartered chemistry and my current research interests range from plant chemistry for decommissioning applications and nuclear fuel modelling. I'm actively involved in collaborative projects with Sellafield Ltd and NDA (decommissioning) and NEA on fuel modelling and thermodynamics.

Dr Andrew Buchan

Dr Andrew Buchan is Senior Lecturer within the School of Engineering and Materials Science at Queen Mary University of London. He obtained his PhD at Imperial College London in 2006 in computational nuclear engineering. He has published around 50 peer reviewed journal and conference articles covering areas of mathematical modelling for neutron transport, single and multi-phase fluids and couple-physics simulation for reactor physics, accident prediction, and sensitivity analysis. In addition to nuclear engineering his interests include spectral wave modelling for oceans, pollutant dispersion around coasts, and more recently the inactivation of microbials in air and water systems using UVC light.

Boyang Chen

I am a Research Assistant at Applied Modelling and Computation Group (AMCG), Department of Earth Science and Engineering, Imperial College London. I am currently working on the UKRIfunded INHALE Project (Health assessment across biological length scales for personal pollution exposure and its mitigation) and the EPSRC-funded CO-TRACE project (Covid-19 transmission risk assessment case studies – education establishments), where I undertake the work on numerical modelling and AI prediction of airborne disease spread at indoor spaces. My area of expertise is Computational Fluid Dynamics (CFD) and my research mainly focuses on multiphase flows,

including the suspension of solid particles in the air, sediment transport in rivers and airborne spread of virus through aerosols. During my PhD, I am the main contributor to the home-made CFD FORTRAN code Hydro3D and developed novel Eulerian-Lagrangian framework applied to solve environmental flows.







5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

Christopher Connolly

Christopher Connolly has a Masters degree in Chemical and Process engineering from the University of Strathclyde, including nuclear engineering. His final year university project involved producing a program to design and model a distillation column to meet a user's specification, for which he received the Scottish Branch Prize from the IChemE.

Following University he took on a 2-year Knowledge Transfer Partnership (KTP) role with NNL and Strathclyde where he developed a steady state hybrid-mechanistic model of the calciner in the Vitrification Test Rig (VTR); this has been used to identify an issue with the primary off-gas coupling seal and led to a re-design.

Christopher then came back to NNL in 2019 and since becoming a permanent member of the Chemical and Process Modelling team he has worked on a variety of projects including creating the high-profile Sim Plant tool for BEIS as part of the Advanced Fuel Cycle Programme. Sim Plant uses process modelling to flowsheet future fuel reprocessing plant options and estimate footprint, sizing and outputs. The project has led to Christopher presenting the work at BEIS, the EU Horizon 2020 conference and the 2021 Waste Management Symposium.

More recently, Christopher has been part of NNL's team working on Nuclear-Derived Hydrogen, tasked with modelling production process options including alkaline electrolysis, PEM, solid oxide steam electrolysis and thermochemical cycles - while supporting collaborative projects with partners in the UK Gas Network.

Dr Marcus Dahlfors

Bangor University

Marcus joined the Nuclear Futures Institute of Bangor University 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 20 odd years, Marcus has worked with LWR analysis and safety including various R&D aspects. Specialisms also include reactor new build and permissioning with regulatory interaction in the UK regime; development, testing and verification of nuclear reactor simulation software; BWR nuclear fuel & core design; core monitoring; reactor physics and thermal-hydraulics related measurements as well as in-core fuel management.

Outside of LWR technology, Marcus has pursued academic research as well as industrial R&D focused on systems operating with fast neutrons. Within this context, he has worked with physics simulations of sub-critical, lead-cooled accelerator-driven systems and molten-salt fast reactor concepts.

Ahmadreza Farrokhnia

Ahmadreza Farrokhnia is a Post doctoral Research Associate for the Nuclear Graphite Research Group at the University of Manchester. His works involves the modelling of irradiation inducted changes in nuclear graphite moderated cores.

He completed his PhD in Nuclear Engineering graduating in 2021 at the same university. His PhD project looked at Large scale Modelling of graphite moderated nuclear reactors.





BIOGRAPHIES

NUCLEAR MODELLING 2022

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

Dr Thomas Haynes

Lecturer in Nuclear Engineering, University of East Anglia

I am a computational modeller focusing upon developing novel local (finite element) and non-local (phase-field and peridynamics) techniques to understand material and component failure at the engineering scale. I have a particular interest in applying these techniques to applications in the nuclear energy sector. I have previously modelled pellet-clad interaction in advanced gas-cooled reactors using finite element analysis; failure of composite SiC/SiC claddings for accident tolerant fuels using peridynamics; coated particle (TRISO) fuels for advanced modular reactors using peridynamics; and, oxidation of the zirconium-based alloys current employed in light water reactors.

Shuisheng He

Shuisheng He Chair in Thermofluids in Department of Mechanical Engineering at University of Sheffield. He is a chartered engineer (CEng) and Fellow of the Institution of Mechanical Engineers (FIMechE). He did his PhD in the Nuclear Research Group at University of Manchester and was Reactor Heat Transfer Analyst at British Energy (now EDF Energy) between 1998-2002, before starting his academic career in 2002. Shuisheng's research focuses on thermal hydraulics modelling for liquid-metal, supercritical-water and gas-cooled reactors using high fidelity DNS and LES as well as conventional RANS CFD. His group has developed several in-house CFD codes including the

DNS/LES package CHAPSim. They have recently developed a new concept coarse-grid CFD referred to as Sub-channel CFD. Shuisheng is Leader of UK Fluids Network Special Interest Group (SIG) in Nuclear Thermal Hydraulics (https://fluids.ac.uk/ sig/Nuclear), and Chair of the Collaborative Computational Project in Nuclear Thermal Hydraulics (https://ccpnth.ac.uk/). He routinely provides expert review/consultancy for EDF Energy.

Robert Hughes

Robert Hughes is a process modeller in the nuclear industry having joined NNL as a 'Chemical with Nuclear Engineering' graduate from Imperial College 6 years ago. In that time, he has developed complex dynamic models and steady state flowsheets for a range of processes – mainly on the Sellafield site (including evaporators, vitrification plants, nuclear fuel storage ponds etc.).

Recent work has focussed on post operational clean out of plants reaching the end of their operational lives at Sellafield. The effluents from this clean out will present challenges to downstream treatment plants and Robert's work uses dynamic models to optimise treatment of these effluents. This will allow effluents to be processed in a safe and responsible manner which minimises the volume of nuclear waste requiring long term storage.

Another of his research interests is modelling of potential radioactivity releases during medium-term storage of spent nuclear fuel. His work is aimed at diagnosing and avoiding such releases. He has presented this 'Activity Release Model' at several international conferences, along with the results of another fuel dissolution model developed in worked funded by the EU (DisCo).

He has also recently performed work for the UK government which will allow high level optioneering of future UK nuclear fuel cycles. The tool 'Sim Plant' will be used to compare the size and cost of next generation nuclear reprocessing flowsheets.

He currently provides a lecture on process modelling in the nuclear industry as part of the 'Dynamic Behaviour of Process Systems' course at Imperial College London.





5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

Dr John Jones

Dr Jones is Technical director of Fairlie Associates. Previously he had technical lead responsibilities for the area of fuel and core at the Office for Nuclear Regulation and also for LWR fault analysis at EdF Energy. He was responsible for the analysis to support the first fuel reload at Sizewell B and he taught fluid mechanics at the Royal Naval College, Greenwich. His PhD thesis was on the topic of fuel clad ballooning and he represented UK on a number of related international initiatives including editing the updated draft of the CSNI state-of-the-art report on LOCA; which is due to be published shortly.

Linfeng Li

PhD Student, Imperial College London

I am a 2nd year PhD student from the Department of Earth Science and Engineering at Imperial College London supervised by Jiansheng Xiang and Chris Pain. My PhD project is on developing advanced simulation methods for fluid-induced vibration in nuclear engineering. My general research interests include finite element methods and AI modelling. Before joining Imperial in 2020, I got my BEng (2017) and MEng (2020) degrees both from Xi'an Jiaotong University.

Andrew Little

Andrew Little has worked for the UK Ministry of Defence as a senior lecturer in nuclear emergency consequence assessment for the last 10 years. He has research interests in atmospheric and marine dispersion modelling and dose consequence assessment. He is currently studying for a PhD in Marine Dispersion Modelling at Imperial College London.

Fulvio Mascari

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 he is investigating severe accident issues in PWR and BWR reactor types, the analyses of the capability of best estimate thermal-hydraulic system code to simulate the main phenomena typical of advanced light water reactor, as small modular reactor, and the thermal-hydraulic phenomena typical of fusion reactor, the analyses of the scaling issues, the analyse of the capability of severe accident code to simulate degradation phenomena, and the application of the probabilistic method to propagate input uncertainty in deterministic safety analyses.

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.









NUCLEAR MODELLING 2022

5th Annual Modelling in Nuclear Science and Engineering Seminar

7-8 April 2022 • Imperial College London

Dr. Simon Middleburgh

Dr. Simon Middleburgh is a Reader in Nuclear Materials at Bangor University (https://nubu.nu/ materials/simon-middleburgh/). He 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 in a timely manner required by the nuclear industry.

Simon has had 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. Paul Nevitt

Dr. Paul Nevitt is the Science and Technology Director for the UK National Nuclear Laboratory (NNL). Paul is responsible for definition and delivery of the science and technology agenda across the four focus areas within the laboratory of Clean Energy, Environmental Restoration, Health and Nuclear Medicine and Security and Non-Proliferation.

Previously Paul was the NNL Technical Director for the UK Advanced Fuel Cycle Programme (AFCP), responsible for the technical and strategic outcomes of this significant programme of investment working with over 100 UK organisations. Prior to AFCP, Paul was Chief Technologist and Senior

Technical Advisor within the Nuclear Innovation and Research Office (NIRO) providing advice to UK Government on all aspects of nuclear research and innovation.

Paul received both his bachelor's degree in Chemistry and a PhD in Actinide Surface Chemistry from Cardiff University.





BIOGRAPHIES

NUCLEAR MODELLING 2022

5th Annual Modelling in Nuclear Science and Engineering Seminar

7–8 April 2022 • Imperial College London

Rebecca Newson

Rebecca Newson has a degree in Physics from the University of Bath and joined Quintessa after graduating in 2017. She currently works as a Senior Consultant within Quintessa's Assessment and Decision Support team, supporting UK and international clients with development, implementation and application of numerical models.

Rebecca works primarily in the areas of post-closure safety assessment for radioactive waste disposal and supporting graphite safety cases for the UK's fleet of operational Advanced Gas-Cooled Reactors (AGRs). She has developed radionuclide transport models in GoldSim and AMBER (Quintessa's compartment modelling software) to assess the safety of deep and near-surface disposal concepts in Norway, Canada, Sweden, Switzerland and the UK.

Rebecca is also leading Quintessa's involvement in the European BEACON project, aimed at modelling the thermo-hydromechanical evolution of bentonite components in engineered barrier systems. She supports EDF Energy in applying statistical modelling techniques and using COMSOL Multiphysics® to understand the evolution of graphite bricks in a reactor core.

Rebecca is an Associate Member of the Nuclear Institute and the Society for Radiological Protection and entered the 2021 NI Young Speakers Competition with a talk entitled 'How (Not) to Predict the Future: Assessing Long-Term Safety of Nuclear Waste'.

Ioannis Nikiteas

I am a final year PhD candidate at Imperial College London, based at the Applied Modelling and Computation Group and supervised by Christopher Pain and Paul Smith. My research focuses on creating high fidelity error estimators to be used in Adaptive Finite Element Methods. These error estimators are optimised for the multi-scale nature of radiation transport phenomena and are capable of driving refinement in both space and angle. In addition, my work focuses on implementing scalable and performant adaptive algorithms capable of running on small local computers to UK's largest HPCs.

Alex Hughes is a postgraduate researcher in the School of Engineering and Materials Science at Queen Mary, University of London. He graduated with a bachelor's degree in Physics from the University of Nottingham in 2018, before moving to QMUL the same year. His research focuses on reduced order modelling of nuclear reactors, with a particular focus on the method of Proper Orthogonal Decomposition and its application to the angular dimension of the Boltzmann transport equation for neutronics modelling. This research aims to develop new and improved methods of reduced order modelling for neutronics applications, with potential uses in the nuclear industry. In addition, the techniques developed may have broader applications within the field of computational modelling. His work has been published in the International Journal for Numerical Methods in Engineering, for which he received a Postgraduate Research Excellence Award from QMUL. He has also presented at several events, including the Universities' Nuclear Technical Forum. He is currently working on his PhD thesis.

Kene Nwegbu

Kene Nwegbu is a 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 Sheeld, then worked as a graduate engineer at Honeywell for a year. Following this, he joining the ESPRC Centre for Doctoral Training in Nuclear Energy Futures in October 2019. His PhD project is exploring using a nite dierence code generation framework for nuclear thermal hydraulics. This is under the supervision of Professor Christopher Pain, Professor Paul Smith, Dr. Gerard Gorman, Dr. Claire Hearney and Professor Alan Jones.







5th Annual Modelling in Nuclear Science and Engineering Seminar

7–8 April 2022 • Imperial College London

Prof Christopher Pain

Prof Christopher Pain (PI and physics lead, ICL) leads the Applied Modelling and Computation Group (AMCG) at ICL. Recipient of the ICL Research Excellence award in 2011 (for high academic achievement and future potential), AMCG is Imperial's largest research group comprising about 60 scientists. He is the director of the data assimilation lab in the Data Science Institute (DSI) at ICL and is co-director of the Centre for AI-Physics Modelling at Imperial-X, leads the modelling for the MEMPHIS (£5M) and MAGIC (£5M) consortia and is PI of Smart-GeoWells (£2M) Newton consortium. Has interests in numerical methods, environmental and engineering fluids (e.g.

multi-phase flows, urban flows). He developed the first Large Eddy Simulation air pollution models, the first 3D tetrahedralbased mesh optimisation and conservative mesh-to-mesh interpolation methods; he was the original developer of the FETCH transient criticality model for nuclear systems; he developed the first Non-Intrusive Reduced Order Model (NIROM) for fluid mechanics. >250 journal papers, supervised 50 PhD students, completed 42 industry and research council grants, h index=51.

Marinos Panayiotou

Marinos Panayiotou is the Digital Products & Services lead at CRA. Marinos joined CRA in 2013 and specialises in safety, risk and reliability helping companies identify and analyse the risks that can impact their assets and business to ensure they are adequately managed for ensuring business continuity. Marinos is now working on creating and deploying safety and risk-based digital solutions to help clients optimise and enhance their processes. He is the designer of CRA's Enterprise Risk Operating System (eROS) and Safety Case powered by Artificial Intelligence (AI).

Toby R.F. Phillips

I am currently working on my PhD thesis titled 'Hierarchical reduced-order modelling applied to neutron transport.' which is funded by the ESPRC Centre for Doctoral Training in nuclear energy.

My research includes involves applying and combining reduced-order modelling, domain decomposition and machine learning methods to neutron transport to model reactor behaviour. The main objective of this research is to reduce the computational cost of modelling reactors, which can be expensive when attempting to model real reactor examples.

Dr Miguel Pineda

Dr Miguel Pineda obtained a BSc in Physics from the University of Los Andes (Merida, Venezuela) and a PhD in Physical Chemistry from Leibniz University Hannover (Hannover, Germany). After his PhD, he worked as a researcher in world-leading interdisciplinary research institutions in Spain, Belgium, and the UK. Dr Miguel Pineda was a Lecturer in Physics at Simon Bolivar University in Venezuela. He joined University College London (UCL) for the first time in 2016. He is currently working on several computational material sciences and catalysis projects and design optimisation of micro-fluidic devices for nuclear waste.











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Eugene Shwageraus

Eugene Shwageraus is a Professor of Nuclear Energy Systems Engineering and Course Director of Nuclear Energy MPhil in the Department of Engineering at the University of Cambridge. He is also a part of the University of Cambridge Nuclear Energy Centre which links and coordinates projects in areas related to nuclear technology, among them advanced reactor concepts as well as safety, waste management, nuclear policy and regulation. Previously, he was an Associate Professor and served as the Head of the Nuclear Engineering Department at Ben-Gurion University in Israel. He also spent two years as a Visiting Associate Professor in the Department of Nuclear Science

and Engineering at MIT and holds a PhD degree from MIT as well. In the course of his career, he was a PI and Co-PI on a number of research projects sponsored by government research organisations, power utilities and private companies. He participated in and was a contributing author to a high-profile interdisciplinary study on "The Future of the Nuclear Fuel Cycle" commissioned by the MIT Energy Initiative. He has long standing academic interests in the development of numerical methods for modelling advanced reactors. In particular, multi-physics coupling of Monte Carlo neutron transport codes. Other projects he took part in include: Light Water Reactor designs for recycling and transmutation of Pu and minor actinides, improving performance of LWRs by using advanced fuels (such as Th and inert fuel matrices) with alternative cladding material (e.g. SiC) and alternative geometries (e.g. annular internally and externally cooled fuel), design of advanced fast gas cooled reactors with super-critical CO2 coolant, design of fast reactors with flexible conversion ratio cooled by sodium, lead as well as molten salt, and fast reactors with low- enriched uranium start-up.

Paul Smith

Paul Smith is the technical director of Jacobs' ANSWERS Software Service. He has worked in mathematical modelling for over 45 years and in the nuclear industry of 38 years. He is also a visiting professor in the Applied Modelling and Computation Group at Imperial College London and in the Nuclear Futures Institute in Bangor University

Magda Stefanowska

Magda Stefanowska (Jacobs) is a Graduate Mechanical Engineer and Physicist. Magda graduated in Physics and Energy Conversion Engineering at Gdansk University of Technology (Poland). Magda joined the ANSWERS team in 2018 where she works as a Reactor Physicist.

As Reactor Physicist/ Engineer Magda has worked on a wide range of problems with main focus on core modelling of various reactor types (PWR, SFR, GFR etc.) using Monte Carlo and Deterministic codes (ANSWERS MONK and WIMS respectively). In addition, Magda supports delivery of MONK and Criticality courses. She is currently involved in is the McSafer project whose aim is to perform coupled neutronic and thermal-hydraulic analysis for NuScale SMR including depletion calculation.







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Dr Rossella Arcucci Lecturer in Data Science and Machine Learning, Imperial College Mr Mark Bankhead NNL Ms Sarah Beacock CEO, Nuclear Institute Dr Matthias Braun Framatome Senior Expert, Framatome GmbH Dr Andrew Buchan Queen Mary University Mr Boyang Chen Student, Imperial College London Dr Marco Colombo Lecturer in Fluid Mechanics, University of Sheffield Mr Christopher Connolly Process Modeller, NNL Dr Marcus Dahlfors Bangor University Dr Steven Dargaville Research Associate, Imperial College London Dr Ahmadreza Farrokhnia University of Manchester Mr Oliver Gamez COMSOL Mr Matthew Gowar Jacobs Dr Thomas Haynes University of East Anglia Ms Claire Heaney University College London Mr Robert Hughes NNL Mr Alex Hughes Student, Queen Mary University Dr Tatiana Ivanova Head of Nuclear Science, OECD, Nuclear Energy Agency Dr Lloyd Jones Fuel Performance Scientist, NNL Mr Alan Jones Imperial College London Dr John Jones Technical Director, Fairlie Associates Mr Linfeng Li Student, Imperial College London Dr John Lillington Chief Technologist Nuclear Reactors, Jacobs Mr Andrew Little Student, Imperial College London Dr Fulvio Mascari ENEA Prof Omar Matar Head of Department of Chemical Engineering, Imperial College London Mr Yuki Narushima Researcher in Sustainability, Lab Hitachi Europe Ltd Dr Paul Nevitt Science and Technology Director, NNL Ms Rebecca Newson Quintessa Mr Giannis Nikiteas Student, Imperial College London Mr Kenechukwu Nwegbu Student, Imperial College London Prof Angeli Panagiota Deputy Head ED&I, University College London Mr Marinos Panayiotou Digital Products & Services Lead, CRA Risk Analysis Mr Toby Phillips Student, Imperial College London

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Dr Miguel Pineda University College London Dr Louis Sgandurra Framatome Prof He Shuisheng Chair in Thermofluids, University of Sheffield Prof Eugene Shwagerus Prof of Nuclear Energy Systems Engineering, University of Cambridge Prof Paul Smith Jacobs ANSWERS Technical Director Mr Miguel Sousa Graduate Consultant, CRA Risk Analysis Ms Magda Stefanowska Reactor Physicist, Jacobs Mr Andrew Sweet Nuclear Physicist, Jacobs Prof Ali Tehrani Imperial College London Ms Panagiota Theodoulou COMSOL Ms Olivia Voyce Physicist, Jacobs Dr Wei Wang Senior Computational Scientist, Science and Technology Facilities Council