



Science and  
Technology  
Facilities Council

# Hartree Centre

# Welcome

We provide UK businesses with access to world-leading facilities and expertise in advanced digital technologies, including supercomputing, data analytics and artificial intelligence (AI). We're here to help you to identify and embed the right digital expertise and technologies that will boost business performance, reduce costs and maximise the productivity of people and processes.

As part of the Science and Technology Facilities Council (STFC) within UK Research and Innovation, the Hartree Centre is underpinned by over £170m of UK Government funding, resulting in access to world-leading scientific infrastructure and a considerable competitive advantage for our customers and collaborators.

We support business of all sizes and across many sectors, helping them to begin or progress on their digital journey. Depending on your needs, our flexible approach allows for both long-term Research and Development (R&D) collaborations, or short-term access to our advanced digital technologies and expertise.

We also support and build digital expertise within existing and future generations of the UK workforce by developing bespoke training for organisations and working closely with universities to provide hands-on educational opportunities.

Seizing the opportunity and harnessing the potential of Industry 4.0 technologies will require innovation and investment. Unleashing the UK's potential is dependent on the speed at which businesses and research organisations can innovate and develop digital technologies to support key economic, social and environmental objectives.

The Hartree Centre is here to support that drive.

**Get in touch to see how the Hartree Centre could help to realise your digital ambitions.**

## Our mission

**To transform UK industry by accelerating the adoption of high performance computing, big data analytics and artificial intelligence technologies.**

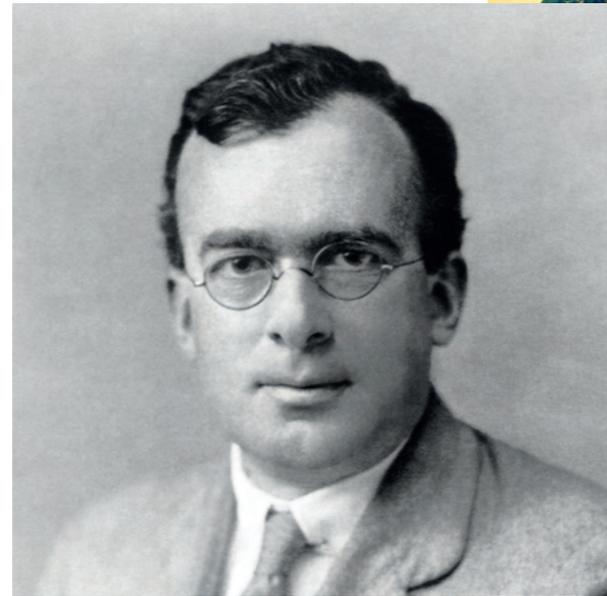
# Who we are

The Hartree Centre is named after Douglas Rayner Hartree, a mathematician, physicist and champion of early electronic computer development. His passion for innovation and technological advancement is at the heart of what we do.

Our team is made up of chemists, physicists, mathematicians, software engineers, data scientists, technical architects, project managers and business development specialists - a community of experts, working to translate the latest computational advances into digital solutions that deliver an effective and sustainable economic impact for UK businesses.

We have access to a network of strategic industry partners including IBM, Atos, Siemens and more. We're also home to the University of Liverpool's Virtual Engineering Centre and one of only two locations to host an IBM Research team in the UK.

As a technology partner in the ERDF-funded LCR4.0 programme, we were recognised by the Financial Times as one of Europe's 100 Digital Champions for helping SMEs in the Liverpool City Region to embrace and integrate Industry 4.0 technologies.



**“It may well be that the high-speed digital computer will have as great an influence on civilization as the advent of nuclear power.”**

**Douglas Rayner Hartree**

**STFC Daresbury Laboratory**

**The Hartree Centre**



# What we do

## Modelling & simulation

The scale of our supercomputers enables high fidelity modelling and simulation, from detailed engineering analysis to understanding chemical reactions at a molecular level. Our code coupling capabilities help expand upon existing models to capture complex multi-scale and multi-physics effects which means we can help your business to carry out iterative research and development processes within a supercomputer, running faster high-fidelity simulations to develop and test prototypes and reduce time to market.

## Software development and optimisation

We are designing, testing and optimising software for the world's most advanced microprocessors – laying the building blocks for tomorrow's supercomputers. With applications ranging from weather and climate forecasting to modelling and optimising electric power trains for a carbon free future. We can modernise existing codes and deliver optimised software suitable for current and future computing architectures.

## Data science

We can help turn your business data into insights to aid decision-making and solve challenges. From increasing accuracy, improving productivity and efficiency with big data analytics to curating, cleaning and integrating existing and live-streamed datasets to create value from your data, our team can help you understand and prepare your data for advanced analytics, visualisation or AI applications.

## Artificial Intelligence (AI) applications

We're enabling businesses to streamline processes and boost productivity by taking full advantage of AI applications. We can help you use deep learning techniques to automate quality control and inspection processes or explore autonomous vehicle technology. Our team can also work with you using natural language processing to create chatbots and intelligent advisors, or sentiment analysis and automatic summarisation to help identify relevant changes in fast-moving global regulations, such as customs, health and safety or data protection.

## Digital product design

We can combine our data, physics, engineering and modelling capabilities with our visual computing facilities to help build "digital twins" of products, production lines and processes and use them to increase quality and efficiency. We can help you explore and understand detailed aerodynamics of a vehicle, an aircraft and even the wind flow around a building using our Virtual Wind Tunnel without the need for a physical prototype, offering an accessible way for you to bring your designs to life and saving time and money for your business.



# How we do it

## Collaborative R&D

We work with clients on a commercial basis, or as a partner in a funded research project, to define a challenge within their business and build a team to deliver a bespoke digital solution that accelerates R&D, reduces costs and improves the productivity of people and processes.

## Platform as a service

We provide the computing power to your own experts as they require it, to improve products and services on a pay-as-you-go basis for a competitive cost per core hour. Only pay for what you need.

## Creating digital assets

We design new industry-led software applications to solve sector-based challenges, which are then made available for industry and the research community to license.

## Training and skills

We offer hands-on training programmes, workshops and events at a variety of levels, from introductory to expert. If our existing events don't suit your needs, we can work with you to design a bespoke course for your team. We also collaborate with UK universities on postgraduate training and support an MSc in Big Data and High Performance Computing at the University of Liverpool.

## Funding opportunities

We can help you to apply for both STFC-based and external sources of funding to carry out collaborative projects with us, such as Bridging for Innovators (B4I), which offers businesses access to a suite of unique high-tech scientific facilities and knowledge to fast-track solutions to industrial challenges.



# Our Technologies



At the Hartree Centre, we host a range of high performance computing platforms and cutting edge facilities, including:

## Scafell Pike

A Bull Sequana X1000 supercomputer, helps key scientific areas including: molecular modelling and material science, life sciences, virtual engineering and simulation, and deep learning.

## JADE

A Bull Atos NVIDIA DGX1 Deep Learning supercomputer, has particular relevance for: GPU-enabled computing, DL-enabled HPC application development, and prototyping and algorithm development.

## Panther

An IBM POWER8 with 512 POWER8 cores, and **Paragon**, an IBM POWER8 with NVLink and 656 POWER8 cores, can help businesses with a focus on: chemistry, life sciences, engineering and manufacturing, and enabling technologies.

## Dawson

An IBM data analytics platform, supports a range of IBM and open source software with particular benefit for: transport planning, healthcare, financial modelling and blockchain.

## Atos Quantum Learning Machine (QLM)

The Atos Quantum Learning Machine is the UK's first quantum computing simulation environment, enabling companies to develop algorithms and become more resilient to the evolving digital landscape.

## Visual Computing Facilities

Our range of visual computing facilities and event spaces are suitable for training, small-scale conferences, product demonstrations and more. Our immersive visualisation capabilities are well-suited to in-depth data analysis, modelling and simulation, while our VR/AR facilities could allow you to explore virtual product development and make design changes early on in your development process.

# Hartree Centre in Action: Engineering and Manufacturing

Our systems and high performance software engineers can open up new possibilities for the engineering and manufacturing sector with high-fidelity modelling and simulation, offering detailed engineering analysis to help accelerate product development and reduce R&D costs. Our code coupling capabilities can expand on existing models to solve complex multi-scale and multi-physics problems, from fluid dynamics and turbulence to combustion modelling. Our team can help to modernise your code and deliver optimised software, accelerating innovation and future-proofing for next generation architectures. Our visual computing facilities can be used to develop and explore digital twins of products, production lines, processes and environments that aid decision-making. Using our data analytics and AI expertise can even help you to automate product inspection, improve understanding of the regulatory environment or drive efficiency improvements by generating insights from production data to optimising manufacturing processes.

# Improving aerodynamic engineering in Formula One

We worked alongside TotalSim – an aerodynamics and CFD company – to understand vortex formation in Formula One cars and improve aerodynamic performance.

Many components on a modern Formula One car are designed by aerodynamicists to shed vortices. These vortices are used to control the air flow around the race car in order to maximise the downforce that can be generated. Understanding the dynamics of vortex structures is important as they have a direct impact on vehicle performance. TotalSim were looking to develop an algorithm that could extract, label and track vortices in vehicle simulation data to help identify the most promising design solutions more efficiently.

The Hartree Centre team used image processing techniques to identify significant

features and went on to develop a versatile algorithm capable of being applied to images from both simulations and virtual experiments as well as analysing large image sets and offering detailed insights into the formation of vortex structures, leading to better vehicle designs with enhanced aerodynamic efficiency.

**“This has provided opportunities to work with experts outside our normal field of experience and allowed us to undertake ‘bluesky’ research projects that would otherwise be too risky or expensive for an SME like us to undertake.”**

Robert Lewis,  
TotalSim

# Hartree Centre in Action: Health and Life Sciences

From understanding how drugs interact at a molecular level to modelling patient flow through hospitals, our ability to analyse large datasets and apply AI technologies can open up new insights for your organisation to aid decision-making, streamline processes and maximise efficiencies. We can also assist in drug discovery by combining simulation and machine learning to generate detailed 2D and 3D visualisations of candidate compounds, accelerating lead optimisation and reducing R&D costs by streamlining prototyping and boosting the innovation cycle.



# Making a difference using AI

Through our collaboration with Alder Hey Children's Hospital, we harnessed the power of artificial intelligence to personalise children's healthcare by creating a chatbot to enhance the patient experience. Our team is also developing ways to further integrate AI into the hospital using IBM Watson. The 'Ask Oli' chatbot uses the hospital's mascot elephant character to interact and answer questions in real time, reducing patient and relative concerns in a way that is both innovative and fun. This is helping Alder Hey to forge a path to more personalised treatment, enhance health outcomes, increase patient satisfaction and save money. From faster identification of clinical trends, to monitoring admission patterns to aid planning, the potential is limitless.

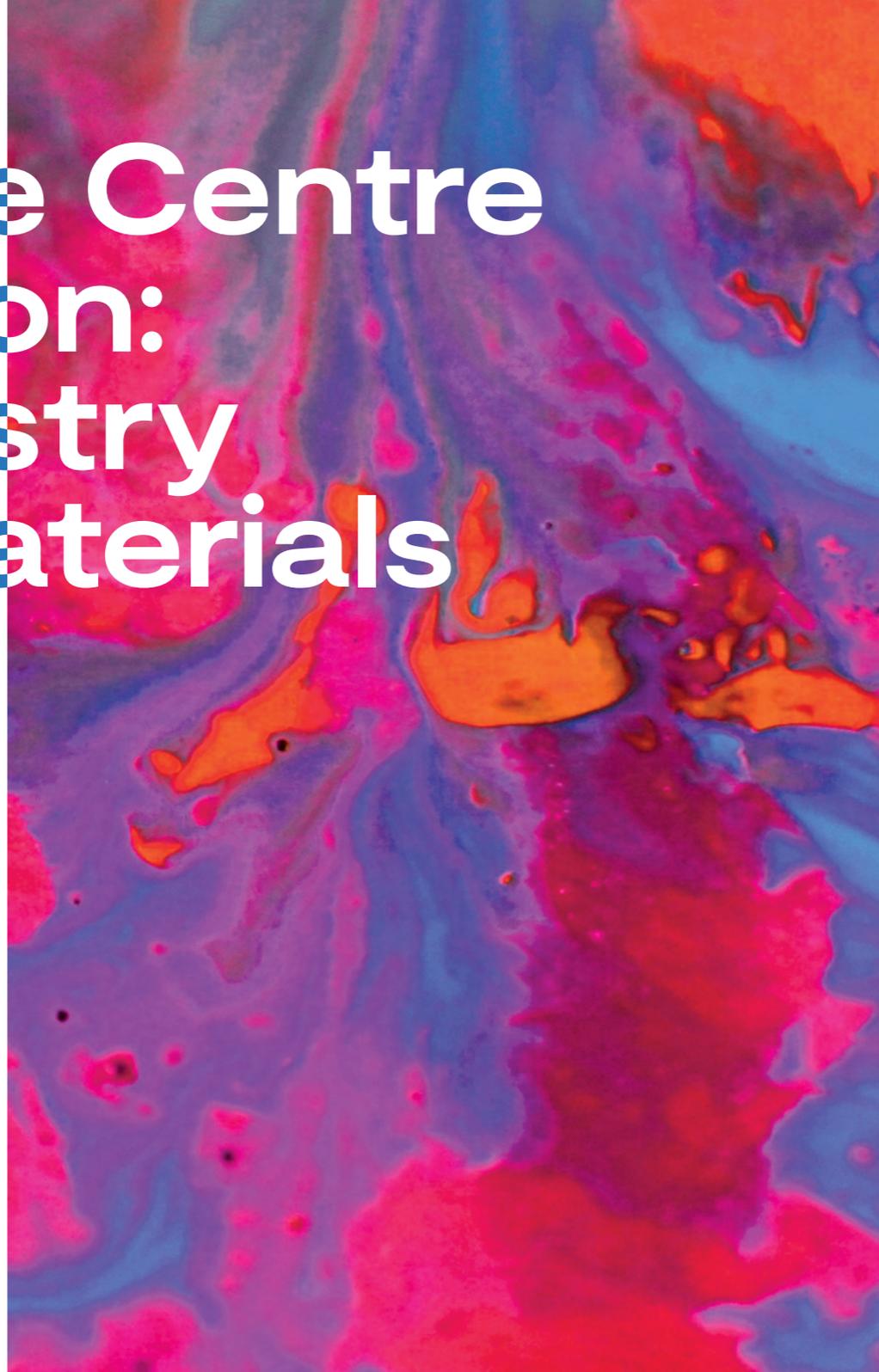
**“This is an unprecedented opportunity to transform working practices in healthcare and enable doctors to spend less time on paperwork and more time with patients.”**

Iain Hennessey  
Alder Hey Children's Hospital



# Hartree Centre in Action: Chemistry and Materials

We help industry to remain competitive using an integrated suite of our data analytics, modelling, and simulation capabilities to address business challenges in chemistry and materials problems with world-class scale and accuracy. Our track record in atomistic and mesoscale modelling can shed light on properties, functions, structures and geometries, with applications from drug discovery and packaging and coatings to energy and environmental infrastructure. We combine our domain specific expertise with an in-depth knowledge of the application of data-driven and AI technologies to transform chemical and materials product design and help industry move away from ad-hoc, labour-intensive and expensive approaches to more robust and adaptive computer-aided paradigms to boost efficiency in the development of new products.



# Optimising drug discovery

The cost of developing new, successful drugs is soaring, with huge implications for productivity. Our researchers worked with AstraZeneca to accelerate lead optimisation by providing insights on a new class of drugs with the potential to reduce costs and bridge that productivity gap. The team developed computational workflows that blend molecular dynamics - a technique that simulates the movements atoms and molecules on a supercomputer - with machine learning. This offered an insight into how chemical modifications influence shape and therefore permeability. This helped identify how to make a drug more permeable or easy to manufacture, saving costs and boosting productivity.

The project included a novel approach to making computational notebooks accessible on supercomputers, helping to democratise computational science, giving domain scientists easy access to high performance computational workflows and analytics.

**“We are excited to build upon this collaboration and work towards large scale benchmarking exercises and adoption of machine learning capabilities”**

**Anders Hogner,  
AstraZeneca**

# Hartree Centre in Action: Data Analytics

We can help you explore how data-driven technologies like advanced analytics, predictive modelling and AI applications can improve business productivity and strengthen your competitive advantage. Our ability to analyse and visualise large datasets fast using the strength of our supercomputing infrastructure, combined with a team of data science experts who can help you collate and clean your data, can enable you to draw valuable insights that enable smarter decision making, more efficient processes and significant cost-savings.



# Using data science to pick the right healthcare app

There are thousands of healthcare apps on the market. Knowing which will be the safest and most effective for patients to monitor or manage their condition can be tricky. ORCHA advise governments, and health and social care organisations, on how to select the highest quality health apps that will have the greatest benefit for a patient and then encourage their take-up. But reviewing and categorising the apps is a time-consuming manual process.

Through the ERDF-funded LCR 4.0 programme, ORCHA worked with data scientists at the Hartree Centre to explore new data-driven techniques that could speed up their evaluation process and develop a more sustainable business model.

The Hartree Centre developed techniques and proof-of-concept tools that have enabled ORCHA to explore a more data-driven approach that will enable it to scale up

and offer even more insight in its app reviews. The project influenced the company's future approach to data collection and analysis and speed up and enhanced the accuracy of the current health app evaluation service. This improved ORCHA's ability to support patients, and the efficiency of healthcare professionals' recommendations.

**“The Hartree Centre has proven the value of data science to our business and led to us expanding our team to create new jobs in data driven roles.”**

Liz Ashall-Payne, ORCHA



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For information about how  
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