

### Hartree Centre

# Hartree Centre Strategy

Hartree Centre

HARTREE

VIRTUAL ENGINEERING CENTRE





# The UK's only supercomputing centre dedicated to industry engagement

Founded in 2012, our purpose is to unlock the high growth potential of advanced digital technologies for UK industry. We're based at the Science and Technology Facilities Council (STFC) Daresbury Laboratory in the Liverpool City Region with additional locations across the UK.

Discover more about us at hartree.stfc.ac.uk

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# Digital solutions that make a difference

We are making the future of computing a reality for UK industry. We work at the intersection of applied digital research and innovation, bridging the gap between theory and practical adoption. We drive productivity, innovation and economic growth in UK organisations, big and small.

Our experts collaborate with industry and the research community to explore the latest supercomputing, data science, quantum computing, cloud and artificial intelligence (AI) technologies, upskill teams and apply digital solutions to individual and industry challenges for the benefit of the UK and its people.

Established in 2012 by the Science and Technology Facilities Council (STFC), the Hartree Centre was created to enable the adoption of advanced digital technologies in UK businesses and the public sector. We are named after Douglas Rayner Hartree, a mathematician, physicist and champion of early electronic computer development. His passion for computing innovation and technological advancement makes him an ideal representative for what we do today. We take this passion forward by solving current business challenges and creating practical solutions, sharing the knowledge and skills required to adopt them. In our first four years of operation we generated £34.6 million net impact GVA for the UK economy. In 2021, the Hartree National Centre for Digital Innovation (HNCDI) was established in collaboration with IBM to enable UK businesses and public sector organisations to acquire the skills needed to adopt AI, develop proofs-of-concept and de-risk investment into emerging digital technologies such as quantum computing.

This strategy sets out our five-year plan to build on our achievements and continue to deliver significant societal and economic impact for the UK. It outlines our key strategic priorities for the period 2024-2029 which are aligned to both UKRI and STFC's strategic objectives. It sets out how we will work with partners in the research and innovation ecosystem to help UK industry to unlock the high growth potential of advanced digital technologies.

# Our purpose

To unlock the high growth potential of advanced digital technologies for UK industry.

# **Our vision**

For UK industry to generate socio-economic growth by exploiting UK compute capabilities to explore and adopt advanced digital technologies.

## **Our mission**

To equip UK industry with the knowledge, skills and compute needed to fully unlock the potential of advanced digital technologies.



## Our strategic objectives at a glance

Training UK industry and the public sector to meet the increasing demand for digital skills so that the UK can actively take advantage of the latest advanced technologies.

Exploiting our facilities and expertise to explore and develop transformative technologies and ground-breaking scientific advancements that address national priorities in HPC, AI, quantum and extreme-scale and cloud computing.

Creating industrial, societal and economic impact across the UK by empowering industry to exploit, embed and adopt the latest advanced digital technologies.



Ensuring the Hartree Centre is recognised as the UK's national facility for providing industry access to world-class compute resources.

Positioning the Hartree Centre as the go-to trusted partner to help UK industry advance understanding and adoption of innovative advanced digital technologies.

Operating a modern, sustainable, and effective Hartree Centre that supports the development, safety and wellbeing of its diverse teams.

We are proud to be members of a thriving and inclusive UK Research and Innovation ecosystem. As part of UKRI, we are a department within STFC, one of the nine councils working together to enrich lives, drive economic growth, and create jobs and high-quality public services across the UK. Our strategic priorities are aligned with UKRI's Transforming Tomorrow Together strategy and STFC's strategic delivery plan, acknowledging our role in delivering our collective mission.

## **Our values**

The Hartree Centre's values embed UKRI's principles of change: diversity, resilience, connectivity and engagement. Our values demonstrate and define the way our teams and individuals work as well as how we, the Hartree Centre, work within our communities and behave as part of the UK's research and innovation ecosystem.

#### Trust

We are proud to operate with integrity and diversity of thought. We are trusted advisors to UK industry.

#### Collaboration

We use the power of our people, partnerships and networks to unlock the high growth potential of advanced digital technologies for UK industry.

#### Innovation

We are driven by curiosity; we are not happy with the status quo and continuously strive to innovate by creating solutions that make a difference for UK society.

#### Knowledge

We can see the bigger picture, connect the dots across technology providers, ideas and challenges. Our people are always open to learning new things and sharing our knowledge to help UK industry explore and adopt advanced digital technologies.



# Strategic objectives and priorities

We want to unlock the high growth potential of compute for industry and empower UK businesses to benefit from integrating advanced digital technologies into their organisations.

## Innovation

Priority 1: Positioning the Hartree Centre as the go-to trusted partner to help UK industry advance understanding and adoption of innovative advanced digital technologies.

- Work alongside IBM to fully exploit the £172 million investment from UK Government in the Hartree National Centre for Digital Innovation (HNCDI) up to March 2026, including the delivery of at least 100 explorative technology demonstrator projects and 32 adoption projects with UK businesses and public sector organisations
- Develop the business case for the next phase of HNCDI that incorporates public and private sector partnerships, ensuring that the UK remains at the forefront of digital technology adoption
- Shape and deliver future funding calls with partners and funding agencies like Innovate UK, demonstrating our capability as a trusted enabler of innovation

- Lead as a key partner in major current and future UK and international funding calls for advanced digital technologies
- Deliver as a consortium partner on current programmes including:
  - **BridgeAl** | A £100 million Innovate UK led programme to support the adoption and diffusion of artificial intelligence and machine learning technologies in the UK economy
  - Smart Manufacturing Data Hub (SMDH) | A £50 million UK Government and industry-backed programme led by Ulster University to support small and medium-sized manufacturers to become more competitive by harnessing the power of data
  - Analysis for Innovators (A4I) | A £3 million UKRIled programme working with UK businesses to solve productivity and competitiveness challenges by working with scientists and research facilities
  - **Industry Impact Fund (I2F)** | Support UK industry through access to STFC facilities and scientific expertise in energy, net zero, health and security and defence

- Expand our private and public sector partnerships by identifying and delivering collaborative programmes and commercial projects in key strategic sectors for UK industry including:
  - Aerospace and Automotive
  - Materials
  - Nuclear, Energy and the Environment
  - · Life Sciences, Health and Wellbeing
  - Security and Resilience
- Actively participate in setting the UK's innovation agenda in partnership with industry:
  - Participate in key innovation advisory boards such as the Liverpool City Region (LCR) Business and Enterprise Board, Digital Twin Hub Advisory Board, Knowledge Centre for Materials Chemistry (KCMC), and Innovate UK activities
  - Develop relationships with key professional trade associations and technical authorities such as the Automotive Council UK, North West Aerospace Alliance (NWAA), Nuclear Industry Association (NIA) and the National Cyber Security Centre (NCSC)
  - Deliver keynotes and convene workshops at leading UK and international industry innovation events showcasing our innovation capabilities and industry impacts such as the Alan Turing Institute's AI UK conference and techUK flagship events

# Powering innovation through collaboration

The Hartree Centre has been our materials chemistry computing partner for over a decade, with several examples delivering into innovation and capability building. It might be no surprise, therefore, that our relationship has grown and developed over time to span several science domains, as a talent hub and for joint exploration into exciting and collaborative horizons such as Al and quantum.

#### Alberto Prado Global Head Digital & Partnerships, Unilever R&D

## **Places**

Priority 2: Ensuring the Hartree Centre is recognised as the UK's national facility for providing industry access to world-class compute resources.

- Deliver the HNCDI programme to update and refresh the Hartree Centre's compute and data infrastructure, ensuring the current and future needs of UK industry are met
- Play our part in delivering on the recommendations from the UK Government's Independent Review of the Future of Compute by providing unmatched compute infrastructure to industry including:
  - The provision of large-scale hybrid-HPC cloud facilities, quantum and extreme scale compute
  - Facilitating access to our large-scale computing and data environments for UK industry
  - Developing attractive and innovative models to enable self-service access to our world-class facilities
- Work with our technology partners to attract more strategic partnerships to the Sci-Tech Daresbury campus including IBM, Microsoft, Amazon Web Services (AWS), NVIDIA, Fujitsu, Eviden (an Atos business), Hewlett Packard Enterprise (HPE), Graphcore, Google and PsiQuantum

- Actively explore novel systems and architectures that have the potential to address current and future economic and societal priorities for the UK
  - Where these don't exist, we will propose, develop and co-design solutions in partnership with technology providers
  - We will work with our national and international collaborators and build strategic partnerships to obtain access to novel and alternative architectures to accelerate our applied industrial research including:
    - IBM Quantum
    - LUMI petascale supercomputer, the fastest supercomputer in Europe via CSC – IT Center for Science, Finland
    - Exascale compute access via the UK Exascale Programme and the US National Laboratories
- Develop and deliver a roadmap for advanced visualisation capabilities that support the UK's National Digital Twin programme and enhance industry uptake of novel technologies

## Expanding our capacity to support UK businesses with a new supercomputing facility

In 2023, construction began on a new £42 million supercomputing centre based at Daresbury Laboratory in the Liverpool City Region. Expected to be completed in 2025, the centre will house new, more powerful supercomputing systems that will expand our capacity to support UK industry and deliver more flexible and secure support for business.

The first system to be installed in our new facility is expected to be one of the largest, publicly owned GPU clusters in the UK, accelerating AI applications for industry. With an anticipated performance capability of between 80 and 100 petaflops (up to 100 trillion calculations per second), our new system will be up to 25 times faster than our existing platforms.

For businesses who are looking to take advantage of Al technologies, our team of experts will be on hand to support their journey without the need for prior technical knowledge. For potential collaborators who are looking to port their existing codes to GPU or supplement their projects with Al, the Hartree Centre will continue to be the trusted partner to support these ambitions.

Our new supercomputing centre will open up the potential to collaborate with more organisations and host larger systems that support the UK Government's Future of Compute Review and ambitions to become a global science superpower.



## Ideas

Priority 3: Exploiting our facilities and expertise to explore and develop transformative technologies and ground-breaking scientific advancements that address national priorities in HPC, AI, quantum, extreme-scale and cloud computing.

#### We will:

- Be recognised internationally as a world leading supercomputing centre for industry, increasing the UKs international influence in advanced digital technologies.
  - Develop new partnerships in regions such as the Asia-Pacific
  - Leverage our existing international and national relationships with other supercomputing centres and national facilities to place the Hartree Centre at the heart of discussions relating to the future of compute and the latest advanced digital technologies
- Become a key pillar of the UK Digital Research Infrastructure and supercomputing ecosystem; influencing, directing and supporting the UK's research and digital infrastructure agenda
  - Write and publish strategic papers to help shape UK research policies in the areas of HPC, AI, quantum, hybrid-cloud and extreme-scale computing

- Participate in key advisory boards and committees nationally and internationally in the areas of extreme scale computing, big data analytics and quantum computing:
  - International:

Society for Industrial and Applied Mathematics (SIAM), ACM Association for Computing Machinery (ACM)

Institute of Electrical and Electronics Engineers (IEEE)

European Technology Platform for High Performance Computing (ETP4HPC)

• National:

STFC e-Infrastructure Advisory Group (SEAG)

Distributed Research using Advanced Computing (DiRAC)

We will also participate in key committees in other UKRI constituent councils including NERC, BBSRC and EPSRC as well as key existing and future committees at the Department for Science, Innovation and Technology (DSIT) level

 Demonstrate our thought leadership in the areas of extreme scale computing, computational and data science, research software engineering, AI and quantum computing on the global stage by organising workshops and presenting keynotes at UK and internationally renowned events such as ISC High Performance (Germany), Supercomputing (SC), Computing Insight UK (CIUK) and others

# Using supercomputers and AI to make fusion energy a commercial reality

Our collaboration with the UK Atomic Energy Authority (UKAEA) uses the latest supercomputing and data science techniques to develop fusion technologies, working towards a low-carbon future. By innovating to develop digital twins of fusion power plants that help scientists and engineers test viable reactor technologies virtually, we are removing the need for expensive, physical prototyping. By exploiting the convergence of supercomputing and AI at the exascale, combined with the fusion expertise from UKAEA, we are working together to accelerate the UK's technology roadmap required to make fusion energy a commercial reality.

This work is seeding the development of a whole new industrial sector – the pioneering SMEs, universities and engineering giants that will deliver and commercialise fusion.

As fusion enters the delivery era and we see the emergence of the world's first exascale supercomputers, there couldn't be a better time for the Hartree Centre and UKAEA to join forces on a mission to help deliver commercial fusion. The Hartree Centre's expertise in supercomputing and AI, combined with UKAEA's domain expertise around fusion science and technology, will enable the co-design of solutions to eliminate large amounts of timeconsuming real-world prototyping. This is an incredibly exciting endeavour that will help to make fusion an environmentally responsible part of the world's future energy supply. In the era of net zero, this is a race, a necessity and a tremendous economic opportunity for the UK.

Rob Akers Director of Computing Programmes, UK Atomic Energy Authority

### Impact

Priority 4: Creating industrial, societal and economic impact across the UK by empowering industry to exploit, embed and adopt the latest advanced digital technologies.

- Collaborate with public and private sector organisations to deliver societal and economic growth to the UK by supporting the exploitation and adoption of the latest advanced digital technologies
- Commit to the publication of our socio-economic impact, commissioning external evaluators to assess the benefit realisation of Hartree Centre activities
  - Publish a collection of Hartree Centre Highlights annually
  - Input into UKRI and STFC frameworks for benefit monitoring and reporting
  - Evaluate our major programmes such as the Hartree National Centre for Digital Innovation (HNCDI) through progress reports, internal process reviews and end point evaluation

- Publish our research through papers and patents that demonstrate our contribution to advancing scientific and technological knowledge and innovation
- Play an active part in developing and delivering local and national impact relating to industry adoption of advanced digital technologies
  - Develop our relationships with innovation boards including Liverpool City Region Combined Authority, Henry Royce Institute and Innovation Greater Manchester
  - Build partnerships with sectorial bodies and Catapults in our key strategic sectors
  - Actively participate in UKRI Clusters such as the Digital, Health and Energy Tech clusters



- Support the ongoing growth of the Sci-Tech Daresbury campus and invest in our presence across other UKRI and STFC locations, creating jobs and delivering societal impact across the UK
  - Help create and shape the North West Quantum Hub
  - Grow and embed our Centre of Excellence for Extreme Scale Computing in Fusion with the UK Atomic Energy Authority (UKAEA)
  - Build our presence at other STFC locations including Rutherford Appleton Laboratory (RAL) and the UK Astronomy Technology Centre (UK ATC)
  - Continue to support the first IBM Discovery Accelerator in Europe, based on site at the Hartree Centre
- Successfully deliver and embed the three Hartree Centre SME Hubs (Northern Ireland, North East and Cardiff) to enhance productivity, engagement and growth across the UK, supporting SMEs regionally as part of the current HNCDI programme
  - Plan to expand and develop the Hartree Centre SME Hubs concept to deliver wider impact across the UK through collaboration with other organisations with a regional focus



**Case study** 

### Improving patient care and fall prevention with data science

safesteps<sup>™</sup> are a digital healthcare company that create personalised patient care plans aiming to reduce the risk of falls. This is particularly significant for the elderly population as falls can lead to serious injury. The company support health care workers to adopt National Institute for Health and Care Excellence (NICE) guidelines that outline over twelve areas of fall risks and fifty types of interventions. Guidelines need mapped against every patient's individual needs which creates a large, unique dataset that has to be processed, standardised and made accessible. safesteps<sup>™</sup> are looking to help GPs and carers access relevant data through a healthcare dashboard that can be integrated into their existing systems and processes, helping them focus on improving patient care.

Our data science team supported the development of the data dashboard by processing and cleaning data into a standardised format, ultimately helping to improve the categorisation of falls. They also integrated new, global industry standard classifications to improve sorting features, simplifying the treatment process for healthcare professionals and patients alike. This data dashboard is now more accessible and connects with NHS Spine, ensuring data gets to the right people at the right time and helping keep people out of hospital. safesteps<sup>™</sup> are looking to do a follow on project with the Hartree Centre and have already hired data scientists into their team.

The Hartree Centre team were really responsive. They understood our needs and helped us frame our challenges in the right way, providing valuable input. With their support, we have managed to make the healthcare system accessible to a lot more people.

#### Lee Omar

Founder and Chief Innovation Officer, safesteps™



### **People and careers**

Priority 5: Training UK industry and the public sector to meet the increasing demand for digital skills so that the UK can actively take advantage of the latest advanced technologies.

- Upskill 5000 mid-career employees across UK industry through the Hartree National Centre for Digital Innovation and engage over 150 SMEs by 2026 to ensure UK industry is best placed to explore and exploit the latest advanced digital technologies. Our support will be focused on understanding and applying emerging technologies and tools enabled by high performance computing, AI, hybrid cloud and quantum
- Advance knowledge of key technology areas across the UK by:
  - Exploiting the benefits of HPC and extreme-scale computing for industry
  - Exploring the development and application of foundation models in AI
  - Developing software for the 'Quantum Computing Age'
  - Understanding the convergence of advanced compute and cloud capabilities
- Deliver training through major collaborative programmes such as BridgeAI, Smart Manufacturing Data Hub and the Industry Impact Fund (I2F) and develop targeted training for C-Suite executives covering the latest advanced digital technologies, to promote board level understanding and investment

- Develop a pipeline of future technologists by supporting and participating in the delivery of Centres for Doctoral Training (CDTs) with UK institutions to support PhD students in their skills development, ensuring they are transferable to work with industry
  - Work with universities and institutes including University of Liverpool, University of Edinburgh, University of Leeds, UCL and the Alan Turing Institute to develop the workforce of tomorrow by delivering tailored training courses alongside AI-focused CDTs and those that support HPC and data analytics skills development in the areas of:
    - healthcare and wellbeing
    - nuclear fusion
    - distributed algorithms
    - quantum computing
- Attract and retain world class talent to work at the Hartree Centre, ensuring that we enable our teams to regularly refresh and update their skills and knowledge to remain at the top of their respective fields
  - Increase the number of upskill apprenticeships across our teams, grow our graduate intake and participation in professional training across the centre
  - Develop people who are skilful working at the intersection of research and industry

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I joined the Hartree Centre as an apprentice, working on data science projects alongside studying for a Digital and Technology Solutions Master's Degree apprenticeship at Manchester Metropolitan University. Being able to apply theory to a diverse range of real-life industry applications has been an ideal way to learn. Exploring how data science can be used to facilitate the digital transformation of organisations has been invaluable when working on industry projects.

One highlight of my apprenticeship was receiving an award for my final project exploring the modelling of Hartree Centre project management data using sequential deep learning methods. I have now been promoted to a Data Scientist role and continue to develop my experience, working on projects in areas such as computer vision, time series analysis and geospatial modelling. Applying these techniques to solve industry challenges across a breadth of sectors is something I really enjoy.

#### Sarah Jackson Data Scientist, Hartree Centre

Hartree Centre Strategy

## Organisation

Priority 6: Operating a modern, sustainable and effective Hartree Centre that supports the development, safety and wellbeing of our diverse teams.

- Develop our funding models to ensure long-term sustainability for our people by balancing grant-funded research, government backed co-funding and commercial income from private sector organisations
  - Strive for a balance of funding models across our portfolio
  - Build the business case for the follow-on programme to the Hartree National Centre for Digital Innovation (HNCDI), with the aim of developing a number of large scale, multi-year programmes that promote public-private sector partnerships
- Increase our diversity and embrace the diverse skills, cultures and experiences of our people
  - Work towards gaining Athena Swan or similar certifications that are recognised frameworks used to support and transform gender equality within research and innovation
  - Embrace cultural diversity by promoting secondments and placements between international supercomputing centres and UK organisations such as the UK Atomic Energy Authority (UKAEA) and others

- Demonstrate our commitment to operational excellence through gaining and maintaining our external accreditations such as ISO9001, ISO 270001 and other relevant best practice certifications such as ITIL
- Develop and promote our Professional Services through a commitment to delivering projects in line with UK Government Project Delivery Profession standards and improve our internal processes and procedures to support our teams in delivering their best work
- Aim to reduce our environmental impact by putting sustainability at the core of our internal operations as well as external projects, aligning to wider STFC and UKRI initiatives where appropriate

# Funding sustainability for operational excellence

As part of our ongoing commitment to operational excellence, we will publish a series of delivery plans that will sit alongside our strategy and contain further detail of our future financial plans. We are backed by funding from the UK Government and are proud to hold strategic partnerships with industry leaders. Our current flagship programme - the Hartree National Centre for Digital Innovation collaboration with IBM - is supported by £172 million over five years via DSIT and UKRI. In the 2022-2023 financial year, we are operating with 60% grant funding, 30% large programme funding via the Department for Science, Innovation and Technology (DSIT) and UKRI and 10% commercial funding.

As we continue to grow the centre, we are looking to transition our funding to a more balanced portfolio spanning government, grant and commercial income so that our teams can continue to deliver maximum impact for society and the UK economy.





# Making the future of computing a reality

#### A note from our Director

I am proud of our continued commitment to the future of digital technologies, their application to real business challenges and their potential to create meaningful societal and economic impact for the UK.

What makes us unique is our ability to work at the intersection of applied research and innovation to place advanced digital technologies into the hands of businesses, regardless of their size. We combine our scientific expertise with our track record delivering solutions for industry to demonstrate the art of the possible and upskill teams to take advantage of emerging technologies for productivity, innovation and economic growth.

Co-created with our staff, collaborators and stakeholders, our strategy sets out our direction of travel over the next five years. I am confident that by fostering collaboration, celebrating innovation, and nurturing talent, we are well positioned as a centre to shape the future of digital innovation in the UK.

> Kate Royse Director, Hartree Centre



What makes the Hartree Centre stand out is the continuous focus on translating emerging digital technologies to solve challenges and deliver meaningful societal and economic impact for UK industry.

Mark Thomson Executive Chair of STFC

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