Science and Technology Facilities Council

Scientific Computing

COMPUTING INSIGHT UK 2021

9 - 10 DECEMBER 2021

Manchester Central, UK

www.stfc.ac.uk/ciuk

CONTENTS

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INTRODUCTION

We are delighted to welcome you all to Computing Insight UK 2021 as we return to a physical, face-to-face conference at Manchester Central on the 9-10 December, following the enforced move to an online, virtual conference in 2020.

The theme for the conference this year is **"Heterogeneous Computing"** with sub-themes including subjects such as "Why Heterogeneous Computing?", "Hardware Sub-Systems", "Co-Design and Environment" and "Emerging Technologies".

CIUK 2021 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 second instalment of the CIUK Student Cluster Challenge. We will also present our annual Jacky Pallas Memorial Award. All of this will take place on-site at Manchester Central with the presentations also broadcast live online.

These safety measures have been agreed with the venue and the CIUK Scientific Advisory Committee, and will be in place throughout the conference.

Please take time to visit the CIUK exhibition and we would also like to invite you to join us on the evening of Thursday 9 December – immediately following the CIUK keynote presentation – for the CIUK networking event.

We remind everyone to please respect social distancing measures where possible. **The wearing of face coverings in communal areas is mandatory.**

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 #CIUK2021 for the latest live updates.

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

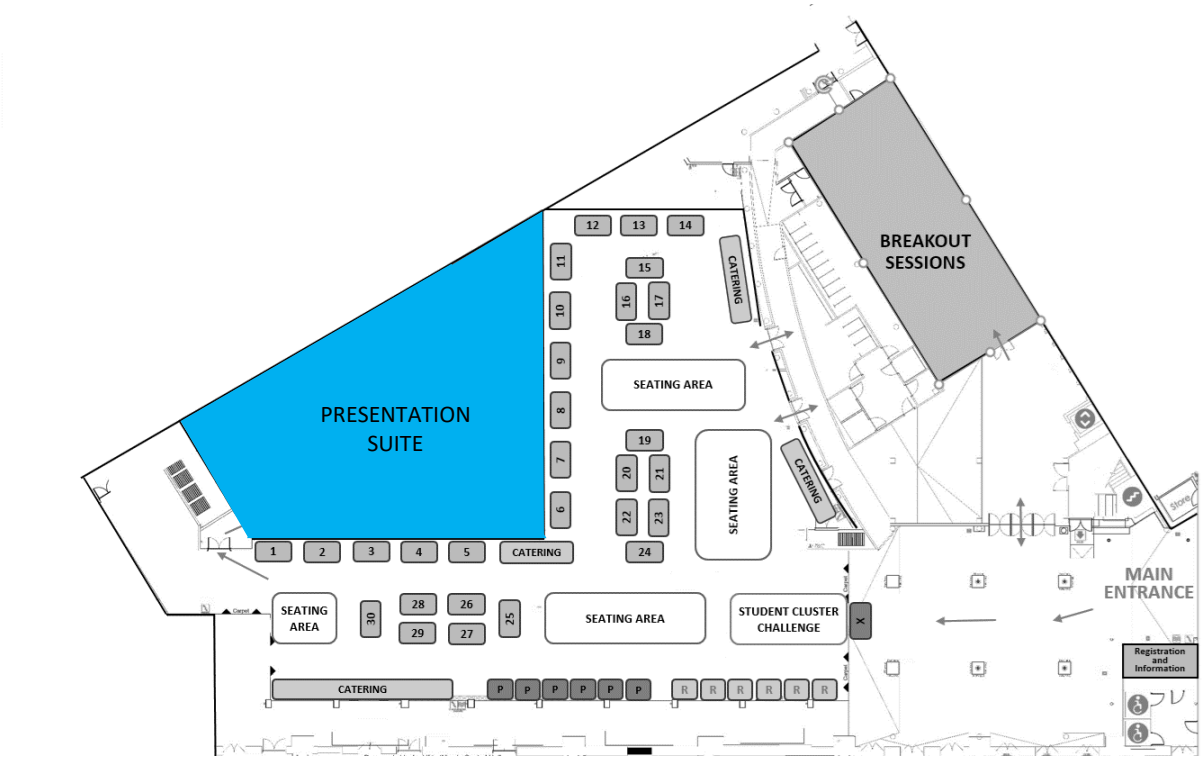
The CIUK team will be happy to assist.

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 2021 PROGRAMME

The main CIUK 2021 programme will take place in Charter Room 1. Look for the BLUE pull-up banners.



Day 1 - Friday 10 December

	Session 1: Why Heterogeneous Computing?
	Session 2: Hardware Sub-Systems
	Session 3: The ExCALIBUR Programme

TIME	MAIN PROGRAMME	BREAKOUT SESSIONS
From 08:30	**Registration Open (Main Foyer)** **Exhibition Open (Gallery)**	
09:15 - 09:30	**Tom Griffin** (Director, Scientific Computing, STFC) *Welcome and Introduction*	
09:30 - 10:00	**Steve Hindmarsh** (Head of Scientific Computing, The Francis Crick Institute) *Heterogeneous Computing at the Crick*	
10:00 - 10:30	**Phil Hasnip** (University of York) *Portable acceleration of materials modelling software: CASTEP, GPUs and OpenACC*	CoSeC Computational Science Centre for Research Communities **Annual Conference 2021** Thursday 9 December @ CIUK 2021
10:30 - 11:00	**Dr Igor Baratta** (Department of Engineering, University of Cambridge) *Heterogeneous Programming for Finite Element: insights from benchmarks*	
11:00 - 11:30	**REFRESHMENTS**	
11:30 - 12:00	**Paul Calleja** (University of Cambridge) *The Modern Cloud Native Heterogeneous Super Computer – A Converged Platform for Simulation, AI & Data Analytics*	
12:00 - 12:30	**Alastair Basden** (Durham University) *The Durham Intelligent NIC Environment (DINE)*	
12:30 - 13:00	**Andrew Edmondson** (Research Software Group Leader, Advanced Research Computing, University of Birmingham) *Installing and curating software for heterogeneous compute environments*	
13:00 - 14:00	**LUNCH**	
14:00 - 14:30	**The ExCALIBUR Programme**	

14:30 - 15:00	**Dr Elizabeth Bent** (Senior Portfolio Manager, UKRI-EPSRC) *Harnessing Exascale Computing – an ExCALIBUR overview*	
15:00 - 15:30	**Rob Akers** (UKAEA) *ExCALIBUR – exploiting the exascale to bottle a star* **Nigel Wood** (Met Office) *ExCALIBUR and the quest for the holy grail of weather & climate prediction* **ExCALIBUR Panel Discussion and Q&A Session**	
15:30 - 16:15	**REFRESHMENTS**	
16:15 - 17:00	**Martyn Guest** (ARCCA, Cardiff University) *Performance of Computational Chemistry Codes. An Analysis of Molecular Dynamics and Electronic Structure Applications on Multi-core Processors*	
17:00 - 18:00	**Keynote Presentation - Simon McIntosh-Smith (Bristol University)** *Heterogeneous Computing: past, present and future*	
18:00 - 20:00	**CIUK 2021 Networking Event** Join us at Manchester Central for wine, beer and nibbles. All registered attendees are invited!	

Day 2 - Friday 10 December

	Session 4: Co-Design and Environment
	Session 5: The Skills Gap
	Session 6: Emerging Technologies

TIME	MAIN PROGRAMME	BREAKOUT SESSIONS
From 08:30	**Registration Open (Main Foyer)** **Exhibition Open (Gallery)**	
09:30 - 10:00	**Professor Mark Parsons** (EPCC Director at The University of Edinburgh / EPSRC Director of Research Computing) *The UK Exascale Project*	
10:00 - 10:30	**Jeff Hammond and Filippo Spiga** (NVIDIA) *Shifting through the Gears of GPU Programming: Understanding Performance and Portability Trade-offs*	
10:30 - 11:00	**The Jacky Pallas Memorial Presentation**	

	Dr Niall Jeffrey (Ecole Normale Supérieure & University College London) *Mapping dark matter with the Dark Energy Survey and AI*	 Spectrum Scale User Group
11:00 - 11:30	**REFRESHMENTS**	
11:30 - 12:00	**The UK Skills Gap** **Richard Gunn** (UKRI) Skills gaps in the context of the wider approach to DRI within UKRI **Michael Ball** (BBSRC) UKRI's approach to supporting DRI skills **Prof Mark Wilkinson** (DiRAC) The DiRAC Facility HPC skills training programme **Christine Kitchen** (Cardiff University) Ideas to address skills gaps **Andrew Medhurst** (Inspire People) Title TBC **Skills Gap Panel Discussion and Q&A Session**	
12:00 - 12:30		
12:30 - 13:00		
13:00 - 14:15	**LUNCH**	
14:15 - 14:30	**Award Presentation** The CIUK 2021 Student Cluster Challenge and Poster Competition	
14:30 - 15:00	**Prof Viv Kendon** (University of Strathclyde) *QEVEC: integrating quantum computing with HPC*	
15:00 - 15:30	**Nick Brown** (EPCC, University of Edinburgh) *FPGAs for scientific workloads: The why and the how*	
15:30 - 16:00	**Gihan Mudalige** (Reader (Associate Professor), University of Warwick, Department of Computer Science) *Multi-Layered Abstractions for Performance Portability - Lessons Learnt and Challenges*	
16:00	**CIUK 2021 CLOSES**	

CIUK 2021 KEYNOTE PRESENTATION

Professor Simon McIntosh-Smith
Professor of High Performance Computing
PI for the Isambard GW4 Tier 2 HPC service
Head of the HPC Research Group
Department of Computer Science
University of Bristol

Twitter: @simonmcs
Web: http://uob-hpc.github.io/SimonMS/
HPC research webpage: http://uob-hpc.github.io

"Heterogeneous Computing: past, present and future"

ABSTRACT: Heterogeneous computing has been a part of HPC almost since the field began, but the current wave, which began 15 years ago, is the most significant revolution in the field since the commodity cluster. In this talk we will explore where this trend has come from, discuss its implications, and consider how our community needs to act in order to be ready for the era of heterogeneous Exascale supercomputers. We will also discuss related initiatives in the UK, such as ExCALIBUR and the UK's Exascale programme.

BIO: Simon McIntosh-Smith is Professor of HPC at the University of Bristol, UK. He began his career in industry as a microprocessor architect, first at Inmos and STMicro in the 1990s, before co-designing the world's first fully programmable GPU at Pixelfusion in 1999. In 2002 he co-founded ClearSpeed Technology where, as Director of Architecture and Applications, he co-developed the first modern many-core HPC accelerators, which lead to the creation of the first modern heterogeneous supercomputers, such as Tsubame 1.0 at Tokyo Tech in 2006. He now leads the HPC Research Group in Bristol, where his research focuses on advanced computer architectures and performance portability. He leads the Isambard supercomputer service which combines Arm-based CPUs with a diverse range of CPUs and GPUs from all the main vendors.

ABSTRACTS AND SPEAKER BIOS

Abstract: The presentation will provide an overview of the current and future Scientific Computing landscape at the Crick, which features a heterogeneous range of compute resources and (crucially) the skills and support for researchers to apply them effectively. It will also show examples of Crick research to understand life and benefit human health, made possible by Scientific Computing.

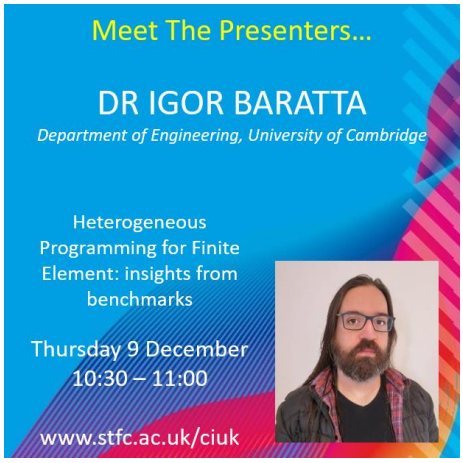
The overall premise of the talk is that our researchers need access to a wide range of computing resources to enable their research, and help to make the best use of them.

Bio: I joined the Crick in 2017 and lead the Scientific Computing Science Technology Platform (core facility) with a team of 20+ staff providing specialist scientific computing services including software development/engineering, machine learning/AI, research data services and databases to over 1500 researchers. We provide specialist support to 100+ research groups and 15 other Science Technology Platforms at the Crick as well as participating in collaborations across the wider biomedical community.

I am a biology graduate that 'defected' to IT, with over 20 years of experience working with scientists to provide the scientific computing tools to enable their research. I was previously Head of IT at the NERC Centre for Ecology & Hydrology, where I was responsible for provision of scientific computing and core IT services and support.

Abstract: CASTEP is a leading first-principles materials modelling program, which uses quantum mechanics to predict the chemical, electronic and physical properties of materials. CASTEP is parallelised using OpenMP and MPI, and is widely used on HPC facilities, including ARCHER2 where it typically consumes 5% of monthly CPU cycles. In this presentation we will present work to extend CASTEP to exploit heterogeneous architectures, in particular GPGPUs, using OpenACC. We discuss the challenges and opportunities presented by accelerator-based architectures, and the approach taken in the CASTEP OpenACC port. Whilst the port is still under active development, early performance results show that significant speed-ups may be gained, particularly for materials simulations using so-called “non-local functionals,” where speed-ups can exceed a factor of ten.

Bio: 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, and is also on the "Materials and Molecular Modelling" working group for the UK's ExCALIBUR exascale HPC programme, working to ensure the key UK materials modelling methods are ready for the next generation of HPC machines.



Abstract: Finite Element software packages have struggled to get good performance from GPUs and accelerators in the past. Partly, this was due to the limited memory capacity of earlier devices, but it is also essential to consider the memory layout, the details of the kernel code, and where it runs.

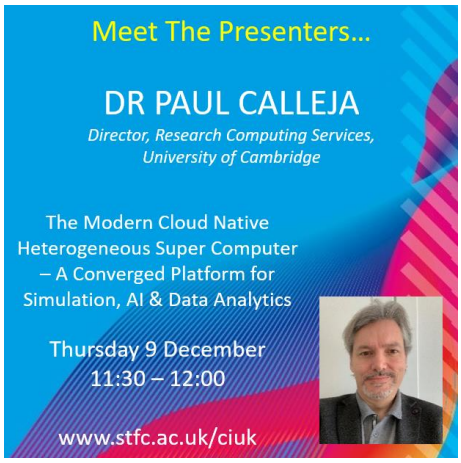
This presentation will consider the performance of the finite element method on different architectures and accelerators using the FEniCS finite element libraries and the SYCL programming model. SYCL is a modern kernel-based parallel programming model that allows one code to be written, which can run on multiple types of computational devices.

This kernel-based model matches nicely with the latest FEniCS data-centric design: the top-level C++ library creates data to operate in parallel (geometry, topology, and dof layout information) and an automatic code generator emits efficient code that can be used as part of the kernel.

Finite element codes have several parts, often subdivided into: mesh and domain handling, formulation of the equations of interest, assembly and linear solve. The linear solve is the most computationally intensive, and for all problems of size worth consideration on HPC systems, a direct solve is not scalable. Iterative solvers are a necessity, and the cost per iteration is strongly affected by the cost of memory access. Various strategies can be used to minimise data movement, and this often means considering some merging of the assemble and solve phases. We will demonstrate some of the approaches we have taken with FEniCS and SYCL to obtain the best performance from the currently available hardware.

We will also discuss how different ways of expressing parallelism can affect the performance of finite element code on heterogeneous architectures. We will consider how arranging memory transfer and allocations can reduce latency and increase throughput in different accelerators. Finally, we will show some performance results from our Excalibur Project (Excalibur-SLE) using our code in the well-known CEED benchmarks from the ECP programme. We will present results for several architectures, including Intel Ice Lake CPU and NVIDIA A100 GPU.

Bio: Igor Baratta is a Research Associate in Scientific Computing at the University of Cambridge. He completed his PhD and undergraduate degrees in Electrical and Computer Engineering at UFMG in Brazil. Prior to completing his PhD, he was an R&D Engineer working on computational electromagnetics at a multinational aerospace company.



Abstract: During the presentation we will position research computing infrastructure as a vital national capability driving research innovation and enabling the knowledge economy and industrial competitiveness whilst also providing vital resources in terms "Urgent Computing" for national emergency response activities. We will look at how modern research computing infrastructure is evolving from the traditional monolithic proprietary, highly specialized supercomputers of the past to cloud native heterogenous high performance infrastructure supporting converged AI, simulation and data analytics workloads. We will illustrate this trend by looking at the Cambridge Research Computing Service, its infrastructure, operational model and a selection of use cases and current development / outreach activities that may be of interest.

Bio: Dr Calleja is Director of Research Computing at the University of Cambridge where he oversees one of the UK's leading large-scale National HPC centres supporting a diverse community of UK frontier science, engineering, and medical research programmes.

Dr Calleja has a strong academic / industrial HPC co-design background focusing on commodity open standards-based solutions. Recently he has pioneered the convergence of OpenStack and Research Computing use-cases, working with industry partners to develop the "Scientific OpenStack", a software defined supercomputing middleware solution making large scale cloud native supercomputing a reality.

Dr Calleja also heads up the Cambridge Open Exascale Lab a prominent UK academic / industrial collaboration aimed at the development and democratisation of exascale computing solutions.

Abstract: We present the DINE cluster which uses NVIDIA Data Processing Unit (DPU) technology in the form of BlueField cards to enable advanced HPC algorithms.

Now entering its second generation, DINE is a 24 node test cluster equipped with AMD Rome processors, 512GB RAM per node and NVIDIA BlueField DPUs. BlueField-2 DPUs contain 8-core ARM processors at >2GHz and offer a 200GBit/s HDR network interconnect which is shared with the host. The DPUs have access to host memory via RDMA.

Here we present the hardware and software configuration of DINE, and discuss how this heterogeneous compute cluster provides insight into future Exascale systems. We provide researcher use cases and describe how codes can be adopted to benefit from the flexibility of the underlying architecture.

Bio: Alastair is the technical manager for the DiRAC Memory Intensive HPC service hosted at Durham.

Abstract: The Advanced Research Computing team at the University of Birmingham operates evolving and constantly-changing heterogenous compute environments. This includes the Baskerville Tier 2 HPC, our BlueBEAR Tier 3 HPC, and own-cloud virtual machines. Across these compute systems we currently have five different CPU architectures: Intel (Haswell, Broadwell, Cascade Lake and Ice Lake) and IBM POWER9, running RedHat, CentOS Stream and Ubuntu operating systems. We also operate multiple different NVIDIA GPU models, from K40 to A100.

We manage a large range of over 1,000 applications across all these systems, using EasyBuild and a suite of our own automation and management tools to maintain quality, consistency and minimise the staff time required. These applications can be seen on the automatically-updated websites https://bear-apps.bham.ac.uk/ and https://apps.baskerville.ac.uk.

In this talk I will tell the story of how our processes, systems and tools have evolved over time from a single, homogenous HPC cluster to our current, complex heterogenous environment. I will explain some of the difficulties and challenges we encountered, and how we have overcome them – including the times we have chosen to spend time in order to save time.

Bio: Known as "Ed", I started my career as a software engineer and team leader at QinetiQ, after completing an MMath at the University of Oxford. I left QinetiQ to complete a BA in Theology at Birmingham Christian College after which I worked part-time as a senior developer at ApplianSys working on embedded Linux and Python firmware for network appliances.

I completed a part-time PhD in New Testament Textual Criticism in the Institute for Textual Scholarship and Electronic Editing (ITSEE) at the University of Birmingham supervised by Professor David Parker. The title of my PhD thesis is "An analysis of the coherence-based genealogical method using phylogenetics" and is available online here. I am currently an Honorary Fellow of ITSEE.

In 2016 I joined Advanced Research Computing at the University of Birmingham and founded the Research Software Group (RSG). The RSG supports researchers using ARC's various compute resources, and offers advice, coaching, coding, mentoring and training to researchers and RSEs across campus.

I am an active member of the Society of Research Software Engineering, and was the Programme Chair of the 2019 UK RSE Conference.

Abstract: ExCALIBUR is a UK research programme that aims to deliver the next generation of high-performance simulation software for the highest-priority fields in UK research. The programme brings together experts across the research landscape to address the efficiency of simulation codes that will transform capability within UK science and develop expertise for the next generation of supercomputers. This presentation will provide an overview of the programme to date and provide an insight into the science highlights so far.

Bio: Elizabeth is a Senior Portfolio Manager in the Research Infrastructure Team. She manages the UK Research and Innovation (UKRI) aspects of the ExCALIBUR Strategic Priority Fund programme including the ExCALIBUR Steering Committee. She joined EPSRC in July 2017 as a member of the Energy Team where she worked in a range of research areas and convened the Energy Programme Scientific Advisory Committee.

Abstract: At the heart of the UK's national capability in weather & climate prediction is a complex, unified modelling system which comprises an observation processing system, a data assimilation system, a dynamical model of the atmosphere, a number of marine modelling systems, a land surface model, a chemistry model, a variety of subgrid-scale parametrisations, as well as all the infrastructure to manage the data flow into, through, and out of the coupled system of models. I will briefly introduce this system and discuss why being able to fully exploit Exascale computers is so important to us in our quest to continually improve the accuracy of weather & climate predictions. This will explain what might be referred to as the holy grail of weather & climate prediction capability. For most of the components of the system, exploiting Exascale machines requires a redesign of the software infrastructure. For some of the components, a complete redesign of the algorithmic approach is also required. Co-design, application of the principle of a separation of concerns, data science, and software engineering

expertise are all key to the success of this venture; they are also the pillars of ExCALIBUR. I will outline the important role that ExCALIBUR has in preparing the path to our holy grail.

Bio: I am the Senior Science Supplier for the Met Office's Next Generation Modelling Systems programme. This is one of the Met Office's corporate strategic actions which aims to reformulate and redesign our complete weather and climate research and operational/production systems, including oceans and the environment, to allow us and our partners to fully exploit future generations of supercomputer for the benefits of society. I am also the Met Office Senior Science Supplier for the Exascale Computing Algorithms and Infrastructure for the Benefit of the UK (ExCALIBUR) Project which has similar aims to NGMS but applied more broadly across the UK's supercomputing landscape. Both the Next Generation Modelling Systems programme and ExCALIBUR are targeting application on supercomputers of the mid-2020s and beyond.

After studying maths at university, I joined the Met Office to work on parametrising the effects on large-scale flows of unresolved turbulent flow over hills. This led to the award of my PhD from Reading University in 1992. At the turn of the millennium I migrated from the area of physical parametrisations to the Met Office's Dynamics Research group becoming responsible for the design and implementation of our operational dynamical core. Since that went operational in 2014 my attention has increasingly turned to ensuring that our modelling systems are ready to fully exploit the supercomputers of the future. This has included leading the GungHo project to develop a highly scalable dynamical core that at least matches the accuracy of our current one. GungHo and the associated infrastructure project, LFRic, were the precursors to the Next Generation Modelling Systems Programme.

Abstract: The UK Atomic Energy Authority (UKAEA) has been set a grand challenge – to help UK achieve Net Zero by delivering fusion energy to grid in the 2040's. Fusion is the process that powers our Sun. Recreating the fusion process here on Earth by confining a hot, thermonuclear plasma inside a "magnetic bottle" or "tokamak" however is challenging, and has often been referred to as the "holy grail" of power production. Since the advent of modern computing and with a growing understanding of the complex physics that describes the fusion plasma, our ability to design a viable fusion reactor concept has for a long time been heralded an "exascale challenge". The exascale itself is, of course, nearly upon us. Rob will briefly describe one of the most challenging areas of tokamak plasma modelling being tackled through the ExCALIBUR programme – the so-called plasma "exhaust", a region of the machine where hot plasma leaves the confined plasma core and encounters the tokamak first wall. This part of the machine is a well established, multi-physics, multi-scale problem. We have therefore assembled a rainbow team of UK researchers and developers to co-design a brand new, "actionable", scalable and performance portable platform that will be capable of exploiting the world's first exascale supercomputers. The project connects across half a dozen ExCALIBUR Cross Cutting (XC) Theme projects together with a Hardware and Enabling Software (H&ES) programme necessary for systems co-design. As we enter the commercial fusion and exascale era, supercomputing and interdisciplinary collaboration will be key to success – a very demanding timeline necessitates that the reactor design process and our journey up the engineering "S-curve" must take place "in-silico" rather than in the

real world via test-based design. The ExCALIBUR programme, with its underpinning four pillars as a core element of UKAEA's mission couldn't, therefore, be more timely.

Bio: Rob is Department Manager and Programme Lead for Advanced Computing at UKAEA. He is leading a rapidly growing team of experts into the exascale and AI era of supercomputing with a mission to "accelerate the delivery of commercial fusion energy by exploiting advances in data science and extreme scale computing". Programmes managed by Rob and his group leaders include the £5M ExCALIBUR High Priority Fusion use case (project NEPTUNE), the Advanced Computing Programme within UKAEA's EPSRC Fusion Grant (focusing upon low TRL research), a new collaboration with STFC HNCDI to grow an Extreme Scale Computing Centre to Advance Fusion Energy at Hartree Centre, Daresbury Laboratory: https://www.hpcwire.com/2021/08/19/uks-new-extreme-scale-computing-center-to-advance-fusion-energy/, collaborations with the University of Cambridge and the Cambridge/Intel Open Exascale Lab (https://www.exascale.hpc.cam.ac.uk) and a new partnership with the University of Manchester focusing upon Fusion Digital Engineering: https://www.gov.uk/government/news/fusion-research-partnership-agreed-between-ukaea-and-the-university-of-manchester).

Rob gained a PhD. in High Energy Physics from the University of Manchester in 1995 (based at CERN) and has worked for UKAEA ever since. His early career was as a plasma modeller and experimentalist, working on the pioneering START Spherical Tokamak and then the EPSRC flagship tokamak MAST. Around a decade ago he became interested in GPU programming after visiting the Machine Evaluation Workshop (predecessor to CIUK) where every stand in the vendor space seemed to be showcasing GPU solutions. After a decade of programming CUDA he must now be content to let his team enjoy delivering technical work while he instead concentrates on how to scale operations in order to deliver the world's first commercial fusion reactor, a machine called STEP: https://step.ukaea.uk.

Abstract: This session will overview application performance on a variety of clusters, focusing on the Intel Ice Lake and AMD EPYC Milan family of processors. Using the Intel Skylake Gold 6148 as the baseline, an assessment is made across a variety of Ice Lake (8358, 8352Y, 8368Q and 8360Y) and Cascade Lake SKUs (e.g., the 9242-AP, 8280, 6252 and 6248), with system interconnects from both Mellanox and Intel. Attention is also focused on the AMD Milan (7713, 7513) and Rome SKUs (e.g., the 7702 and 7502). Our analysis is based on the familiar parallel benchmark performance using popular chemistry community codes – from Molecular Dynamics (DL_POLY, Gromacs and LAMMPS), Quantum Chemistry (GAMESS-UK) and Materials Science (VASP, CASTEP). 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 in now 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 Group Leader of the HPC Chemistry Group at PNNL, before returning to the UK as Associate Director of Daresbury's Computational Science and Engineering Department. He joined Cardiff University in April 2007 and is

their Director of Advanced Research Computing as well as Technical Director of both the HPC Wales and successor Supercomputing Wales programme.

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 250 journal articles.

Abstract: The Exascale era is upon us. China is already operating two Exascale systems and the first Exascale system in the USA – Frontier – will go live soon. The UK Government has committed to have a UKRI Exascale supercomputer in operation by 2025. This talk will summarise the UK Exascale Project with insights into the hosting of such a system and what the system is likely to look like from a technical standpoint. The Exascale system will enable the UK's internationally respected computational science community to cement the UK as a global science and technology superpower.

Bio: Mark Parsons is Director of EPCC, the supercomputing centre at the University of Edinburgh. He has a Personal Chair in High Performance Computing at the University and has worked for EPCC since 1994 following his PhD in Particle Physics at CERN in Geneva. In addition to being in charge of the most of the UK's national supercomputers at EPCC's data centre outside Edinburgh, he also has responsibility for the Edinburgh International Data Facility, a key part of the Edinburgh & SE Scotland City Region Deal. One day per week he works for UK Research & Innovation as EPSRC's Director of Research Computing. He is best known internationally, particularly in the Europe, for his work with the industrial applications of HPC with a specific focus on SMEs. He also has had the honour in 2021 of being the Chair of the ACM Gordon Bell Prize committee.

Abstract: This talk will show implementations of standard linear algebra algorithms in a range of programming models, including standard language parallelism, directives/pragmas, and CUDA, and how the performance and productivity varies across these. Unlike my GTC talk, this one will show Python results, in addition to Fortran, C and C++.

Bio: Jeff Hammond is a Principal Programming Model Architect at NVIDIA, working on open standards, the ARM HPC software ecosystem, and scientific applications. He is based in Helsinki, Finland. Previously, Jeff worked at Intel and Argonne on a wide range of HPC hardware and software projects. He received his PhD in Chemistry from the University of Chicago for work on NWChem.

Filippo Spiga works as EMEA HPC Developer Relations manager and Arm HPC ecosystem Alliance manager at NVIDIA. In these roles, he works closely with computational scientists from several science domains to understand their needs and help them prepare their software to run efficiently on current

and future Arm-based GPU-accelerated. Prior NVIDIA, Filippo worked at Arm Research, University of Cambridge, ICHEC, CINECA and IBM Research. He has been developing and contributing in various HPC codes (mainly Physics, Chemistry and Engineering) for more than a decade. He is based in Cambridge (UK).

Abstract: ExCALIBUR cross-cutting project QEVEC - quantum enhanced and verified exascale computing - contributes to the development of exascale computing by focusing on how to add quantum computers as co-processors to HPC. Early quantum computers will be much smaller -- in terms of the amount of classical data they can process in one go -- than current HPC.

But the processing power on that data can be much faster due to their quantum properties of superposition and coherence. The most promising way to use them is thus to accelerate those parts of the computations that are slow for HPC. This requires detailed study of the algorithms, both quantum and classical, which QEVEC will do for two specific applications areas, fluids simulations and materials simulations. I will explain why quantum computing is so promising for enhancing computational capability, while avoiding the current hype, and focusing on the hard work required to realise this potential for useful applications.

Bio: Prof Kendon joined Strathclyde in Nov 2021 as Professor of Quantum Technology, has been working on quantum computing for the past 20 years, including three fellowships, most recently EPSRC Established Career Fellow in Hybrid Quantum Computing (2014-19 at Durham University). She is PI of QEVEC, ExCALIBUR cross-cutting project Quantum Enhanced and Verified Exascale Computing incorporating quantum computing into future exascale high performance computing, and chairs CCP-QC, the Collaborative Computational Project in Quantum Computing, an EPSRC-STFC funded network linking quantum computing and scientific computing experts in applications suitable for quantum enhancement.

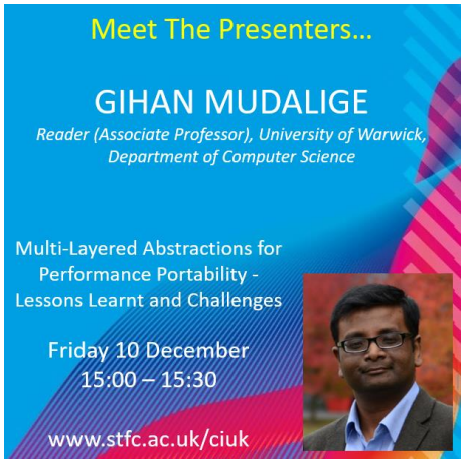
Abstract: Field Programmable Gate Arrays (FPGAs) enable the electronics of the chip to be configured to represent a specific kernel or application.

Such tailoring of the electronics to the code means that we bypass the general purpose micro-architecture of CPUs and GPUs, thus being able to organise aspects such as the logic and cache memory to entirely suit what is being executed. Whilst FPGAs have been popular in embedded computing for years, they are yet to gain wide acceptance for HPC workloads. There are a variety of reasons for this, but in the past couple of years there has been massive investments made by vendors in FPGA hardware and software ecosystems, making them a much more attractive choice than ever before.

In this talk I will use real-world applications and kernels to describe the role we see for FPGAs complimenting other hardware technologies at the exascale. I will describe that, whilst high performance is possible, the devil is in the detail and the programmer must recast their algorithm into a dataflow algorithmic style. Lastly I will provide access details for the ExCALIBUR H&ES FPGA testbed, where audience members can sign-up to for free and experiment with FPGAs for their workloads.

Bio: Dr Nick Brown is a Research Fellow at EPCC the University of Edinburgh with interests in HPC application development, novel heterogeneous architectures, data science, programming language design, and compilers.

He is involved with running the UK's FPGA testbed system, which aims to encourage HPC developers to experiment with exploring FPGAs for their scientific and engineering workloads. Nick is a course organizer on EPCC's MSc in HPC and data science courses, as well as supervising MSc and PhD students.



Abstract: The rapid evolution of High Performance Computing architectures has resulted in highly complex systems with massively parallel heterogeneous processors, deep and multiple memory hierarchies and interconnects. As a result, maintaining performance as platforms change has becomes increasingly difficult. On the one hand, open standards have been slow to catch up with supporting new hardware, and for many real applications have not provided the best performance achievable from these systems. On the other hand, proprietary solutions have only targeted narrow vendor-specific devices resulting in a proliferation of parallel programming models and technologies. The only practically viable approach to addressing the above issue, is through the development of appropriate application-oriented, high-level programming abstractions such as Domain Specific Languages (DSLs). In this talk I will present how two of the earliest DSLs developed in the UK, OP2 and OPS, have been able to build on multi-layered abstractions techniques to address these challenges. I will detail how simple source-to-source and automatic code-generation techniques using maintainable software technologies have enabled us to develop frameworks that has remained agile in delivering performance portability in the face of nearly a decade of hardware and parallel programming innovations. I will also discuss lessons learnt and my outlook for our DSLs in the run-up to deploying exa-scale systems.

Bio: Dr. Gihan Mudalige is an Reader (Associate Professor) in High Performance Computing at the University of Warwick's Department of Computer Science. His research focuses on the development of next-generation high performance computing numerical simulation software libraries through the utilization of domain–specific languages and high-level abstraction frameworks. As part of this work Dr. Mudalige acts as one of the main developers of the OP2 and OPS embedded domain specific languages (eDSLs), two of the earliest high-level frameworks to demonstrate the utility of these techniques for developing production-grade HPC applications. In 2018, he was awarded a four-year Royal Society Industry Fellowship with Rolls-Royce plc., focusing on developing future-ready massively-parallel CFD simulations for Exascale HPC systems. Previously Dr. Mudalige worked as a Research Associate and Senior Researcher at the University of Oxford's eResearch Centre before joining the Warwick Computer Science faculty in 2016. He has also worked as a research intern at the University of Wisconsin-Madison's (US) Department of Computer Science and holds a PhD. in Computer Science from the University of Warwick. Dr. Mudalige is a member of the AC

CIUK 2021 EXHIBITION

The CIUK 2021 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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Swarm for HPC Environments

Hassle-Free, Multi-Tenant Object Storage Platform

BENEFITS

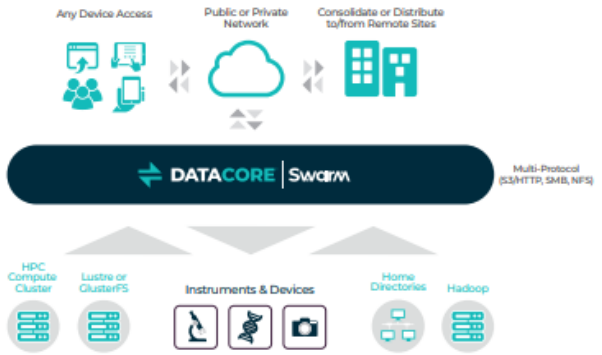
- Scale from TBs to 100s of PBs on any mix of standard hardware
- Eliminate tedious manual processes for infrastructure, data protection and tenant management
- Decrease time to discovery with integrated search and simple private/public file sharing

In high-performance computing (HPC), time to insight and discovery is determined by how quickly and easily your organization can ingest data from various sources, search for data and securely share data with authorized researchers, regardless of location. Due to performance requirements, HPC infrastructure managers have historically solved these issues using a mix of networked attached storage (NAS), distributed or parallel file systems, file transfer protocol (FTP) servers, web servers and tedious manual data authorization and access management. However, increasing capacity needs, more researchers in various locations capturing and analyzing data, along with a shift in access from traditional file protocols to RESTful interfaces are straining the status quo and hindering analysis and time to discovery.

The solution is DataCore Swarm that delivers a high-performance production infrastructure at scale simplifying content management and data access on highly resilient and cost-effective object storage. With Swarm, you no longer need to migrate data into disparate solutions for distribution, ongoing analysis and long-term preservation.

DELIVER PRIVATE OR PUBLIC STORAGE SERVICE

With Swarm you can rapidly deliver web-based storage services and provide secure access to internal or external users. Swarm snaps into existing access control systems (LDAP, AD, PAM, or token based) and comes with an integrated management portal for easy web- or API-based administration of tenants, quotas, data access and data protection policies.



SOLUTION BRIEF
NAS

RIVAL PARALLEL FILE SYSTEMS FOR READ INTENSIVE WORKFLOWS

DataCore Swarm does not require the use of any front side-caching mechanism or load balancers. Swarm's simple, flat architecture makes it low latency, self-balancing and highly symmetrical. This enables Swarm to handle many concurrent requests in parallel yielding the full throughput potential of all the drives in the system—resulting in 35 GB/s read and 12.5 GB/s write aggregate throughput via the S3 protocol on deployed HPC environments.

SIMPLE CONTENT MANAGEMENT, FILE SHARING AND SEARCH

In addition to the robust storage management user interface (UI), Swarm also has a built-in web-based UI and RESTful application program interface (API) for tenant and content management. Administrators can create buckets with capacity and bandwidth quotas and set unique data protection policies and access controls. Metadata, searches and queries are all customizable and interoperable with Elasticsearch 5 and the Elasticsearch application ecosystem. And, because the native interface to Swarm is based on HTTP, all files can be shared privately with those who have authorized access or publicly via a URL.

A BRIDGE FROM POSIX TO RESTFUL WORKFLOWS

Swarm's multi-protocol support enables interoperability with various HPC use cases making it easy to migrate data from compute clusters and network and direct attached storage (NAS and DAS) devices freeing up expensive primary storage and experimentation space. Swarm's native RESTful interface is based on HTTP 1.1 and supports the S3 protocol. The optional SwarmFS interface provides a method for S3 access to NFS data through rapid conversion of NFS data to Swarm objects delivering up to 1.6 GB/s sustained streaming in a single NFS server instance (over 3 PB per month) in HPC environments.

OPTIMIZE FILERS WHILE ELIMINATING STORAGE SILOS

In addition, DataCore offers FileFly, a Windows Server application that automates movement of cold and warm data from on-premises NAS devices and Windows filers to Swarm, Amazon S3, Google Cloud Storage or Microsoft Azure Blob Storage. FileFly enables you to consolidate data from disparate filers and tier data to the cloud for disaster recovery (DR) without disruption to end users or applications.

HPC CUSTOMERS COUNT ON DATACORE SWARM

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TEXAS TECH UNIVERSITY
UMC Utrecht
NIH National Institutes of Health
MAX PLANCK FLORIDA INSTITUTE FOR NEUROSCIENCE

0321

CIUK 2021 EXHIBITORS

X	CIUK Information Point
R	Research Zone - BEDE
R	Research Zone - SULIS
R	Research Zone - CIRRUS
R	Research Zone - MMM Hub
R	Research Zone - NI-HPC
R	Research Zone – JASMIN
R	Research Zone – Baskerville
P	Poster – Thomas Johnson
P	Poster – Megan Ratcliffe
P	Poster – Adam Tuft
P	Poster – Kieran Woodward
P	Poster – Jemma Bennett
P	Poster – Shrey Bhardwaj
1	
2	Cornelis Networks
3	Atos
4	Atempo
5	Boston Limited
6	BIOS IT
7	NEC Deutschland GmbH
8	DUG Technology
9	DDN
10	SambaNova Systems Inc
11	
12	Alces Flight
13	Kao Data
14	
15	SCAN
16	StrongBox Data Solutions
17	Scientific Computing World
18	GigaIO
19	NVIDIA
20	YellowDog
21	SoftIron
22	Panasas
23	Nexstor
24	Altair
25	VAST Data
26	Intel
27	Lenovo
28	IBM
29	OCF
30	DataCore Software / NAS

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NEC HPC Solutions

High Performance Computing (HPC) is a way to tackle complex mathematical, scientific or engineering problems. Alongside theory and experiment, computer-supported simulations of natural or technical processes have established themselves as a third pillar in the field of science and research.

It is nowadays inconceivable that an aircraft manufacturer or a Formula One racing team would operate without using simulation software. Scientific calculations, such as in the field of astrophysics, weather prediction, medicine, pharmaceuticals or life sciences, depend on supercomputing to a very large extent.

https://www.nec.com/en/global/solutions/hpc/

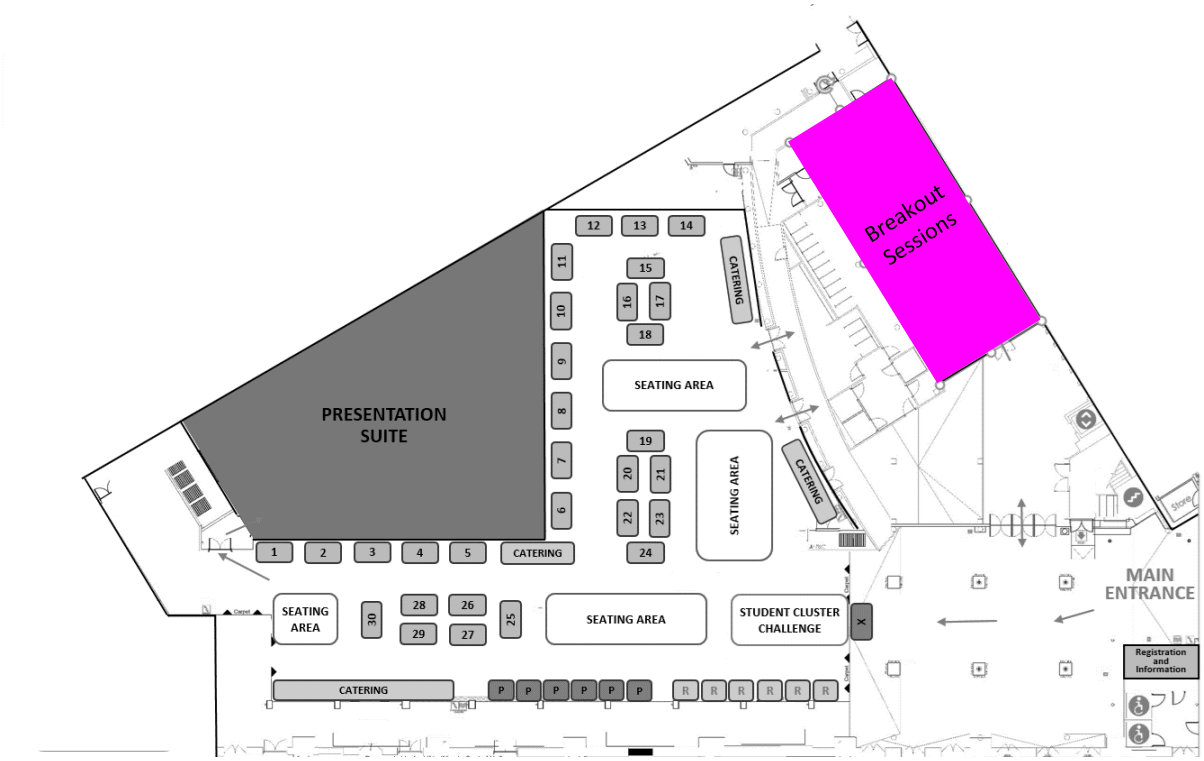
Range of services:

- x86 based High Performance Computing platforms
- Vector Computing with SX-Aurora TSUBASA
- GPU Computing with NVIDIA CUDA
- Storage Solutions
- HPC Network Technology
- Infrastructure Solutions with Water Cooled Racks and Direct Liquid Cooling
- Service and Support
- R&D with NEC Labs

\Orchestrating a brighter world NEC

CIUK 2021 PARALLEL BREAKOUT SESSIONS

The CIUK 2021 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 2021
Thursday 9 December @ CIUK 2021

CIUK is excited to welcome the first ever CoSeC Annual Conference to Manchester on Thursday 9 December (10:00-16:00).

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
Computational Science Centre for Research Communities

CoSeC@CIUK – 9th December 2021, Manchester Central

Session 1: Introducing CoSeC

- 10:00 - 10:20: ***Introduction to CoSeC*** (Barbara Montanari, *CoSeC director*)
- 10:20 - 10:40: ***Software citation & cataloguing*** (Alejandra Gonzales-Beltran & Gemma Poulter, *Data & Software Engineering Group*)
- 10:40 - 11:00***: CoSeC impact activities and wider lessons learned*** (Dawn Geatches, *CoSeC project office*)

11:00 - 11:30 - Break

Session 2: Exascale Computing

- 11:30 - 11:50: ***A Million Cores and Beyond: Opportunities and Outlook for Exascale Computing*** (David Emerson, *Computational Engineering Group*)
- 11:50 - 12:10: ***Materials modelling and particle simulations at exascale*** (Phil Hasnip, *University of York*)
- 12:10 - 12:30: ***CRYSTAL22 - Thanks for the memory*** (Ian Bush, *Theoretical & Computational Physics Group*)

12:30 - 13:30 - Lunch

13:30 - 14:30: Data Science

- 13:30 - 13:50: ***CoVal: Understanding SARS-CoV-2 variants by integrating genome and 3D structure data*** (Agnel-Praveen Joseph, *Biology and Life Sciences Group*)
- 13:50 - 14:10: ***The CCPi core imaging library, a versatile software for tomographic imaging*** (Edoardo Pasca, *Biology and Life Sciences Group*)
- 14:10 - 14:30: ***Simulation meets Machine Learning for supercharging science*** (Keith Butler, *Scientific Machine Learning Group*)

14:30 - 15:00 - Break

Session 3: Scientific Challenges

- 15:00 - 15:20: ***Nuclear thermal hydraulics for low-carbon applications - understanding energy and mass transport in advanced nuclear reactor systems*** (Wei Wang, *Computational Engineering Group*)
- 15:20 - 15:40: ***Towards a quantum annealing algorithm for determining crystal structures*** (Ronan Keegan, *Biology and Life Sciences Group & Adam Callison, University College London*)
- 15:40 - 16:00: ***Machine Learning for interatomic potentials*** (Alin Elena, Computational Chemistry Group)

Spectrum Scale User Group – Friday 10 December

Spectrum Scale User Group

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

CIUK 2021 RESEARCH ZONE

The CIUK 2021 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 2021 STUDENT CLUSTER CHALLENGE

Following the success of our first ever Student Cluster Challenge at CIUK 2020 the competition returns in 2021 with some changes that we think will improve the experience for everyone. As CIUK is returning to a physical, face-to-face conference the Student Cluster Competition became 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.

- Wednesday 13 October – Alces Flight (ONLINE CHALLENGE)
- Wednesday 27 October – Boston (ONLINE CHALLENGE)
- Wednesday 10 November – OCF (ONLINE CHALLENGE)
- Wednesday 24 November – Lenovo (ONLINE CHALLENGE)
- Wednesday 8 December – OCF (pm)
- Thursday 9 December – Lenovo (am) / Alces Flight (pm)
- Friday 10 December – Boston (am) - Results announced (pm)

This year we welcome back our defending champions Team Durham who are looking to defend their title against the new challengers from a combined Team Bristol / Bath.

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…

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 #CIUK2021_SCC.

The winning team will be announced before the final presentation session on Friday 10 December with the champions going forward to represent CIUK at the ISC'22 Cluster Challenge in Germany next summer.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CIUK 2021 JACKY PALLAS MEMORIAL AWARD

In 2019 we lost an incredibly important member of the CIUK Scientific Advisory Committee with the sudden and unexpected passing of Jacky Pallas at the age of just 54. Jacky was head of e-Research at King's College London and for the previous three years had been an active and vocal member of the CIUK SAC, helping to shape the direction our event has taken and pushing through many positive changes, whilst championing diversity and the inclusion of young researchers.

In her memory, and in recognition of her passion for our conference, we introduced an annual award that will highlight the work of an early career researcher and will allow the award winner a slot in the main programme at CIUK. Researchers are nominated by their supervisors and we are looking for nominations for presentations that highlight the impact of a project that early career researchers have been working on.

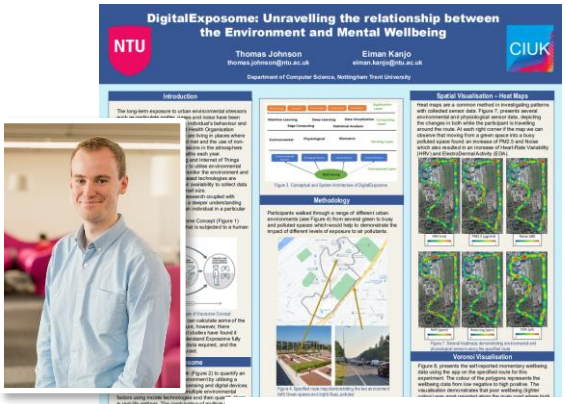
Congratulations to the winner of the CIUK 2021 Jacky Pallas Memorial Award… Dr Niall Jeffrey

Abstract: In the Dark Energy Survey (DES), we have created the largest ever map of dark matter – invisible matter thought to account for 80% of the total matter of the Universe – using gravitational lensing of galaxies. I will share the exciting developments used for this cosmic cartography over a quarter of the Southern Hemisphere. Exploiting this map to understand the unknown physics of the Universe, in the DiRAC project "Likelihood-free inference with the Dark Energy Survey", we combine GPU-accelerated cosmological simulations with novel artificial intelligence techniques. By using deep learning in a Bayesian framework, I will demonstrate how we can now quantify our belief in different cosmological models using information encoded in the new DES map.

Bio: Niall's research interests combine cosmology, statistical methods and machine learning. After completing his MSci in Theoretical Physics at Imperial College London, he completed his PhD at University College London supervised by Prof. Ofer Lahav. It was during his PhD that he became involved in the Dark Energy Survey and the European Space Agency's future Euclid mission.

CIUK 2021 STUDENT POSTER COMPETITION

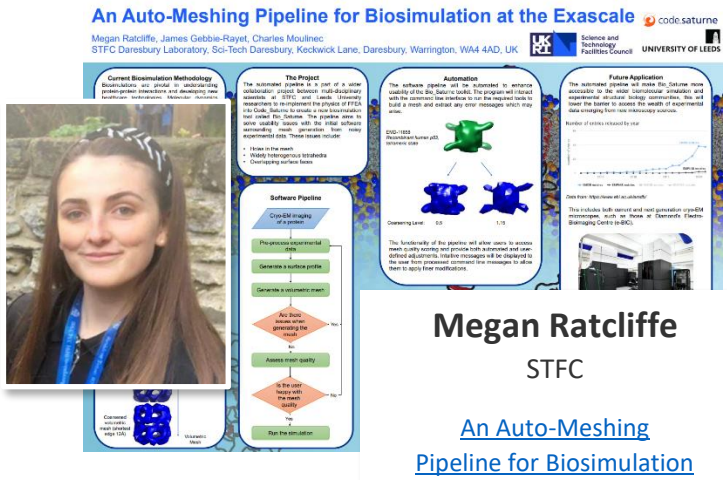
Six finalists have been chosen for the CIUK 2021 Student Poster Competition. Their posters can be viewed on the exhibition floor and also online. The winner will be announced prior to the final presentation session on Friday 10 December.



Thomas Johnson

Nottingham Trent University

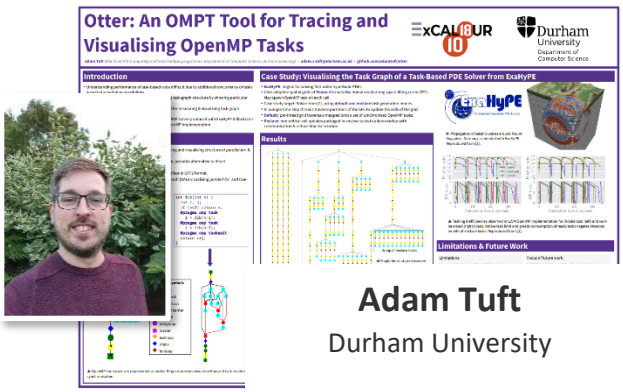
[DigitalExposome: Unravelling The Impact of the Environment on Mental Wellbeing]



Megan Ratcliffe

STFC

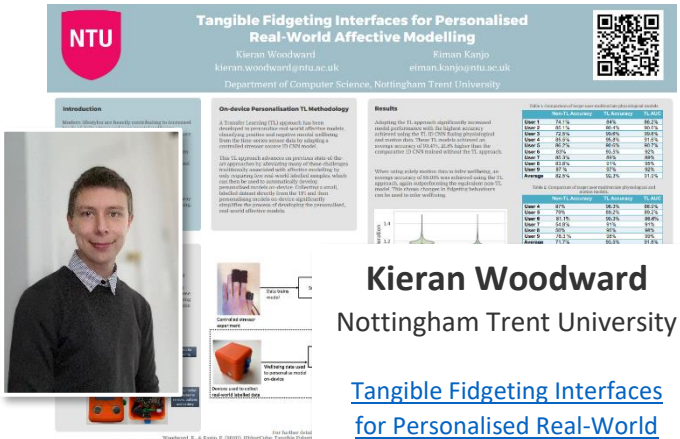
[An Auto-Meshing Pipeline for Biosimulation at the Exascale]



Adam Tuft

Durham University

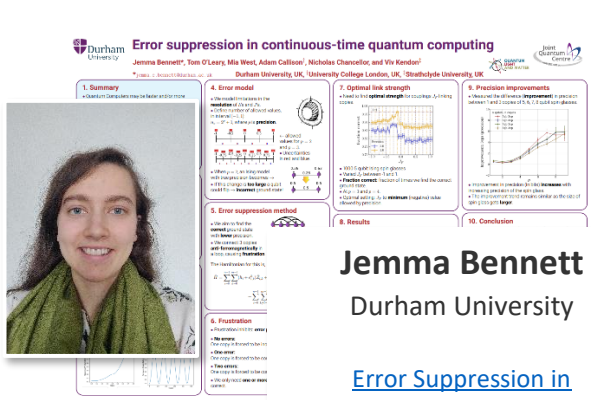
[Otter: An OMPT Tool for Tracing and Visualising Task Creation and Synchronisation in OpenMP Programs]



Kieran Woodward

Nottingham Trent University

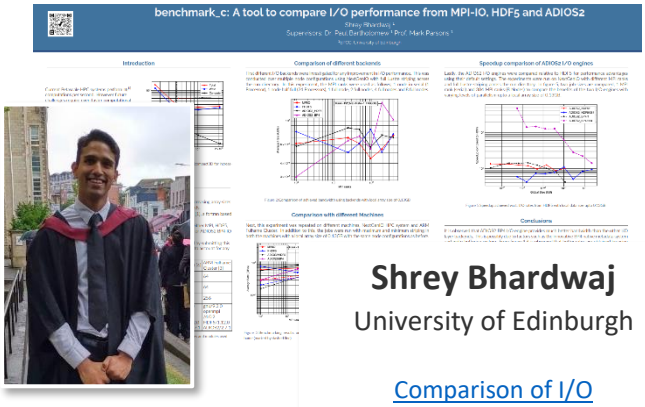
[Tangible Fidgeting Interfaces for Personalised Real-World Affective Modelling]



Jemma Bennett

Durham University

[Error Suppression in Continuous-time Quantum Computing]



Shrey Bhardwaj

University of Edinburgh

[Comparison of I/O performance of ADIOS 2 using benchmark_c]

See you in 2022…