Science and Technology Facilities Council

Scientific Computing

# COMPUTING INSIGHT UK 2022

"Sustainable HPC"

**1 - 2 DECEMBER 2022**

**Manchester Central, UK**

**www.stfc.ac.uk/ciuk**

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# INTRODUCTION

We are delighted to welcome you all to Computing Insight UK 2022.

The theme for the conference this year is **"Sustainable HPC"** with sub-themes including "Sustainable Computer and Data Centres", "Sustainability and Systems Administration", "Software Engineering to Improve Code Performance" and "Industry Perspective on Sustainability".

CIUK 2022 will include an exhibition of the latest hardware and software releases plus a full, two day programme of presentations and a series of parallel breakout sessions, including the first annual CoSeC Conference. There will be a student poster competition plus the third instalment of the CIUK Student Cluster Challenge. We will also present our annual Jacky Pallas Memorial Award.

Please take time to visit the CIUK exhibition and we would also like to invite you to join us on the evening of Thursday 1 December – immediately following the CIUK keynote presentation – for the CIUK networking event at Revolucion de Cuba, 11 Peter St, Manchester M2 5QR (*CIUK lanyard and badge required for entry*).

We hope that you enjoy the conference.

All information about the conference can be found on the event website… www.stfc.ac.uk/CIUK.

You can also follow us on Twitter @CompInsightUK (#CIUK2022) and LinkedIn for the latest live updates.


**Need help during the conference?**
**Have a question about the event?**

The CIUK team will be happy to assist.

You can find them at the main reception desk in the foyer or on the exhibition floor… look for the yellow shirts!

You will also find an information screen at the start of the exhibition.

# CIUK 2022 PROGRAMME

The main CIUK 2022 programme will take place in Charter Room 1. Look for the BLUE pull-up banners.


## Day 1 - Thursday 1 December

| | |
|---|---|
| | Session 1: Sustainable Computer and Data Centres |
| | Session 2: Sustainability and Systems Administration |
| | Session 3: ExCALIBUR in Practice |

| TIME | MAIN PROGRAMME | BREAKOUT SESSIONS |
|---|---|---|
| From 08:30 | **REGISTRATION OPEN (Charter Foyer) EXHIBITION OPEN (Gallery)** | |
| 09:15 - 09:30 | *Welcome and Introduction* **Tom Griffin (Director, Scientific Computing, STFC)** | |
| 09:30 - 10:00 | **Dr Peter Oliver (Scientific Computing, STFC)**<br>*Design considerations for an environmentally sustainable datacentre for STFC* | |
| 10:00 - 10:30 | **Pekka Lehtovuori (CSC - IT Center for Science Ltd)**<br>*Reaching zero carbon footprint in HPC operations* | CoSeC<br>Computational Science Centre for Research Communities<br>**Annual Conference 2022**<br>Thursday 1 December @ CIUK 2022<br>10:00-16:00 |
| 10:30 - 11:00 | **Thomas Eickermann (Jülich Supercomputing Centre)**<br>*Towards more sustainable HPC at the Jülich Supercomputing Centre* | |
| 11:00 - 11:30 | **REFRESHMENTS** | |
| 11:30 - 12:00 | **Jacob Newman (University of East Anglia)**<br>*Optimising HPC Workflows: Three Case Studies from a Research Software Engineer's Perspective* | |
| 12:00 - 12:30 | **Gabryel Mason-Williams (Rosalind Franklin Institute)**<br>*DisTRaC: Accelerating High-Performance Data Processing* | |
| 12:30 - 13:00 | **Simon Atack (University of Bristol)**<br>*Creating A Cluster - Going it Alone* | |
| 13:00 - 14:00 | **LUNCH** | |
| 14:00 - 14:30 | **Ed Threlfall (UKAEA)**<br>*Project NEPTUNE - sustainable software for sustainable fusion energy* | |
| 14:30 - 15:00 | **Joseph Hickson, Lewis Sampson and Victoria Smart (Met Office)**<br>*Preparing the Met Office for the next generation of supercomputers* | |
| 15:00 - 15:30 | **Ben Rogers (University of Manchester) and Phil Hasnip (University of York)**<br>*PAX-HPC - Modelling particles at exascale: from atoms to galaxies* | |
| 15:30 - 16:15 | **REFRESHMENTS** | |
| 16:15 - 17:00 | **Martyn Guest (ARCCA, Cardiff University)**<br>*Performance of Community Codes on Multi-core Processors.*<br>*An Analysis of Computational Chemistry and Ocean Modelling Applications* | |
| 17:00 - 18:00 | **Keynote Presentation - Professor Michèle Weiland (EPCC, The University of Edinburgh)**<br>**Net Zero HPC - noble dream or inevitable goal?** | |
| 18:30 - 23:00 | **CIUK 2022 Networking Event**<br>**Revolucion de Cuba, 11 Peter St, Manchester M2 5QR** (*CIUK lanyard and badge required for entry*). | |

## Day 2 - Friday 10 December

| | |
|---|---|
| | Session 4: UKRI Net Zero Digital Research Infrastructure Project |
| | Session 5: Software Engineering to Improve Code Performance |
| | Session 6: An Industry Perspective on Sustainability |

| TIME | MAIN PROGRAMME | BREAKOUT SESSIONS |
|---|---|---|
| From 08:30 | **REGISTRATION OPEN (Charter Foyer) EXHIBITION OPEN (Gallery)** | WHPC WOMEN IN HIGH PERFORMANCE COMPUTING<br>08:30-10:30 |
| 09:30 - 10:00 | **UKRI Net Zero Digital Research Infrastructure Project**<br>09:30 - 09:50 Project Overview **(Martin Juckes)**<br>09:50 - 10:00 HPC-JEEP **(Alastair Basden and Andy Turner)**<br>10:00 - 10:10 IRISCAST **(Jonathan Hays)**<br>10:10 - 10:20 ENERGETIC **(Deepan Bhowmik and Teymoor Ali)**<br>10:20 - 10:30 CARBON-QUANDRI **(Daniel Schien)**<br>10:30 - 11:00 Panel Discussion **(Wim Vanderbauwhede, Justin O'Byrne, Martin Juckes)** | |
| 10:00 - 10:30 | | |
| 10:30 - 11:00 | | Spectrum Scale User Group<br>10:30-12:30 |
| 11:00 - 11:30 | **REFRESHMENTS** | |
| 11:30 - 12:00 | **Ilektra Christidi (Senior Research Software Developer, UCL Advanced Research Computing Centre)**<br>*Coupling the Time-Warp algorithm with a Kinetic Monte Carlo framework for exact distributed simulations of heterogeneous catalysts* | |
| 12:00 - 12:30 | **Elizabetta Boella (Lancaster University & Cockcroft Institute)**<br>*ECsim: a massively parallel Particle-In-Cell code for plasma physics with OpenACC support* | |
| 12:30 - 13:00 | **The Jacky Pallas Memorial Presentation**<br>**Dr Djenifer Kappel (Centre for Neuropsychiatric Genetics and Genomics - Cardiff University)**<br>*The genomic basis for precision medicine in treatment-resistant schizophrenia* | |
| 13:00 - 14:15 | **LUNCH** | |
| 14:15 - 14:30 | **Award Presentation - The CIUK 2022 Student Cluster Challenge and Poster Competition** | UK Research and Innovation<br>**ENERGETIC: A workshop regarding Energy Benchmarking on Heterogeneous Systems**<br>14:00-16:00 |
| 14:30 - 15:00 | **Dr Rosemary Francis (Chief Scientist HPC, Altair)**<br>*Ten Ways in Which Altair is Saving the Planet with HPC* | |
| 15:00 - 15:30 | **Dr Crispin Keable (Senior HPC Architect, Global HPC Strategic Sales, Atos)**<br>*Sustainability issues as we move towards exascale class HPC architectures* | |
| 15:30 - 16:00 | **Laura Foster (techUK)**<br>*Why is HPC integral to becoming a "science and technology superpower?"* | |
| 16:00 | **CIUK 2022 CLOSES** | |

# CIUK 2022 KEYNOTE PRESENTATION


**Professor Michèle Weiland**
Director of Research and Met Office Joint Chair at EPCC, the supercomputing centre at the University of Edinburgh

Twitter: @micheleweiland
Web: https://www.epcc.ed.ac.uk/about-us/our-team/prof-michele-weiland


## "Net Zero HPC - noble dream or inevitable goal?"


**ABSTRACT:** In the face of the climate emergency, the term 'Net Zero' has sprung up in every context of daily life, and HPC is no exception. But how far away are we from achieving Net Zero? Where is the community doing well already, where are we falling short, and why? How hard and how quickly should we push for Net Zero HPC - what sacrifices (if any) are acceptable? In this talk, I will explore what the concept of 'Net Zero' might mean for users, operators and hosts of HPC systems going forward, and show examples of research and activities that are trying to push HPC in the direction of Net Zero and sustainability.


**BIO:** Prof Michèle Weiland is the Director of Research and Met Office Joint Chair at EPCC, the supercomputing centre at the University of Edinburgh. She leads Edinburgh's involvement in the Met Office Academic Partnership, as well as the technical work in the UKRI-funded ASiMoV Strategic Prosperity Partnership with Rolls-Royce, building and performing highly complex multi-physics simulations of aircraft engines. She led the EU H2020 project NEXTGenIO which, in collaboration with Intel and Fujitsu, developed a new HPC platform using non-volatile memory to accelerate I/O performance, and the ExCALIBUR ELEMENT project that investigated meshing for and at Exascale. She also led the EU FP7 project Adept, which investigated methods for energy and power efficiency measurements on parallel hardware. Michèle is a member of the EPSRC Strategic Advisory Team for e-Infrastructure.

# CIUK 2022 JACKY PALLAS MEMORIAL AWARD PRESENTATION


## Dr Djenifer B. Kappel

Centre for Neuropsychiatric Genetics and Genomics
Cardiff University

Twitter: @dbkappel
Web: https://www.cardiff.ac.uk/people/view/2520281-kappel-djenifer


## "The genomic basis for precision medicine in treatment-resistant schizophrenia"


**Abstract:** Mental illness is currently the main worldwide driver of health problems and disability, and one of the main challenges in adequately addressing and treating mental illnesses is the fact that the most commonly prescribed drugs are not equally effective for everyone. Genetic differences between individuals are known to contribute to how one responds to pharmacological treatment, but few guidelines in implementing this knowledge exist. My research seeks to explore how to use genomic information to make psychiatric treatments, particularly antipsychotics, more beneficial for everyone who needs them. As part of Cardiff University's CLOZUK project, I have accessed genomic and clinical data from thousands of individuals with schizophrenia that take an antipsychotic called clozapine. Clozapine is particularly effective in treating this condition, however due to a range of potentially severe adverse effects, it is currently only employed when other treatments have failed and not everyone eligible gets access to it. To identify avenues for a safer and more efficient way to use clozapine, my work has leveraged clinical treatment records on over 4000 CLOZUK samples. Some insights from this dataset involve the discovery of genetic variants associated to clozapine metabolism, and the establishment of a metric of genetic predisposition to schizophrenia (a construct called a “polygenic risk score”) as a marker of individuals receiving higher doses of the drug than commonly prescribed. These results suggest that the genomics-aware healthcare of the near future might realise the personalisation of medication doses, a process which can currently take months and ultimately relies on trial-and-error procedures, even in conditions as complex as psychiatric disorders.


**Bio:** Dr. Djenifer Kappel is a Brazilian Early Career Researcher currently working as a Post-doctoral Research Associate at Cardiff University with Dr. Antonio Pardiñas. She initially graduated in Biomedical Science at Federal University of Rio Grande do Sul in Brazil, later obtaining a Master’s and a PhD in Human Genetics (2020) at the same institution. Over the last 10 years she’s been interested in the biological underpinnings of mental illness and the use of bioinformatics and statistical genetics in their discovery. Her current research is based on understanding how genetics can predispose us to psychiatric disorders and impact on their treatment and management.

# ABSTRACTS AND SPEAKER BIOS


**Abstract:** The process of turning data into knowledge lies at the heart of research and innovation. Today, the use of digital technologies is as fundamental to modern research as theory, observation and experiment. A new environmentally sustainable datacentre is required to house computing to support the UKRI Digital Research Infrastructure (DRI) requirements of national facilities, science programmes and instruments. The presentation will explore the implications of an environmentally sustainable datacentre in both build and operation.

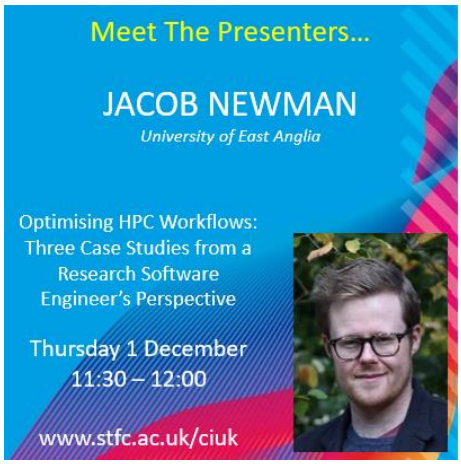
**Bio:** Dr Peter Oliver is Head of Operations for Scientific Computing (SC) at the Scientific and Technology Facilities Council (STFC) and is leading a new initiative to build an environmentally sustainable datacentre with a very high target for power efficiency. Peter gained his PhD from the University of Bath in 1994 with his thesis entitled "Computer Simulation of the Effects of Temperature on Oxide Surfaces." Inspired by high performance computing (HPC), Peter joined the Rutherford Appleton laboratory in 1997, to provide user support on the national HPC service Cray J90. Since then, Peter has developed his expertise and was responsible for the specification, procurement and management of High Performance Computing Systems such as STFC's Facilities (SCARF), national e-infrastructures (NGS & NeS) and climate and earth-system science (JASMIN). In 2013, Peter changed roles to lead the Scientific Computing Technology Division with expertise in visualisation, code optimisation, software engineering and computational mathematics and in 2016 became Head of Operations for Scientific Computing.


**Abstract:** Operating HPC data centers is very energy intensive business. In this presentation we explain how LUMI datacenter was designed to be one of the world most energy efficient data centers and how we achieved carbon negative foot print for our HPC operations..

**Bio:** Director Pekka Lehtovuori (PhD) leads the Services for Computational Research unit at CSC. He is responsible for CSC's national HPC services, scientific and user support as well as cloud and data intensive computing services. He is a member of the board for Nordic e-Infrastructure Collaboration. Dr Lehtovuori has extensive experience in development, implementation, and operation of national and European research infrastructure projects, such as FCCI, PRACE, EGI, ELIXIR, NeIC, EOSC, and EuroHPC.

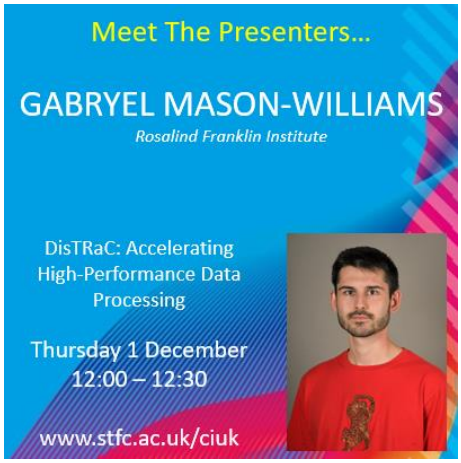

**Abstract:** With the increasing energy demand of high-end HPC systems, their efficient operation becomes ever more important both from an economic and ecologic perspective. JSC follows a holistic approach, ranging from the selection of HPC technology to the reuse of waste heat. The presentation gives an overview of its activities in this respect.

**Bio:** Thomas Eickermann is working at Jülich Supercomputing Centre (JSC) since he finished his PhD in Physics at the University of Düsseldorf in 1994. His activities cover system administration, Grid computing, and networking. In 2002, he became head of the communication systems division of JSC. Between 2008 and 2015, Thomas Eickermann has been project manager of PRACE preparatory and implementation phase projects and served on the PRACE aisbl Board of Directors. Currently, he is a deputy director of JSC and engaged in the preparations for a EuroHPC Exascale computer in Jülich.




**Abstract:** The University of East Anglia's HPC service has recently appointed a Research Software Engineer (RSE) to address the challenge of optimising users' jobs to make more efficient use of the available resources. In this talk, I will present three case studies of users requesting assistance to optimise their computational workflows on our HPC. I will describe how their requests were presented, the solutions considered and selected, and quantify the speed improvements obtained. Solutions explored will range from identifying simple idiosyncrasies due to software versioning, through to utilising GPU technology more effectively.

**Bio:** Jacob studied an undergraduate degree in Computing with Electronics, and a PhD in Computing entitled, "Language Identification Using Visual Features". He worked as a researcher for 11 years in the areas of speech recognition, computational biology, and medical computing. In 2021, Jacob joined the University of East Anglia's Research and Specialist Computing Support team, where his main responsibilities are to develop and optimise user workflows on the HPC.



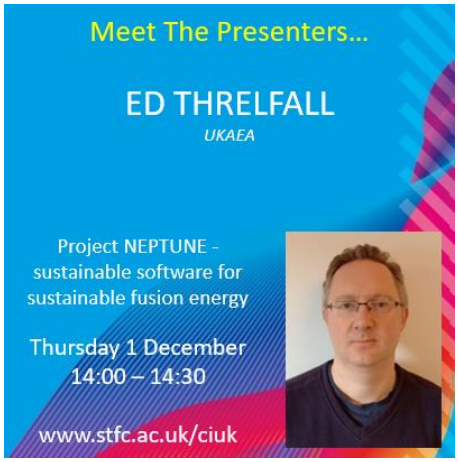

**Abstract:** Clusters in high-performance computing (HPC) are composed of four main components: a job scheduler, compute nodes, networking, and storage - each of which plays a role in the performance and sustainability of the system. DisTRaC is a Ceph deployment tool for creating temporary distributed RAM-disk file/object stores across job compute nodes. DisTRaC can remove the need for a parallel filesystem and the out-of-cluster network IO, reducing competition between concurrent jobs. Increasing efficiency while lowering external network and storage utilisation lowers CO2 emissions and costs associated with HPC, helping move towards Net Zero. In this talk, we introduce DisTRaC as a mechanism to increase the efficiency of applications without needing modification and showcase benchmark results against real-world HPC tasks.

**Bio:** Gabryel Mason-Williams is a computer science graduate from the University of Plymouth. During their studies, they did a year in industry with Diamond Light Source conducting research into "High-Performance

Object Stores for Big Data Processing" and a dissertation project titled "ALaBDaC- Automated Lab Book Data Collection" in collaboration with the Rosalind Franklin Institute. After this, Gabryel worked at the Rosalind Franklin Institute, building upon the success of the research conducted at Diamond Light Source and focusing on novel approaches to HPC, cloud, compression and storage. They are currently studying an MSc in Artificial Intelligence at Queen Mary University of London whilst continuing to work with the Rosalind Franklin Institute. Following the MSc, they plan to do a PhD in Machine Learning.


**Abstract:** In 2019 Bristol University went live with its homemade cluster. This is our experience of the trials and tribulations encountered during this endeavour from a sysadmin perspective. I will discuss the technical aspects and design considerations (including networking, deployment, scheduling [software stack] etc). And will finish with our reflections on this experience.

**Bio:** Simon is the HPC Team Leader at the Advanced Computing Research Center(ACRC), University of Bristol for the last 5 years, and has been with the center for the last 8 years. Involved in a wide variety of technical areas of HPC, sysadmin, networking and storage. Previously employed at the University of Nottingham for many years in a variety of roles, including software development, HPC, software licencing, system deployment, user support etc.




**Abstract:** Modelling the edge region of magnetically-confined nuclear fusion plasmas brings many computational challenges including plasma turbulence and the significant kinetic effects. Project NEPTUNE, part of the UK's ExCALIBUR programme, aims to apply modern numerical methods and software engineering techniques to address these issues using current and next-generation (i.e. exascale) HPC. One key theme is the application of spectral / hp finite element methods, which, due to their intrinsically large number of arithmetic operations per unit of data, are well-suited to today's exascale architectures - this contrasts with existing finite-difference codes, which are not expected to scale well. A second key theme is the use of particle methods for matter that is out of thermal equilibrium owing to low collisionality.

This presentation will outline applications of spectral / hp methods and particle methods to fusion-relevant problems, including heat transport and the dynamics of charged and neutral particles, intended as the initial steps toward a full-featured plasma edge simulation code. These applications serve to illustrate the NEPTUNE project's aims for software sustainability (software capable of significant evolution during a 30-year lifecycle) and embody an approach to multi-site opensource software development encompassing `separation of concerns' and `co-design'.

**Bio:** Ed Threlfall holds a degree and a Masters in physics from Cambridge University and a PhD in theoretical particle physics from the University of Southampton. Following a postdoctoral position at Durham University, he joined a software company to pursue the development of advanced physics simulation codes and wrote a commercially successful finite-element simulation engine for solving problems in photonics and nonlinear optics, using C++.

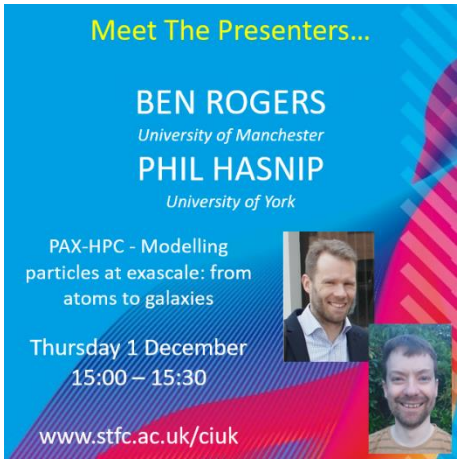
After ten years' experience in industry, he joined UKAEA in 2020, in order to explore the challenge of numerical fusion simulations. Ed has extensive experience with implementing efficient finite-element codes, particularly Discontinuous Galerkin methods.


**Abstract:** As part of ExCALIBUR funded projects at the Met Office there have been projects exploring multiple approaches towards a sustainable computing future, from general compute optimisations to GPU studies, all to enable Exascale weather & climate modelling. In this talk we hear about the results of some of these technical developments and the experiences of two early career software engineers who have been developing the skills needed to work on these projects.

**Bio:** Having spent most of his working career developing cloud-based business software, Joe Hickson joined the Met Office in 2019 as a Scientific Software Engineer working on developing the next generation modelling system. Since then, he's worked on the ubiquitous Covid Modelling projects before moving into managing the ExCALIBUR Pool of Scientific Software Engineers in 2021.

Lewis Sampson started higher education at the University of Plymouth, completing a PhD in "Ocean modelling with novel data assimilation techniques" under Professor Georgy Shapiro. Lewis joined the Met Office as a foundation scientific software engineer during lockdown in 2020, working for the Ocean Forecasting Research and Development team, while still being part of the ExCALIBUR Pool. His work focuses on the analysis of the WaveWatch III model, using the options surrounding parallel processing such as OpenMP, OpenACC, MPI, and hybrid implementations.

Victoria Smart joined the Met Office in 2020 as a member of the ExCALIBUR pool. Since joining, Victoria has been deployed into multiple teams, previously working on improving the testing infrastructure for the IMPROVER post-processing code and investigating the method of launching coupled models on the supercomputer. Now Victoria is working on porting the ocean data assimilation code, NEMOVAR, to GPU.




**Abstract:**

**Bio:** Prof Benedict D. Rogers (Manchester) is Chair of Computational Hydrodynamics and is leader of the Smoothed Particle Hydrodynamics (SPH) specialist group in the Department of Mechanical,

Aerospace and Civil Engineering at the University of Manchester. He is a founder of the SPH rEsearch and engineeRing International Community (SPHERIC), the international organisation for SPH and was chair from 2015-2021. He is a core developer of the open-source GPU-accelerated code DualSPHysics with more than 100,000+ downloads and has been at the heart of the development of massively parallel incompressible SPH solvers. He is a co-Investigator on 2 projects for the UK's ExCALIBUR exascale HPC programme including the Particles At eXascale (PAX-HPC) project. He has twice received the Thomas Telford Premium Award from the Institution of Civil Engineers (ICE) for his work on SPH applied to tsunami-structure interaction.

Phil Hasnip is a physicist and computer programmer in the Department of Physics at the University of York. He grew up in the 1980s, where he learned physics at school and computer programming on his Sinclair ZX Spectrum. He is an EPSRC Research Software Engineering Fellow, and writes computer software to tackle problems in physics research, with a particular interest in making scientific software user-friendly, scalable, efficient and reliable. Phil is a lead developer of the quantum mechanical materials modelling program CASTEP, chairs the UKCP High End Compute Consortium, and is the Knowledge Exchange Coordinator for the Particles At eXascale (PAX-HPC) project for the UK's ExCALIBUR exascale HPC programme, working to ensure that key UK modelling methods are ready for the next generation of HPC machines.

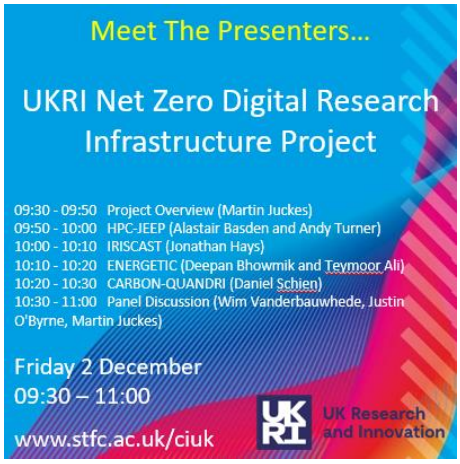

**Abstract:** This session will overview the parallel benchmark performance of a variety of popular community codes on a number of HPC systems, with our analysis based on both computational chemistry and ocean modelling applications. The former feature codes from Molecular Dynamics (AMBER, LAMMPS and NAMD) and Materials Science (VASP, CASTEP), while representative codes from the ocean modelling community include NEMO and FVCOM.

The variety of systems considered focus on both the Intel Ice Lake and AMD EPYC Milan family of processors. Using the Intel Skylake Gold 6148 and AMD EPYC Rome 7502 as the baselines, an assessment is made across a variety of Ice Lake (8358, 8352Y, 8368Q, 8360Y and 8380) and Cascade Lake SKUs (e.g., the 9242-AP and 6248), with system interconnects from both NVIDIA Networks and Cornelis Networks. Attention is also focused on systems featuring the 64-core Milan and Rome AMD processor (the Rome 7702 and Milan 7713, 7763 & 7773X) and the corresponding 32-core processors (the Rome 7502 and Milan 7543 & 7573X).

The benefit of the Intel® oneAPI Toolkit is demonstrated throughout this analysis. To best capture a 'like for like' comparison amidst the extensive array of core densities, our analysis remains based on both a “node-by-node” and the more traditional “core-by-core” consideration.

**Bio:** Professor Martyn Guest has led a variety of high performance and distributed computing initiatives in the UK. He spent three years as Senior Chief Scientist and HPC Chemistry Group Leader at PNNL, before returning to the UK as Associate Director of Daresbury’s Computational Science and Engineering Department. Martyn joined Cardiff University in April 2007 as their Director of Advanced Research Computing. He is also Technical Director of the Supercomputing Wales programme and is co-I on the Isambard 2 system at the GW4 Tier-2 HPC regional centre.

Martyn’s research interests cover the development and application of computational chemistry methods. He is lead author of the GAMESS-UK electronic structure program and has written or contributed to more than 260 journal articles.




**Abstract:** UK Research and Innovation (UKRI) is committed to becoming net zero by 2040. Across the nine component organisations, there is an extensive range of computers and peripherals, which we refer to as digital research infrastructure (DRI). The UKRI Net Zero DRI Scoping project (NZDRI) will cover all the UKRI-owned and majority-funded digital research infrastructure. It will produce evidence and recommendations for the delivery of a carbon neutral DRI by 2040 or sooner. NZDRI will present recommendations at a workshop in May 2023.

HPC-JEEP is analysing the compute node energy use data available from the ARCHER2 and DiRAC COSMA HPC services to understand what meaning can be extracted from this type of data to help users, service providers and funders analyse the energy/emissions and how they can contribute towards net zero goals. In particular, we are looking at how we can analyse energy use by project, research area or software across the whole services; how you might implement a charging scheme with a component of energy use; and what energy/emissions metrics can be reported back to users, service providers and funders based on compute node energy use data.

Current, leading-edge HPC systems are often heterogeneous, comprised of combinations of multiple compute units and accelerators, including (but not limited to) CPUs, GPUs and FPGAs. HPC is a significant contributor to energy usage. However, the energy-to-solution varies between these architectures. In terms of minimising

energy consumption, this choice of possible architectures presents a set of challenges to HPC system maintainers and algorithm developers, such as, a) which configuration of architectures provides the lowest energy consumption? or b) which combination of architectures should a code target in order to minimise its energy consumption.

The ENERGETIC project is conducting research to answer these questions through energy measurement benchmarks on prototypical algorithms. In this talk, we shall present our initial findings and energy profiles obtained from both existing HPCs as well standalone computing systems.

**Bio:** Martin Juckes is Head of CEDA Atmosphere and leading the UKRI Net Zero Digital Research Infrastructure Scoping project

Alastair Basden is a HPC manager for the DiRAC Memory Intensive service at Durham University, and a member of the DiRAC technical directorate.

Andy Turner is a Principal Architect at EPCC and provides technical leadership for the ARCHER2 Computational Science and Engineering (CSE) service.

Dr Deepayan Bhowmik is a Senior Lecturer in Data Science in the School of Computing at Newcastle University, UK. He is conducting research in fundamental signal and image processing, applications and their system implementations. His research interests include heterogeneous computer architecture with CPU, GPU and FPGAs, embedded and low power vision systems, computer vision, and other image processing applications. Dr Bhowmik received research fundings from various UK research councils, Royal Academy of Engineering, EU and industries.

Teymoor Ali is a research associate in School of Computing at Newcastle University, UK. His research interests include image processing, heterogenous architectures, image sensor characterisation methods and high-level synthesis tools.

Professor Wim Vanderbauwhede is the lead of the Low Carbon and Sustainable Computing activity at the School of Computing Science of the University of Glasgow. He received a PhD in Electrotechnical Engineering from the University of Gent, Belgium in 1996. He has been a lecturer in the School of Computing Science at the University of Glasgow since 2004. His research has resulted in over 150 refereed conference and journal papers as well as several books and book chapters. Before returning to academic research, Prof. Vanderbauwhede worked in the electronics industry as a Design Engineer and Technology R&D Engineer.

Justin O'Byrne works in STFC as an Associate Director within the Programmes Directorate, and also as UKRI's Acting Co-Director for Digital Research Infrastructure (DRI). The DRI programme has £130m to allocate over the next few years and we are extremely conscious of the choices that face us on the net zero front.


**Abstract:** Kinetic Monte-Carlo (KMC) simulations have been instrumental in multiscale catalysis studies, enabling the elucidation of the complex dynamics of heterogeneous catalysts and the prediction of macroscopic performance metrics, such as activity and selectivity. However, the accessible length- and time-scales have been a limiting factor in such simulations. I will present a recently established approach for exact, distributed, lattice-based simulations of catalytic kinetics, which couples the Time-Warp algorithm, an optimistic approach to Parallel Discrete Event Simulation, with the Graph-Theoretical KMC framework in the "Zacros" software package, enabling the handling of complex events within large lattices.

The performance of this MPI-based parallel KMC implementation broadly depends on the amount of available memory. Therefore, its performance as a function of parameters that control its memory usage will be presented, as well as its weak and strong scaling benchmark results.

Performance improvements of 1-4 orders of magnitude were observed, depending on the simulated chemical system, memory available, parameter choice, and number of MPI processes used. The results of a simulation of a system with 16M sites that exhibits large-scale pattern formation, which was not feasible with the serial algorithm, will also be shown.

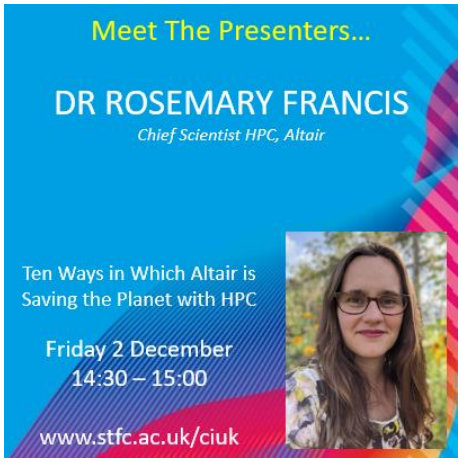
**Bio:** Dr Ilektra Christidi is a particle physicist by calling and research software engineer by profession. She received her PhD from Stony Brook University in NY, for research on the rarest physical process ever observed, a rare decay of charged Kaon particles that provides insight into the matter-antimatter asymmetry of the universe. As a postdoctoral researcher with the ATLAS experiment of the LHC at CERN, she studied background processes to the detection of the Higgs particle that involve lepton pairs, the identification of high-momentum b-jets and measurement of their production rate, the commissioning and data quality assurance of the Muon Spectrometer sub-detector, and the software-level trigger of the Inner Tracker sub-detector.

She moved to software engineering first in industry, developing algorithms and libraries for processing geophysics data for oil and gas searches, and moved to UCL as a research software developer in its central Research IT Services team in 2016. While being a generalist RSE, she mostly focuses on computational projects, often involving HPC. She enjoys working with researchers all over the university to develop robust, sustainable, and performant software to deliver research results, and has so far been involved in various projects, including parallelising simulation software for surface catalysis, single-core optimisation of a particle physics event generator, development of data analysis and visualisation software for yeast genome studies, benchmarking of image analysis codes for radio astronomy, as well as the ExCALIBUR benchmarking project, to name a few.


**Abstract:** The Particle-In-Cell (PIC) method is a computational technique used to explore the physics of plasmas at a microscopic level. The plasma is described through a statistical distribution of positive and negative charges sampled via computational particles. These computational particles interact via electromagnetic fields that they produce. These fields are obtained solving Maxwell's equations on a fixed grid, where source terms are computed by interpolating the particles to the grid.

In this talk, we describe our massively parallel PIC code ECsim. We discuss the inclusion of OpenACC directives in the code to port particle kernels to GPUs. For typical numerical parameters used in our simulations, we show that the version of the code that leverages GPUs runs up to 5 time faster than the CPU version. We compare code performance on different generations of NVIDIA GPUs. Finally, we report on scaling tests obtained on different supercomputers.

**Bio:** Dr Elisabetta Boella is a lecturer in Physics at Lancaster University & the Cockcroft Institute of Accelerator Science and Technology. She has a long-time experience in the development of kinetic codes for exploring the microphysics of space and laboratory plasmas. She has also extensive expertise in High-Performance-Computing. She is one of the main developers of the plasma code ECsim. Her most recent effort regarding the code concerns the tentative to off-load some of the code calculations to GPU via OpenACC. She is a volunteer for Women in High Performance Computing.



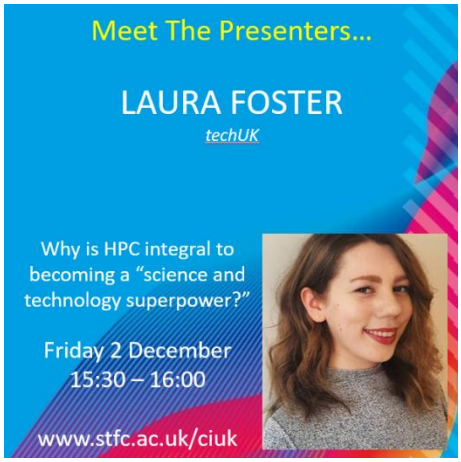

**Abstract:** Most of the HPC community know Altair for HPC infrastructure products such as PBS Professional or Altair Grid Engine, but most of our business is in the manufacturing and simulation space as a user of HPC. In this presentation I'll be looking at ten ways in which Altair and our customers are saving the planet through reducing the environmental cost of manufacturing, increasing product life spans, and using HPC in place of expensive real-life experiments. The quest for net zero needs to be done at every level so I'll also be talking about what you can do in the datacentre to increase efficiency, reduce power consumption and increase the life span of your hardware. HPC is usually cost efficient and power efficient compared with the alternatives, but we owe it to the planet to ensure that HPC is as green as possible and that every gram of carbon emissions count.

**Bio:** Dr Rosemary Francis founded Ellexus, the I/O profiling company, in 2010, and Ellexus was acquired by Altair in 2020. Rosemary obtained her PhD in computer architecture from the University of Cambridge and worked in the semiconductor industry before founding Ellexus. She is now chief scientist for HPC at Altair, responsible for the future roadmap of workload managers Altair® PBS Professional® and Altair® Grid Engine®. She also continues to manage I/O profiling tools, Altair® Breeze™ and Altair® Mistral™ and is shaping analytics and reporting solutions across Altair's HPC portfolio. Rosemary is a member of the Raspberry Pi Foundation, an educational charity that promotes access to technology education and digital making. She has two small children and is a keen gardener and windsurfer.


**Abstract:** High performance Computing is evolving from limited options with high costs towards flexible and simple computing resources available to end-users. At the same time with increased parallelism the journey towards Exascale entails numerous challenges. As energy costs spike, ignoring these costs is not an option. While an exascale system can consume the electricity of a small city, how to reconcile "performance" with "sustainability"?

A trade-off has to be made between achieving results, computational performance and energy consumption. "Greener" is as important as "faster", in defining the scientific value delivered by these systems. We need to consider user goals to reach net zero, and also looming carbon pricing as we evaluate what "Greener" really means. At the same time, more options are opening up to deliver scientific value using HPC in the cloud.

**Bio:** With over 30 year's experience in the HPC industry, I have worked through the evolution from proprietary supercomputers to Unix and then Open systems. While the development of technology is critically important, it is only there to do a job – forecast the weather, design new materials or drugs, build better cars or improve energy systems. I have always tried to keep this maxim at the forefront in my design choices.




**Abstract:** Through techUK's Future of Compute workstream, techUK members – a group of over 950 tech sector companies in the UK - have emphasised that HPC should be viewed as a key part of the UK's ambition to remain a world leader in science and innovation. In this sense, HPC should be seen as strategic national infrastructure, as important to our economic future in an information age as steel was in the industrial age. Lack of investment in this vital infrastructure could make the UK less competitive in both academia and key industries like life sciences, aerospace, and financial services.

Furthermore, there is a real danger that lack of investment in HPC will undermine growth in other technology ecosystems like artificial intelligence and quantum, both of which have been identified in current government policy as key pillars of the UK's science and technology ecosystem.

With this in mind, techUK will present the key themes from its Future of Compute work, such as technology convergence, international collaboration, and sustainability, before looking at how the UK tech sector envision the future of HPC in the UK. In doing so, we will ultimately explore how the UK tech sector, policy makers and academia in HPC could work together to support the UK's ambition of becoming a science and technology super power.

**Bio:** Laura is techUK's Head of Programme for Technology and Innovation.

She supports the application and expansion of emerging technologies across business, including Geospatial Data, Quantum Computing, AR/VR/XR and Edge technologies.

Before joining techUK, Laura worked internationally in London, Singapore and across the United States as a conference researcher and producer covering enterprise adoption of emerging technologies. This included being part of the strategic team at London Tech Week.

Laura has a degree in History (BA Hons) from Durham University, focussing on regional social history. Outside of work she loves reading, travelling and supporting rugby team St. Helens, where she is from.

# CIUK 2022 EXHIBITION

The CIUK 2022 Exhibition will take place in the main hall. The exhibition will include the exhibition stands, the student poster competition, the cluster challenge and the research zone.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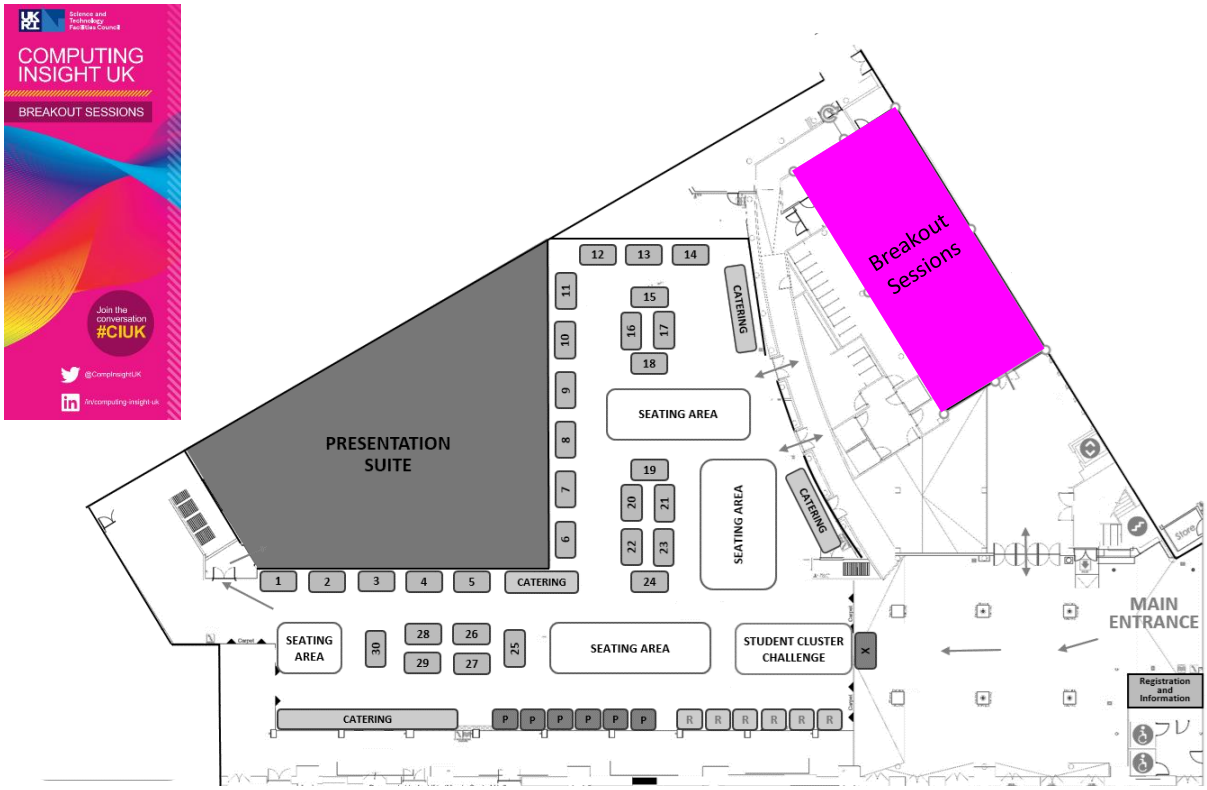
# CIUK 2022 PARALLEL BREAKOUT SESSIONS

The CIUK 2022 Breakout Sessions will run alongside the main CIUK programme in Charter Room 4. Look for the PINK pull-up banners.




## CoSeC Annual Conference - Thursday 9 December

CoSeC
Computational Science Centre for Research Communities
**Annual Conference 2022**
Thursday 1 December @ CIUK 2022

The Computational Science Centre for Research Communities (CoSeC) supports the advancement of scientific research by developing and strengthening software to analyse and solve increasingly complex problems in multiple disciplines - physics, chemistry, life sciences, engineering, and more.

Funded by EPSRC, MRC, and BBSRC, CoSeC also provides a hub for exchanging knowledge and expertise through training and outreach. Long-term partnerships and collaborations with universities and other research establishments are at the heart of what CoSeC does. Together, they convey longevity to the software and expertise that, alongside continued advancement of computational hardware and the nurturing of strong collaborations, provide what is necessary for scientific communities to flourish.

# CoSeC Conference 2022

**Thursday 1 December**
**Manchester Central**

CoSeC
Computational Science Centre for Research Communities
Annual Conference 2022
Thursday 1 December @ CIUK 2022

## AGENDA

| TIME | SPEAKER | PRESENTATION TITLE |
|---|---|---|
| 09:30 - 09:45 | Barbara Montanari (Director CoSeC, STFC) | Welcome and Introduction |
| **09:45 - 11:15** | **Data Science & Machine Learning** | |
| 09:45 - 10:15 | Stefano Mensa (Hartree Centre) | Quantum Machine Learning Framework for Virtual Screening in Drug Discovery: a Prospective Quantum Advantage |
| 10:15 - 10:45 | Jiayun Pang (University of Greenwich) | A Natural Language Processing (NLP)-Based Deep Learning Approach to Predict Solubility Parameters for Drug Discovery |
| 10:45 - 11:15 | Yuhan Wang (University College London) | Using molecular dynamics simulation to predict the aggregation propensity of mAb formulations & accelerate development |
| 11:15 - 11:45 | **REFRESHMENTS** | |
| **11:45 - 13:15** | **Coupling & Data Workflows** | |
| 11:45 - 12:15 | Wendi Liu (STFC) | ParaSiF: A Partitioned Fluid-Structure Interaction Simulation Framework |
| 12:15 - 12:45 | Raz Benson (University College London) | Fast pattern detection in kinetic Monte Carlo simulations of heterogeneous catalysis |
| 12:45 -13:15 | Chien Nguyen (Bangor University) | Reusing Previous Simulation Runs: Applications in Environmental Fluid Dynamics |
| 13:15 - 14:00 | **LUNCH BREAK** | |
| **14:00 - 16:00** | **High Performance & Future Computing** | |
| 14:00 - 14:30 | Stefano Rolfo (STFC) | Modernisation of the 2DECOMP&FFT Library for Hybrid Architecture |
| 14:30 - 15:00 | Jianping Meng (STFC) | Domain specific languages for exascale fluid simulations |
| 15:00 - 15:30 | Jian Fang (STFC) | Study of High-Speed Aerodynamics based on High-Fidelity Simulation |
| **15:30 - 16:00** | **Panel Discussion and Wrap Up** | |
| 15:30 - 15:55 | Panel Discussion (Chair: Sylvain Laizet) | |
| 15:55 - 16:00 | Stephen Longshaw (STFC) | Wrap Up |

## Women in HPC Networking Breakfast – Friday 10 December

We are pleased to launch our first ever Women in HPC (WHPC) Networking Breakfast on Friday 2 December starting at 08:30.

This breakfast is included in the conference registration and is open to all conference delegates. Tea, coffee and food will be available and there will be a selection of presentations.

By attending you will be able to:

- Learn more about how to be an ally for diversity, equity and inclusion in HPC.
- Engage in talks and conversation around the barriers and skills gaps which face those who wish to enter the field.
- Meet WHPC leaders from our UK and EMEA Chapters and Affiliates.

More information and a schedule can be found on the WHPC website. We look forward to seeing you there.

## Spectrum Scale User Group – Friday 10 December

We are delighted to welcome the Spectrum Scale User Group back to CIUK in 2021. Their meeting will take place on Friday 10 December.

The Spectrum Scale (GPFS) User Group is free to join and open to all using, interested in using or integrating Spectrum Scale. We welcome Spectrum Scale users from a wide range of industries and are not sector specific. Our membership represents media, academia, research, automotive, defence, pharmaceutical industries, etc.

The Spectrum Scale User Group aims to:

- Bring together users of Spectrum Scale and Spectrum Scale with Spectrum Protect with ILM (TSM/HSM) into a collective environment
- Represent the needs of the Spectrum Scale User Group members
- Liaise with IBM and our User Group members to improve Spectrum Scale and Spectrum Scale with Spectrum Protect
- Provide a “localised” community for support and knowledge sharing
- Raise awareness of Spectrum Scale as a capable data management platform

## ENERGETIC: A workshop regarding Energy Benchmarking on Heterogeneous Systems – Friday 10 December

This session will be led by the "Energetic" sub-project - part of the UKRI "Net Zero Digital Research Infrastructure Project" - which is (i) exploring potential role of heterogenous architectures to reduce energy consumption of HPC codes and (ii) to initiate discussion on how to reliably and accurately monitor energy usage of HPC systems and how to share this information at a job level with all users.

ENERGETIC: Energy Benchmarking on Heterogeneous Systems

The ENERGETIC sub-project (part of the UKRI Net Zero DRI Project) is investigating the potential role of heterogeneous architectures in reducing the energy consumption of digital research infrastructure. Our aim is to investigate which accelerators may give an energy advantage and in what circumstances, how can DRI users reliably and accurately benchmark energy usage of their own codes on heterogeneous systems, and how do we ensure that energy benchmarking results are fairly compared. Ultimately, we hope that UK DRI users will be empowered to benchmark their own applications using standardised tools and methodologies, and as a result will be able to choose most energy efficient way to do their science. In this session we will present some of our own findings from benchmarking applications on heterogeneous systems, and then initiate a series of discussion groups. In particular, we will discuss the following points:

- In what areas might we see energy advantage from accelerators?
- What barriers exist to user-level benchmarking of applications on UK DRI?
- How do we fairly compare application energy usage across architectures?

We invite DRI stakeholders at all levels: users, vendors, administrators, and policymakers to come and join the discussion.

## CIUK 2022 RESEARCH ZONE


The CIUK 2022 Research Zone will allow all EPSRC Tier-2 Centres, and other sites with significant size computing facilities, the opportunity to join the CIUK exhibition and update attendees on their progress. You can visit them in the exhibition hall to find out about their systems, discuss potential projects and discover how to get access.

## CIUK 2022 STUDENT CLUSTER CHALLENGE

Following the success of our first two Student Cluster Challenges at CIUK 2020 and CIUK 2021 the competition will return in 2022 for its third edition. As in 2021 this years' Student Cluster Competition will be a hybrid competition with a series of online challenges leading up to the conference followed by some physical, hands-on challenges during the conference itself.

Meet the teams…

| University of Birmingham | University of York | UCL | Durham University | University of Bristol | University of Bristol |
|---|---|---|---|---|---|
| **Runtime Terrors** | **Team York** | **Team UCL** | **Team ClusDur** | **Team Bristol (A)** | **Team Bristol (B)** |

As we head into the face-to-face challenges at CIUK 2022 Team ClusDur hold a narrow lead over the two Bristol teams with plenty of points still to play for.

You can find the Cluster Challenge teams at the entrance to the exhibition hall, by the information point. Please feel free to pay them a visit as they complete their challenges during the conference. You can also follow the competition on Twitter #CIUK2022_SCC.

The winning team will be announced before the final presentation session on Friday 2 December with the champions going forward to represent CIUK at the ISC'23 Cluster Challenge in Germany next summer.

As always, we could not host the cluster challenge without the support of our cluster challenge partners and we thank them for their time, efforts and the opportunity to access their systems…

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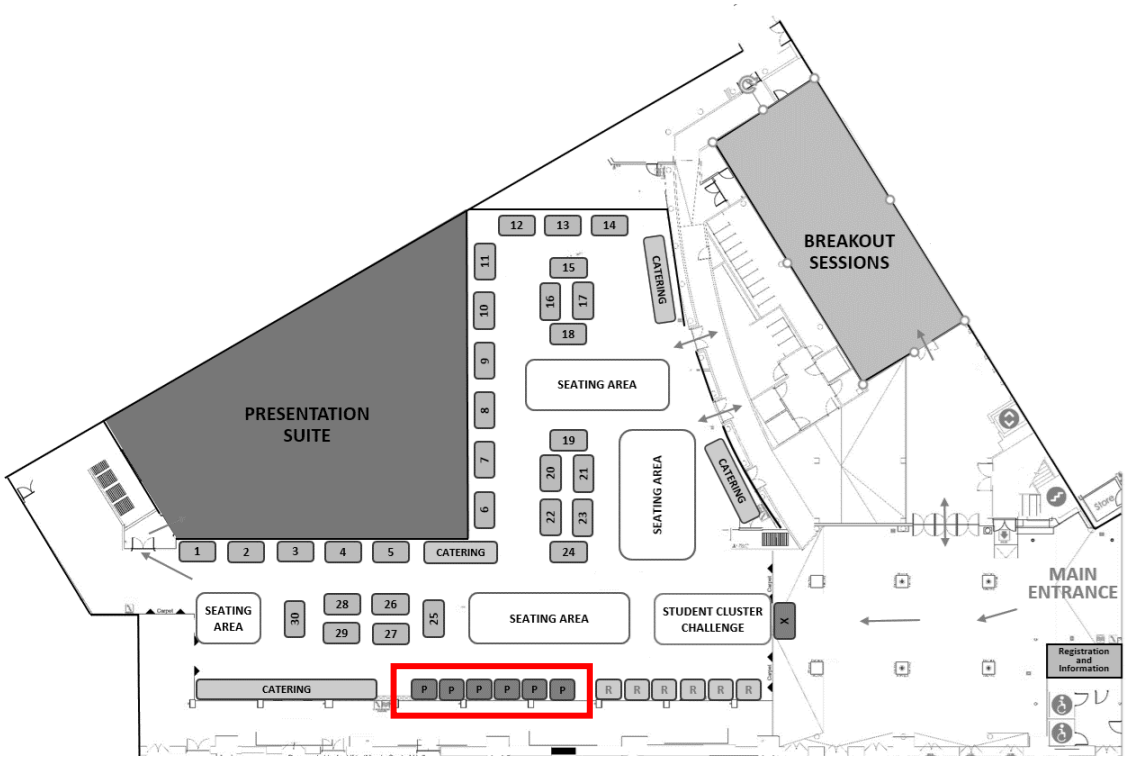
# CIUK 2022 POSTER COMPETITION

Nine finalists have been chosen for the CIUK 2022 Student Poster Competition. Their posters can be viewed on the exhibition floor and also online. The winner will be announced prior to the final presentation session on Friday 2 December.

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| **Jakub Adamski**<br>*University of Edinburgh* | **Energy Efficient Quantum Computing Simulations**<br><br>As we are entering the era when quantum advantage becomes viable, it is especially important to push the boundaries of classical simulations of quantum computing. It involves running exponentially complex algorithms, so the use of high-performance computing is essential and entails huge energy consumption. The simulation can be performed via state vector evolution or by contracting a tensor network of matrix product states and operators. Each method offers different advantages, and allows potential optimisations to save energy. Various benchmarks have been set up and run on ARCHER2 to determine the most economical approach. It was found that by downclocking the CPU, a state vector simulation can consume up to 30% less energy. On the other hand, tensor networks proved exponentially more efficient when the entanglement was limited. The goal of this poster is to present and explain the benchmarking results, and encourage greener HPC use when simulating quantum computing. |
| **Bruno Camino**<br>*University College London* | **Applications of quantum computing for quantum chemistry**<br><br>Quantum chemistry has been predicted to be one of the first fields to benefit from the development of quantum computing. In this work we explore applications of quantum annealing for the study of solid solutions. These materials are of great interest for energy store applications and simulating their properties with classical computers is particularly challenging because of the large configuration space to explore. Using vacancies of graphene as a model system, we show how quantum annealers can be used to tackle these type of problems. |
| **Shayantan Chaudhuri**<br>*University of Warwick* | **Long-range dispersion-inclusive machine learning potentials for hybrid organic-inorganic interfaces**<br><br>The computational prediction of the structure and stability of hybrid organic–inorganic interfaces provides important insights into the measurable properties of electronic thin film devices and catalyst surfaces, and plays an important role in their rational design. However, the rich diversity of molecular configurations and the important role of long-range interactions in such systems make it difficult to use machine learning potentials (MLPs) to facilitate structure exploration that would otherwise require computationally expensive electronic structure calculations. We present an ML approach that enables fast, yet accurate, structure optimisations by combining two different types of deep neural networks trained on high-level electronic structure data for gold nanoclusters on diamond (110) surfaces. |
| **Kenneth Chinembiri**<br>*University of Sheffield* | **An Immersed Boundary Method for the DNS Solver CHAPSIM**<br><br>CHAPSim 2.0 is a Direct Numerical Simulation code developed by the Collaborative Computational Project – Nuclear Thermal |

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| | Hydraulics (CCP-NTH) as an open-source UK nuclear community code. The solver is fast, efficient, and capable of simulating turbulent thermal flows with strong physical property variation. This paper discusses the methodology and validation of an Immersed Boundary Method (IBM) for complex geometries in the solver CHAPSim 2.0. When adopting this method, the effect of the solid body to flow field is mimicked by introducing a forcing term to the governing momentum equations of the CFD solver. The forcing term allows the user to impose a desired target velocity at the grid nodes of the complex solid boundary and is computed courtesy of the direct forcing approach. This function enables CHAPSim2 to simulate flow over arbitrary geometry without complicated grid generation process. |
| **Asa Hopkins**<br>*University of Strathclyde* | **Introducing Incoherence to Artificial Neural Networks**<br><br>Artificial neural networks (NNs) at their core are an attempt to emulate the biological NNs found in the brains of animals, and can accomplish tasks with lower energy consumption than more traditional computing methods.However, there are still ways that artifical NNs fall short of their biological counterparts. Most artificial NNs are made up of layers of nodes, with edges only being formed between adjacent layers. This kind of strict ordering is not seen in nature and the existence of edges connecting non-adjacent layers is important to the stability of larger natural systems, such as food chains and metabolic pathways. The extent to which this strict layering is broken is known as the trophic incoherence.This work investigates methods of adding trophic incoherence to artificial NNs, and the effectsdoing so has on the convergence speed during training (fast convergenceis more energy efficient) and the accuracy after training is completed. |
| **Lara Janiurek**<br>*University of Strathclyde* | **Using Machine Learning Techniques to Determine Photometric Redshifts for Gravitational wave Cosmology**<br><br>The inference of the Hubble constant using gravitational waves has allowed for a new way for the expansion of the universe to be probed, which may shed light on the current Hubble tension. Galaxy redshift surveys are a required for the application of these dark sirens. Photometric redshift surveys contain significant errors and spectroscopic redshifts are much more energy intensive than simply using an algorithm to estimate these values. Here, the random forest (RF) algorithm GALPRO is implemented to generate photometric redshift posteriors. GALPRO is calibrated using a truth dataset, which is successful, meaning it is useful when presented with an incomplete survey with missing redshift values. Analysis suggests that the redshift posterior distributions are non-Gaussian. Tests were run which determined that training and testing datasets must overlap by least 90% in range to give accurate results. However, the algorithm failed when the training and testing datasets came from different surveys meaning there is some underlying fundamental difference in galaxy surveys that must be recognised when using RFs. |

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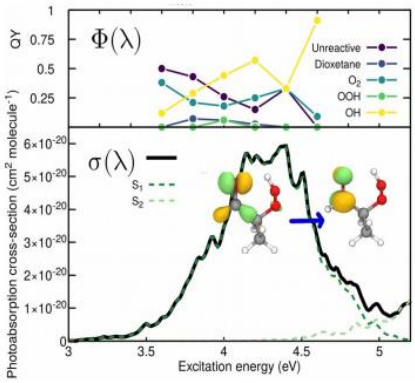
| **Harriet Jones**<br>*STFC / University of Chester* | **Validation and Application of Lagrangian Stochastic Methods for Indoor Air Quality**<br><br>This STFC Air Quality Network (SAQN) project uses EDF's computational fluid dynamics software Code_Saturne to model the dispersion of a key hazardous aerial pollutant, particulate matter (PM), during cooking experiments within a test house. This is done via the implementation of Code_Saturne's Lagrangian Particle Tracking module. The basis for the model is the EPSRC funded DOMestic Systems Technology InCubator (DOMESTIC) test house, a controlled environment designed to simulate a full-scale kitchen/diner and bathroom. Early results indicate that the model appears to effectively replicate the evolution of PM2.5 (particulate matter with a diameter of 2.5 microns or less) during cooking episodes, and further experimental validation results are pending. |
| **Emanuele Marsili**<br>*University of Bristol* | **A Theoretical Perspective on the Actinic Photochemistry of 2-hydroperoxypropanal**<br><br>Determining the chemical composition of the Earth's troposphere and its evolution over time is crucial for shaping the political and societal decisions regarding global warming. Presently used chemical mechanism models - encompassing experimental and theoretical data for many ground-state reactions of volatile organic compounds (VOCs) - allow estimating the outcomes of VOCs reactions. Interestingly though, the role of light-induced, excited-state processes is still largely unexplored and photochemical reactions of transient VOCs are mostly neglected in predictive atmospheric models.<br><br>  <br><br><br>One important family of VOCs is the α-hydroperoxycarbonyls. Since experimental studies on these transient molecules are hardly feasible, we have employed high-level<br><br>quantum chemical methods to fully characterize the photochemistry of the 2-hydroperoxypropanal (2-HPP) [1]. Using the nuclear ensemble approach we calculated the photo-absorption cross-section (σ(λ)) [2] while we resorted to nonadiabatic molecular dynamics to determine the wavelength-dependent photolysis quantum yield (Φ(λ)). These two ingredients, together with the solar actinic flux (F(λ)), allow us to predict the photolysis rate constant J, a |

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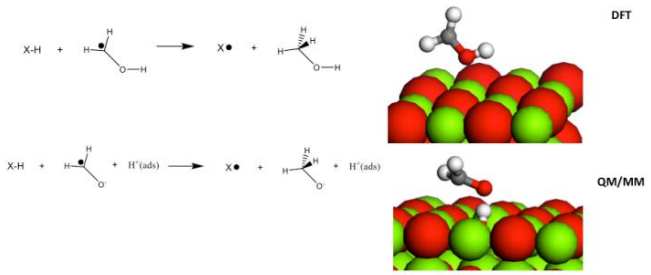
| | crucial piece of information required by predictive chemical mechanism models.<br><br>[1] Marsili E., et al. The Journal of Physical Chemistry A 2022, 126, 5420–5433<br>[2] Prlj A., Marsili E., et al., ACS Earth and Space Chemistry 2022, 6, 207-217 |
| **Mala Alhaji Sainna** | **A combined periodic DFT and QM/MM approach to understand the radical mechanism of the catalytic production of methanol from glycerol**<br><br>The production of methanol from glycerol over a basic oxide, such as MgO, using high reaction temperatures (320 °C) is a promising new approach to improving atom efficiency in the production of biofuels. The mechanism of this reaction involves the homolytic cleavage of the C3 feedstock, or its dehydration product hydroxyacetone, to produce a hydroxymethyl radical species which can then abstract an H atom from other species. Obtaining a detailed reaction mechanism for this type of chemistry is difficult due to the large number of products present when the system is operated at high conversions. In this contribution we show how DFT based modelling studies can provide new insights into likely reaction pathways, in particular the source of H atoms for the final step of converting hydroxymethyl radicals to methanol. We show that water is unlikely to be important in this stage of the process, C-H bonds of C2 and C3 species can give an energetically favourable pathway and that the disproportionation of hydroxymethyl radicals to methanol and formaldehyde produces a very favourable route. Experimental analysis of reaction products confirms the presence of formaldehyde. The calculations presented in this work also provides new insight into the role of the catalyst surface in the reaction showing that the base sites of the MgO(100) are able to deprotonate hydroxymethyl radicals but not methanol itself. In carrying out the calculations we also show how periodic DFT and QM/MM approaches can be used together to obtain a rounded picture of molecular adsorption to surfaces and homolytic bond cleavage which are both central to the reactions studied.<br><br>  <br><br><br>Reference:<br><br>• Sainna, MA; et al. Faraday Discuss. 229, 108 (2020)<br>• E. Lotero, Y. et al. Ind. Eng. Chem. Res., 44, (2005) |

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