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# Sustainable Reality 2025



**October 7, 2025**

Royal Society of Chemistry  
Burlington House, London

*Conference Preview*



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# Conference Preview

- About Sustainable Reality
- The RSC Library at Burlington House
- Conference Agenda
- 2025 Alces Flight Travel Fellows
- Main Session Speakers and Abstracts





# About Sustainable Reality

Sustainable Reality began in 2023 as a UK community event focused on making HPC and AI more practical and approachable.

The aim of our annual event is to spark conversations, share real experiences, and show how people and technology can work together to create lasting, sustainable solutions. Our goal is to cut through the jargon, keep things simple, and make sure everyone feels part of the journey.



# Royal Society of Chemistry

Since 1857, the Royal Society of Chemistry has been a home for ideas, innovation, and collaboration.

Located at Burlington House, alongside fellow learned societies and the Royal Academy of Arts—its historic Library and Information Centre (dating back to 1842) remains a living archive of scientific discovery.

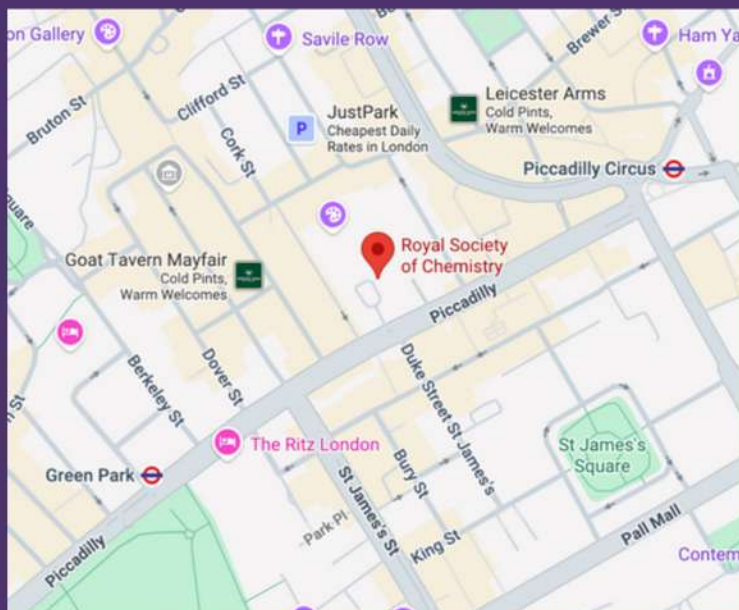
## How to get to the RSC

Burlington House  
Piccadilly, W1J 0BD

### **Closest Tube Stations:**

Green Park  
(Jubilee, Piccadilly, Victoria Lines)

Piccadilly Circus  
(Bakerloo, Piccadilly)



## **Come as you are.**



The RSC is known for hosting diverse audiences, from tourists to fellows and academics. No need to dress up! Whether you're a hoodie person or prefer a blazer and tie, you'll fit right in.





# Royal Society of Chemistry

The Burlington House courtyard provides an oasis of calm outside of Piccadilly - one of the busiest streets in London.

Upon entry to the courtyard the Royal Society of Chemistry is located to the right of the statue of Sir Joshua Reynolds.

*There are a few short steps into the main building with a lift available inside. If you require step-free access, please contact us.*



Entrance to Burlington House



RSC is to the right of the statue

**RA**

## Royal Academy of Arts (RA)

In the middle of Burlington House's courtyard, you'll find the Royal Academy of Arts (RA). It's both an art school and an exhibition space, with a mix of free and paid shows to check out. Right now, the main exhibition is Kiefer/Van Gogh, featuring works by both artists.



# Agenda

Welcome and Keynote



Time	Talk Title	Presented By
from 9:30	Arrival (Tea & Coffee)	
10:00	Welcome	Cristin Merritt <i>Alces Flight</i>
10:15	<u>Keynote Address</u> Catalysts for Change in Digital Chemistry: Redefining Drug Discovery Through Predictive Modelling and Supercomputing Synergy	Nathan Brown <i>RSC Fellow</i>
10:45	Break (15 minutes)	

catalysts for change





# Agenda

## Session One: "Designing for Better"

Time	Talk Title	Presented By
11:00	HPC in Formula One: Designs for Speed	Paul Cusdin <i>Alpine F1</i>
11:20	Quantum Computing - Roadmap, Uses and the Continuing Role of HPC	James Thorne <i>NQCC</i>
11:40	Compilers, Creatives, and Collaboration: What HPC Can Learn from DJs and Game Devs	Perry Gibson <i>Fractile</i>
12:00	Keynote and Speaker Q&A	
12:20	Lunch (40 Minutes)	

# Agenda

## Session Two: "Energy States"



Time	Talk Title	Presented By
13:00	Practical Approaches to Energy-Efficient Supercomputing	Wil Mayers <i>Alces Flight</i>
13:20	Lessons from the edge – what we've learnt when scaling data centre heat reuse	Mark Bjornsgaard <i>Deep Green</i>
13:40	Decoding Carbon: Energy Reporting in Supercomputing	Stu Franks <i>Concertim</i>
14:00	Break (20 minutes)	





# Agenda

## Session Three: "Rising Elements"

Time	Talk Title	Presented By
14:20	Reflections of a Technology Recruiter	John Fergusson <i>JDF Solutions</i>
	<b>Travel Fellows: Lightning Talks</b>	
14:40	Evaluating the Accuracy of Energy Measurement Tools for Data-Parallel Workloads in HPC Environment	Urooj Asgher TU Dublin
14:45	From Pixels to Pedigree: Visual-Transformer based Re-Identification and Genetic Inference of Guppies	Daniel (Danny) Ash <i>University of Oxford</i>
14:50	Beyond Code: How the Underlying Math Shapes HPC Performance	Xinger Tang <i>University of Edinburgh / EPCC</i>
14:55	GPU offloads for gravity in the SWIFT cosmology code	Sarah Johnston <i>Durham University</i>
15:05	Student Cluster Competitions: Empowering the next generation of HPC	Joseph Moore <i>University of Bristol</i>  Thomas Shtasel <i>Imperial College London</i>
15:35	Break (15 Minutes)	



# Agenda

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## Session Four: "Opportunities & Conclusion"



Time	Talk Title	Presented By
15:40	Green Computing Initiatives: UKRI and beyond	Dawn Geatches <i>UKRI</i>
15:55	Computing Insight UK and the Cluster Challenge	Damian Jones <i>STFC</i>
16:00	Closing Address: The Next Steps in Supercomputing	
16:20	Q&A and Wrap	
17:00	Event Concludes	



# Travel Fellows

*As part of our ongoing commitment to supporting the next generation of supercomputing leadership, the Alces Flight Crew created four pre-paid travel fellowships for SR25. We are delighted to announce the honoured recipients, who will be presenting their research to our community.*



## **UROOJ ASHGER, TU DUBLIN**

Urooj is a PhD researcher at Technological University Dublin Ireland (TU Dublin), focusing on energy-efficient high-performance computing. She is a recipient of the prestigious Irish Research Council Postgraduate Award for her doctoral studies. Her research aims to reduce the energy consumption of computing systems, particularly for data-parallel workloads on modern HPC platforms. She has conducted experimental studies comparing hardware and software-based energy

measurement tools using data-parallel kernels, as well as energy and performance benchmarking of machine learning algorithms. Her research goal is to contribute to greener and more efficient computing through accurate energy profiling, hybrid energy measurement strategies, and application-level optimisation.

She will be presenting, **"Evaluating the Accuracy of Energy Measurement Tools for Data-Parallel Workloads in HPC Environment"**

## **DANIEL (DANNY) ASH, OXFORD**

Daniel (Danny) Ash is a first-year DPhil candidate at the University of Oxford, where he applies machine-learning techniques to monitor and predict biodiversity. Danny's work fuses remote-sensing data, ecological field records and AI models to detect individuals within a species and understand the spatial dynamics across different species. Before returning to academia, Danny worked on R&D projects for methane-removal and anaerobic-digestion start-ups, using GIS data to find suitable locations. Originally trained as an astrophysicist, Danny completed a masters focussed on exoplanet detection. Across industry and research, Danny sought to use quantitative techniques to understand complex natural signals.



He will be presenting, From **"Pixels to Pedigree: Visual-Transformer based Re-Identification and Genetic Inference of Guppies"**





# Travel Fellows



## **XINGER TANG, EDINBURGH/EPCC**

Xinger Tang is an MSc student in High Performance Computing at EPCC, University of Edinburgh, with a strong mathematical foundation from an Honours Bachelor's degree in Applied Mathematics. She also works as a research assistant at Highlander Lab, Roslin Institute, University of Edinburgh. Her interests lie in research software engineering, with hands-on experience in parallel computing, GPU acceleration, and scientific simulations gained through both coursework and

collaborative projects. With a background bridging computer science and applied mathematics, Xinger is passionate about developing efficient, reliable tools for real-world research. Her current work includes implementing GPU versions of Lanczos methods with selective reorthogonalization and contributing to computational genetics projects in bioinformatics.

She will be presenting, "**Beyond Code: How the Underlying Math Shapes HPC Performance**"

## **SARAH JOHNSTON, DURHAM**

Sarah Johnston is a third-year astronomy PhD student in the Institute for Computational Cosmology at Durham University. She holds an MPhys in Astrophysics from University of St Andrews and is passionate about engaging with HPC and harnessing the full power of modern computing in astronomy.

Her PhD centres around implementing a GPU offload in the SWIFT cosmology code, where she is currently developing the GPU port for gravity calculations. Having already demonstrated a proof of concept, she is currently working on optimisation and effective implementation within SWIFT's task-based system. She also works separately on constraining mixed dark matter cosmologies using large-scale simulations.



Beyond her research Sarah is actively involved in outreach and skill development. She leads research groups for young people to get hands-on with coding and simulations and facilitates training for other researchers, helping them develop the computational expertise needed for modern astrophysics.

She will be presenting, "**From GPU offloads for gravity in the SWIFT cosmology code**"





# Main Session

*We are delighted to welcome our main session speakers. Hailing from academia, industry, and government institutions, we hope these speakers inspire you on your journey in creating sustainable supercomputing practices.*



## KEYNOTE: NATHAN BROWN

Globally recognised as a thought-leader in cheminformatics and computational drug discovery, Nathan is the inventor of the first multi-objective de novo molecular design system, published in 2004, and has published over 50 papers and four books on the field. Nathan is the 2017 recipient of the Corwin Hansch Award – an award given by the Hansch-Fujita Foundation for significant contributions to the field of computer-aided drug design. He is also an elected Fellow of the Royal Societies of Chemistry, Biology, and The Arts.

Nathan has worked in senior leadership positions at BenevolentAI and Healx, building and leading large interdisciplinary teams. Prior to this, Nathan was Head of In Silico Medicinal Chemistry at The Institute of Cancer Research in London where he founded and led the In Silico Medicinal Chemistry team for over ten years. In this capacity, he delivered significant scientific impact on drugs in active clinical trials, and was responsible for the development of new algorithms for drug discovery. He was also a Presidential Research Fellow at the Novartis Institutes for BioMedical Research and a Marie Curie Research Fellow at Avantium.

He will be presenting: **“From Catalysts for Change in Digital Chemistry: Redefining Drug Discovery Through Predictive Modelling and Supercomputing Synergy”**

In this talk, Nathan will trace the evolution of Digital Chemistry over the past 25 years: from a behind-the-scenes function to a central driver of drug discovery. He'll explore how predictive modelling techniques, from classical QSAR (the method for determining the relationship between chemical structures and biological activity) to quantum computing and LLMs, are being combined in increasingly powerful and sustainable ways to accelerate discovery and reduce experimental waste. His message is clear: the fusion of supercomputing and molecular science is more than just a technical achievement, it's a catalyst for real-world impact.

The keynote will explore themes including:

- Hybrid Predictive Modelling: Combining classical, physics-based, quantum, and AI-driven methods to enhance accuracy and speed in drug discovery.
- Sustainable Supercomputing: Using automated design and High-Performance Computing (HPC) to reduce experiments, cut resource use, and accelerate time to clinic.
- Collaborative Innovation: Driving progress through community platforms, open science, and empowering the next generation of digital chemists.







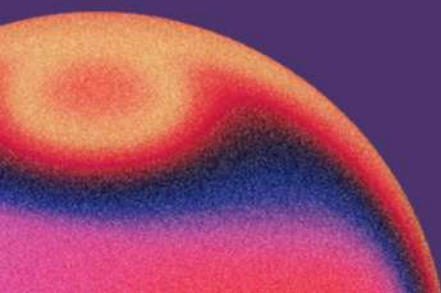
## **PAUL CUSDIN, ALPINE F1**

Paul Cusdin is the Head of CFD at Alpine F1 Team, a role he has held since 2018. He leads the team's efforts in applying advanced computational fluid dynamics to extract maximum performance from the car. Under his leadership, Alpine leverages cutting-edge simulation techniques and high-performance computing to analyse vast datasets, delivering actionable insights on downforce, drag, and cooling. Paul's focus is on empowering engineers with precision and clarity, ensuring every aerodynamic decision contributes to improved laptime.

Beyond motorsport, Paul advocates for the broader impact of CFD in solving real-world challenges. The same techniques used to optimize airflow over an F1 car have been applied to model the dispersion of COVID-19 particles during the pandemic and to improve understanding of wildfire behaviour. His work exemplifies how high-performance simulation can drive innovation not only on the racetrack but also in public health and environmental safety.

He will be presenting: **"HPC in Formula One: Designs for Speed"**

In the relentless pursuit of performance, Formula One teams rely heavily on High Performance Computing (HPC) to simulate, refine, and validate aerodynamic designs that can shave milliseconds off lap times. This talk explores the critical role of HPC in modern F1 development, with a particular focus on Computational Fluid Dynamics (CFD) as a cornerstone of aerodynamic optimization. Over the past two decades, the evolution of hardware—from single-core workstations to massively parallel architectures—has driven transformative changes in simulation capability. Rather than algorithmic breakthroughs, it is the exponential growth in computational power that has enabled engineers to resolve increasingly complex flow phenomena with greater spatial and temporal fidelity. This presentation will trace the trajectory of hardware development in F1, highlighting how improvements in memory bandwidth, processor speed, and parallel scalability have allowed for more accurate discretisation of the governing physics. By aligning computational resolution with the physical scales of interest, teams can better capture transient effects, boundary layer behaviour, and turbulent structures that are critical to performance. Ultimately, this talk will argue that in the context of CFD for F1, precision is not just a function of clever algorithms, but of the raw computational muscle that enables them to be applied meaningfully.





## **PERRY GIBSON, FRACTILE**

Perry Gibson is an ML Compiler Engineer at Fractile, who are working on hardware to accelerate next generation frontier model inference, with significant energy efficiency gains. He completed his PhD in Across-stack DNN Acceleration at University of Glasgow, and is interested in the new forms of expression that HPC can enable.

He will be presenting: **“Compilers, Creatives, and Collaboration: What HPC Can Learn from DJs and Game Devs”**



High performance computing (HPC) has long been foundational to scientific discovery, technological advancement, and new business opportunities. But the landscape is rapidly shifting. Today, interdisciplinary collaboration is not just beneficial; it's becoming critical for project success.

A significant contributor to this shift is the combination of open-source ecosystems, highly capable and accessible software tools, and a flood of free educational content. Emerging technologies like large language models (LLMs) now offer real-time knowledge translation between domains, enabling teams to bridge skill gaps and collaborate across disciplines faster than ever before. But tooling alone isn't enough. Culture and interpersonal dynamics remain the linchpin.

This talk brings together some personal experiences (from working with illustrators, DJs, and game developers), as well as the challenges we face at Fractile. Fractile is a UK-based HPC AI hardware company with a tight knit team of machine learning researchers, compiler monkeys, firmware and driver engineers, hardware designers, and physicists.





## **JOHN FERGUSSON, JDF SOLUTIONS**

John Fergusson is a seasoned technology recruiter with over 20 years of experience in talent acquisition, partnering with global blue-chip corporations including Microsoft, Novartis, Royal Mail, and William Hill, as well as high-growth, VC-backed startups. He has also successfully supported software houses and consultancies across a broad spectrum of technology domains.

John is known for his ability to act as a trusted advisor to client organisations, guiding recruitment strategies, implementing best practices, and coaching hiring teams to ensure effective and aligned hiring processes that support business objectives.

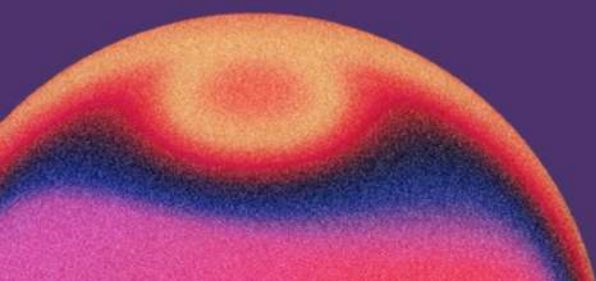
Beyond client advisory, John has a strong track record in supporting technology professionals across all levels of seniority. He provides career coaching, interview preparation, and guidance on career progression, helping individuals navigate their next steps and achieve their full potential in the tech industry.

He will be presenting: **“Reflections of a Technology Recruiter”**

The best career lessons don't always show up on a CV – they come from the stories, surprises, and stumbles along the way. In this talk, recruiter John pulls back the curtain on what he's learned from years of helping people land jobs, grow teams, and navigate career twists and turns.

From writing job descriptions that actually speak to humans, to designing interviews that spark real conversations, to coaching people through big (and sometimes scary) transitions, John has seen what works, what doesn't, and what makes all the difference. His stories are funny, honest, and full of “aha” moments you can take with you.

Whether you're just getting started, building a dream team, or eyeing your next move, you'll leave this session with fresh perspective, practical takeaways, and hopefully a little inspiration to take your own next step.





## **JOSEPH MOORE, BRISTOL**



Joseph is a PhD student working on Design Space Exploration of Microarchitectures for High Performance Computing applications at the University of Bristol. He also organises and runs the Bristol Centre for Supercomputing Student Cluster team, breaking new ground in the UK's participation in international Student Cluster Competitions. Starting as an undergraduate at Durham, he has competed, and more recently mentored, in eight competitions, winning three. He hopes to enable HPC education for students across the UK and continues pushing this alongside his PhD studies.

He will be presenting: **"Student Cluster Competitions: Empowering the next generation of HPC"**

Student Cluster Competitions (SCCs) are where curiosity meets challenge and teamwork meets technology. They give students the chance to design, build, and optimize real high-performance computing systems—learning as much from each other as from the problems they solve. For many, it's the first time they apply classroom knowledge to messy, real-world situations while collaborating under pressure.

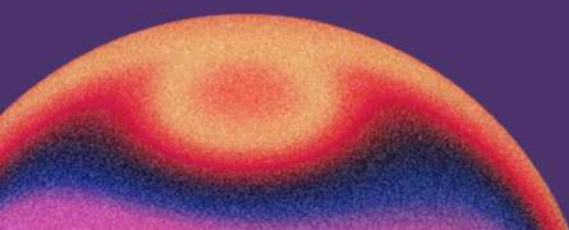
This talk will introduce SCCs and explain the different ways students and institutions can get involved. From virtual competitions to in-person events like CIUK, there are opportunities to participate, support teams, and cheer students on. We'll also explore what makes SCCs so impactful: the confidence they build, the skills they sharpen, and the doors they open into careers across research and industry.

## **THOMAS SHTASEL, IMPERIAL**

Tom is a 3rd year Computing Student at Imperial College London, with special interests in HPC, low-level programming & computer systems. He participated on the Bristol Centre for Supercomputing team at the ISC 25 Student Cluster Competition, where the team worked on configuring a cluster and compiling large programs. Tom is set to participate in the SC 25 Student Cluster Competition, and hopes to work in HPC in the future.



He will be co-presenting as part of **"Student Cluster Competitions: Empowering the next generation of HPC"**







## **DAWN GEATCHES, UKRI**

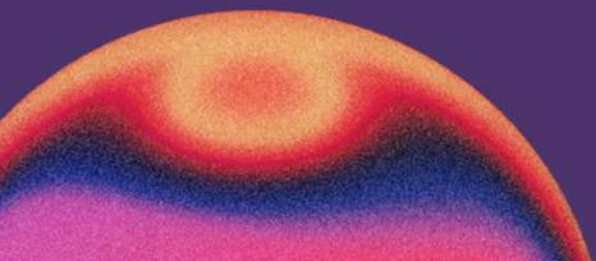
After returning to education as a mature student, Dawn studied part-time with the Open University for a degree in Mathematical Sciences before pursuing a full-time PhD in Computational Physics at Durham University. She then spent two years as a postdoctoral researcher at Stanford University, exploring the properties of clay minerals and their interaction with methane and CO<sub>2</sub> in the context of carbon sequestration.

Following this, Dawn joined STFC as a computational researcher, where over the course of eight years her role expanded to include writing about the impact of research for a community of Collaborative Computational Projects (CCPs).

When her research career reached a natural conclusion, Dawn drew on her strong mathematical background to transition into her current role at Innovate UK Business Connect. There, she works with academics to support knowledge exchange with businesses, industry, government, and not-for-profit organisations. Dawn particularly values this role as it allows her to see how mathematics underpins much of our everyday world in all its variety, while continuing to learn from the wide range of applications it inspires.

She will be presenting: **"Green Computing Initiatives: UKRI and beyond"**

What does 'green computing' mean in the context of UKRI whose digital research infrastructure serves 8000+ staff from administrative to high-end computing tasks? What initiatives are underway to reduce the carbon footprint of this digital infrastructure? Looking beyond UKRI, there are diverse groups addressing green computing, such as the newly launched special interest group – Climate and Environmental Sustainability – of the Institute of Mathematics and its Applications. Additionally, Innovate UK supported an Innovation Challenge: 'Component-level energy monitoring for greener IT operations'. Are there opportunities to bring these initiatives together in a coordinated 'Green Computing' movement?







## **STU FRANKS, CONCERTIM**

Stu cut his teeth as a linux HPC sysadmin and through the years has grown to create and evolve tools and solutions he wishes he had back then. He's focussed on empowering end-users and improving service efficiency with accessible products targeting HPC service delivery, improved time-to-science and environmental consciousness.

He will be presenting: **"Decoding Carbon: Energy Reporting in Supercomputing"**

POV: You'd like to be more sustainable, but you have no idea how much carbon you're currently using and no one seems to be able to tell you why that's even important.

As an industry, IT has been pretty poor at explaining why our computers need to use so much power and how you and your users can help to minimise that. HPC and AI chase maximum performance - and that race to infinity has meant a complete disconnect from what power efficiency really means. In this talk we'll be looking at how you can use a "building-blocks" concept to help model your HPC or AI facility to help understand the component parts and how they relate. Once this is defined, we demonstrate how that model can be used to estimate the carbon footprint of your facility, and highlight some opportunities for future efficiencies.

## **CRISTIN MERRITT, ALCES FLIGHT**

Cristin Merritt is the Head of Communications at Alces Flight, bringing over 20 years of experience in enterprise technology, including nearly a decade in High Performance Computing (HPC). She specializes in market analysis, strategic communications, and driving innovation in HPC integration. At Alces Flight, Cristin has led successful hybrid HPC projects, earning global recognition for their impact.



Her leadership has helped position Alces Flight as a pioneer in HPC integration, subscription-based solutions, and workload management. She plays a key role in shaping the company's messaging, outreach, and industry engagement.

Cristin is also actively involved in the HPC community, serving as an Advisor for the Women in HPC Executive Committee and chairing communications for SC25. She frequently contributes to industry discussions, publications, and events, helping bridge the gap between technology and business strategy.

Cristin will be introducing us to this year's conference theme, **"Catalysts for Change"** and will be SR25's Master of Ceremonies (MC).





## **DAMIAN JONES, STFC**

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Damian is the Computational Science Centre for Research Communities (CoSeC) Programme Manager and has been a member of STFC's Scientific Computing Department for over 25 years, joining in 1999. With a degree in business administration as well as qualifications in project management and years of involvement with various projects within the department, Damian brings a wealth of experience to the CoSeC programme. Alongside his role in the CoSeC programme Damian is also the Conference Chair for the department's annual conference Computing Insight UK and has overseen the impressive growth of the event over recent years to its current position as one of the UK's premier HPC conferences.

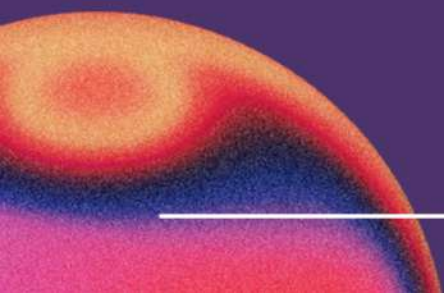


He will be presenting: **"Student Cluster Competitions: Empowering the next generation of HPC"**

Since its inception in 1990, Computing Insight UK (CIUK) has brought the HPC community together to share the latest technologies, real-world applications, and emerging "hot topics." The 2025 conference takes place on 4–5 December in Manchester with the theme "Computing Unites."

In this short presentation, we'll look at how CIUK has been energising the next generation of supercomputing talent. The Student Cluster Challenge, launched in 2020, has quickly become a standout success — giving students the chance to work hands-on with real HPC systems, build networks, and showcase their skills. More importantly, it has sparked lasting engagement that reaches well beyond the competition itself.

We'll highlight how this initiative is helping sustain enthusiasm for supercomputing and how the lessons learned can shape the future of the HPC community.







## **MARK BJORNSGAARD, DEEP GREEN**

Mark Bjornsgaard is Deep Green's Chief Innovation Officer. Mark founded the company and was formerly the CEO. He has grown numerous businesses from scratch to scale. Other investments include Lifted (Senior care - JV British Gas), Altogether (US healthcare, JV GSK) and Secret Source (augmented tech teams). Mark was a founding investor in Elmo (EV subscriptions sold to BCA group) and is an investor in Caldera (Heat Batteries), Ctrl Alt (Asset tokenisation) and NewChange FX (FX data) amongst others.

He is the CEO of System Two, holds a number of board positions and consults to a range of FTSE 100s on M&A strategy and innovation. His 1st Book "The Manual - How to Define a Value Hypothesis" is out next year.

He will be presenting: **"Lessons from the edge - what we've learnt when scaling data centre heat reuse"**

Deep Green has been described as the vanguard of distributed edge computing. What we offer - free heat energy - makes common sense. More than this, Mark Bjornsgaard, founder of Deep Green, will make the case that integrating vast forthcoming data centre capacity into the fabric of urban ecologies is essential for the effective electrification of heat. This being true, how do we expedite its adoption and progress?





## **Wil Mayers, Alces Flight**

Wil Mayers has 20 years experience in high-performance compute and storage systems having built large environments for UK government, University and commercial customers. He has worked for both corporates and SMEs, helping customers to optimise their scientific computing workflows across many different domains including engineering, bioinformatics, physics, media and finance. In 2010 Wil joined Alces Flight, where he is responsible for building and delivering solutions for customers utilising a wide range of open-source and custom-developed software.



He will be presenting: **“Practical Approaches to Energy-Efficient Supercomputing”**

In a world that seems increasingly complex, choosing the right equipment, power and cooling for your HPC or AI seems harder than ever. Do you need liquid cooling? Will your GPU burn your data-centre down? How can you build something sustainable that will meet tomorrow's requirements?

In this talk, we review the current state of the art around compute equipment, data-centre power options and cooling solutions that you can use to plan your next upgrade and keep your users in FLOPs. Catering for a wide range of different workloads and scenarios, we look at some example deployments in use across the UK and Europe that demonstrate how you can plan your sustainable future without breaking the bank.

## **JAMES THORNE, NQCC**



James is HPC/IT Manager at the National Quantum Computing Centre, responsible for all things “classical computing”. He has been in public and university sector roles his whole career: Diamond Light Source, Oxford University, Large Hadron Collider computing and Kew Gardens. He is a lifelong scout leader and likes caving, cycling and hillwalking.

He will be presenting: **“Quantum Computing - Roadmap, Uses and the Continuing Role of HPC”**

Quantum computers have the potential to tackle some of the most computationally complex problems, beyond the reach of even the most advanced supercomputers today.

Although the technology is still in its infancy, progress on its development continues to accelerate rapidly across the world. As a trusted authority, the National Quantum Computing Centre's vision is to enable the UK to solve some of the most complex and challenging problems facing society by harnessing the potential of quantum computing. We will explore the UK roadmap for quantum computing, its potential uses and why HPC is not going away any time soon.





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# **Get in Touch**

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