



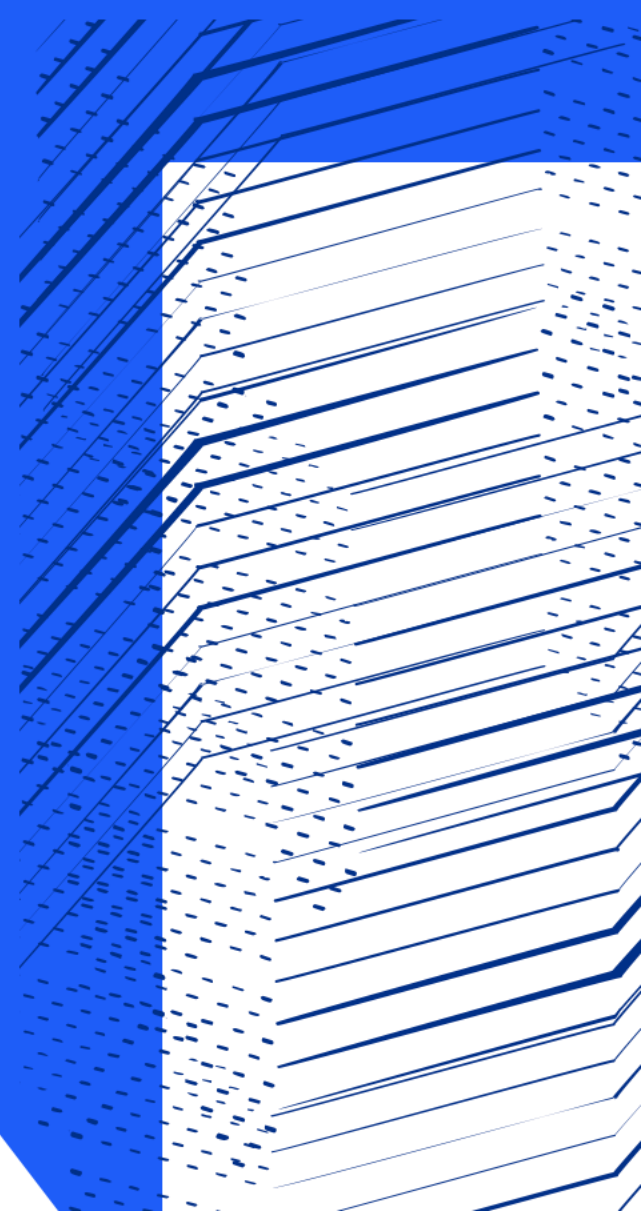
Science and  
Technology  
Facilities Council

# The Hartree Centre

Challenge-led applied research & innovation

**Francis Lee**

Business Development Manager



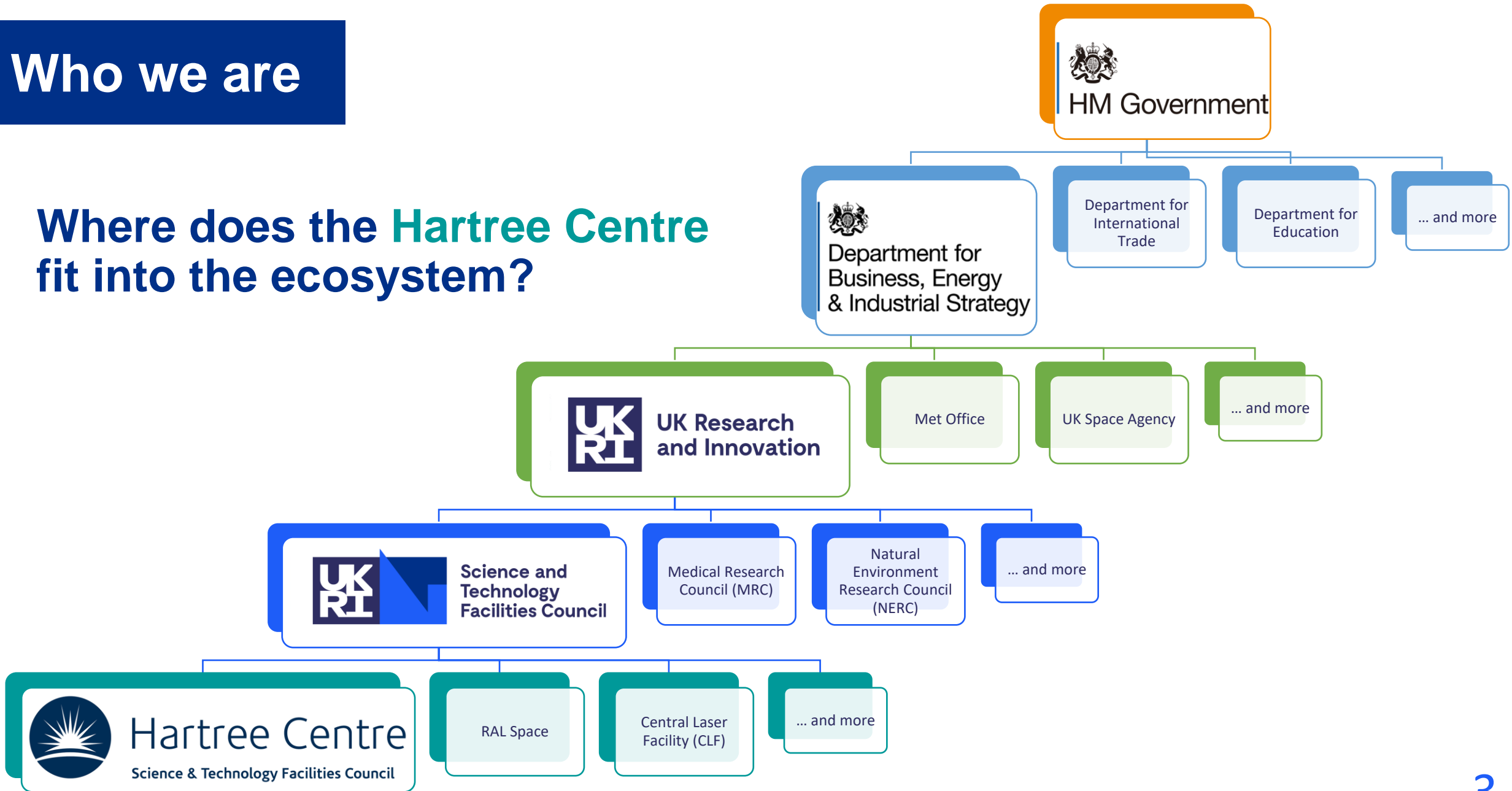
# Our mission

**Transforming UK industry by accelerating the adoption of high performance computing, big data and AI technologies.**

- Primary purpose is to apply the latest capabilities in emerging technologies to industrial challenges to deliver transformative gains in performance, productivity and time to market
- Provides industry and applied researchers access to advanced data and AI technologies, HPC facilities and scientific computing expertise
- Based at the Science and Technology Facilities Council within the Sci-Tech Daresbury campus in North West England.

# Who we are

## Where does the Hartree Centre fit into the ecosystem?



# STFC facilities

## UK Astronomy Technology Centre

Edinburgh, Scotland

- National centre of excellence for development of scientific instrumentation & facilities for ground & space based astronomy



## Polaris House

Swindon, Wiltshire

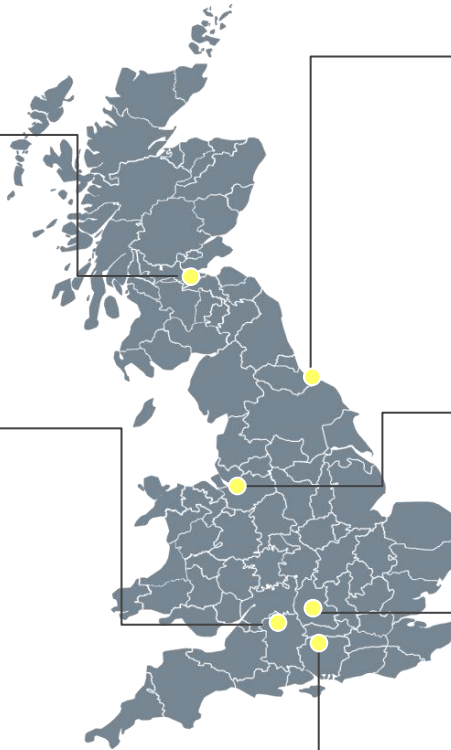
- STFC Headquarters
- Manages international subscriptions & core research grants
- Home to Governments other 6 Research Councils, Innovate UK & UK Space Agency



## Chilbolton Observatory

Stockbridge, Hampshire

- One of worlds most advanced meteorological radar facilities
- Home of the worlds largest steerable meteorological radar (CAMRa), Chilbolton Facility Atmospheric & Radio Research (CFARR), Low Frequency Array Radio Telescope (LOFAR), the Met Office Upper Air Monitoring Facility & the Space Monitoring Facility



## Boulby Underground Laboratory

North Yorkshire

- UK's underground science facility
- One of a handful of worldwide facilities – search for dark matter, studies of cosmic rays, astrobiology & life in extreme environments



## Daresbury Laboratory

Sci-tech Daresbury Campus, Liverpool City Region

- Hartree Centre – HPC, Big Data, AI
- ASTeC - deliver world-class particle accelerator R&D
- CTH - rapid prototyping through additive manufacturing



## Rutherford Appleton Laboratory

Harwell Didcot, Oxfordshire

- Diamond Light Source Ltd - UK's national synchrotron - giant microscope using electrons to study anything from fossils to jet engines to viruses and vaccines
- Central Laser facility – reveals how life & matter works from molecules to cells to supernova
- RAL Space – space research & technology development, test facilities (210 space missions)
- ISIS Neutron & Muon Source – studies materials at atomic level

# Network of Expertise



# Our Platforms & Facilities

## Intel Platform

Bull Sequana X1000 (4.3PFlop/s, ~80000 cores)

- Normal Compute Nodes – Skylake (Xeon Gold)
- Accelerator Nodes – Knights Landing (Xeon Phi)
- High Memory Nodes – Xeon
- GPU Nodes – nVidia V100

## JADE – Oxford University

Deep learning supercomputer, one of largest in UK

NVIDIA DGX SuperPOD™ architecture

Atos Bull 63x DGX nodes

- 504 NVIDIA V100 Tensor Core GPUs
- 2,580,480 CUDA Cores



## Atos Quantum Learning Machine (QLM)

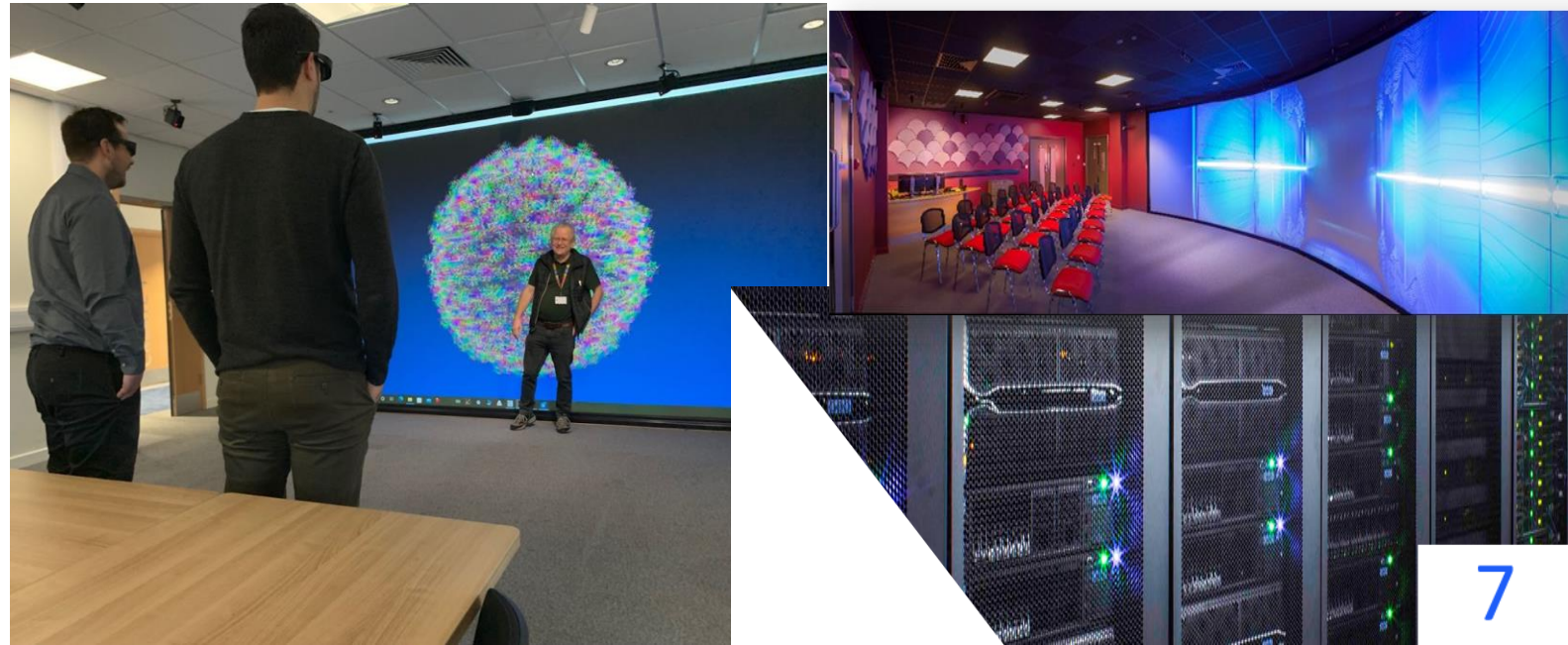
Discovering and delivering next-generation algorithms for future quantum computers

## Cloud Computing Platforms

We have access to multiple cloud vendor platforms. We are vendor agnostic, so can deploy to a variety of different cloud runtimes during and after projects. Post project, this can simplify handover of solutions into customer production environments.

## Visual Computing Suite

Collaborative visual computing technologies enabling exploration of data analytics and computational modelling



# Our People

- Chemists
- Physicists
- Life Scientists
- Mathematicians
- Engineers
- Software Developers
- Research Software Engineers
- Data Scientists
- High Performance Computing Scientists
- Technical Architects
- Programme Management
- Business Development
- Customer Services



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# What we do

## – Collaborative R&D

Define a challenge in your business and we build a team to deliver a solution in the areas of:

- Modelling & simulation
- Code optimisation
- Data Science and AI
- Digital product design

## – Platform as a service

Give your own experts pay-as-you-go access to our compute power

## – Creating digital assets

License the new industry-led software applications we create with IBM Research

## – Training and skills

Drop in on our comprehensive programme of specialist training events or design a bespoke course for your team





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# Our track record

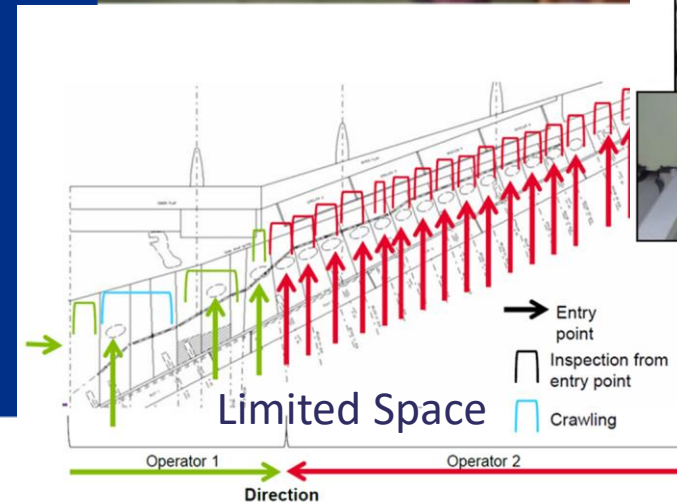


# Case study

## Airbus | Deep Learning for Wing Tank Inspection

Faster quality control process for wing tank inspection (A320 & A321)

- Check correct standard of: sealant, fasteners, paint, adhesion, liquids
- Detection of flaws: Missing/damaged sealant, excess paint, scratches and foreign objects (nuts, bolts, misc tools, swarf, safety glasses, wire, etc.)



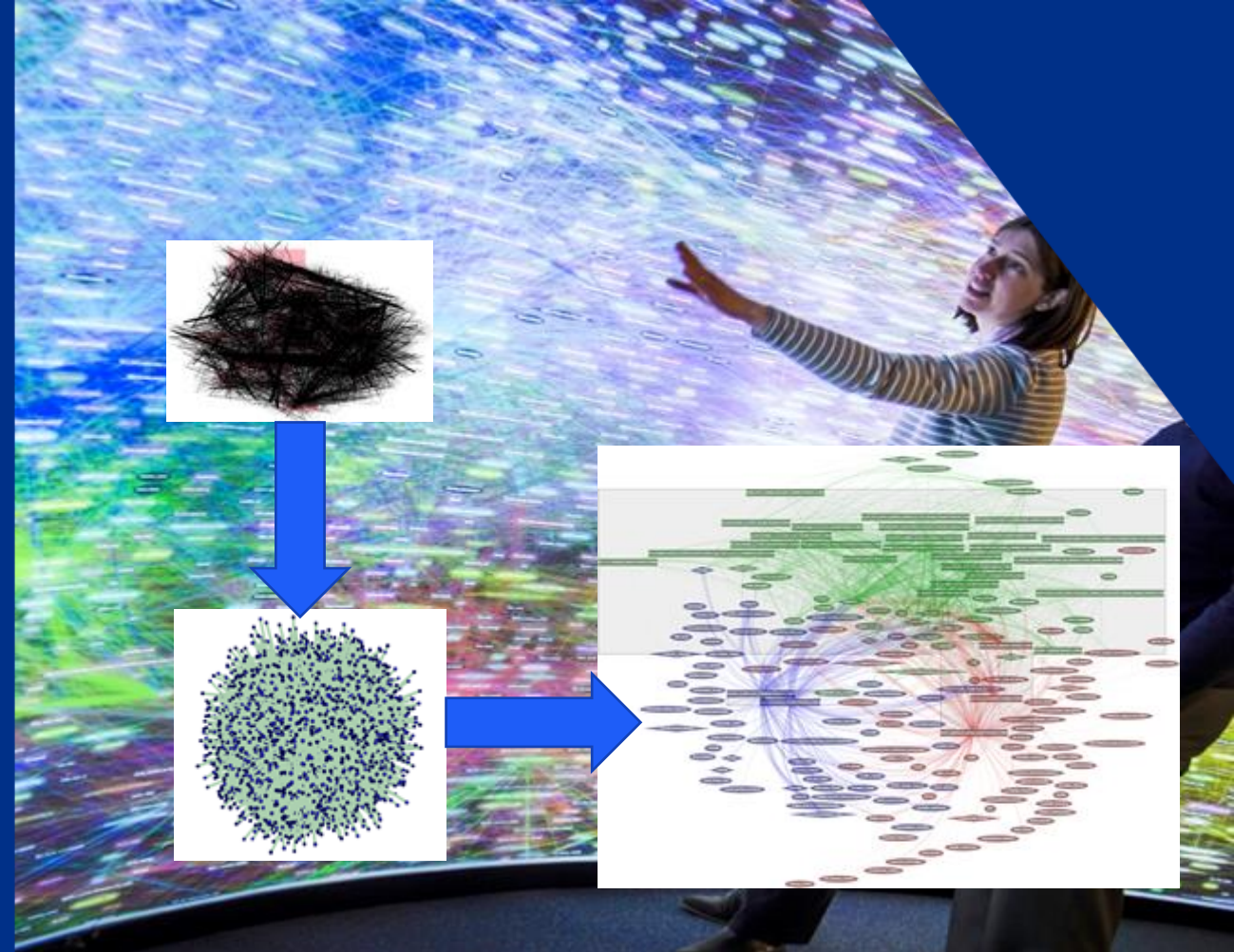
- Model Creation with >1000 Images
- Train/Validate 80:20
- Test Set >50 Images

# Case study

## Data-driven disease mapping

Drug discovery and identifying new uses for existing treatments using big data

- PubMed – 24 Million citations
- All known human diseases, genes, pathways & proteins
- 22,000 Node, 1,000,000 edge hairball

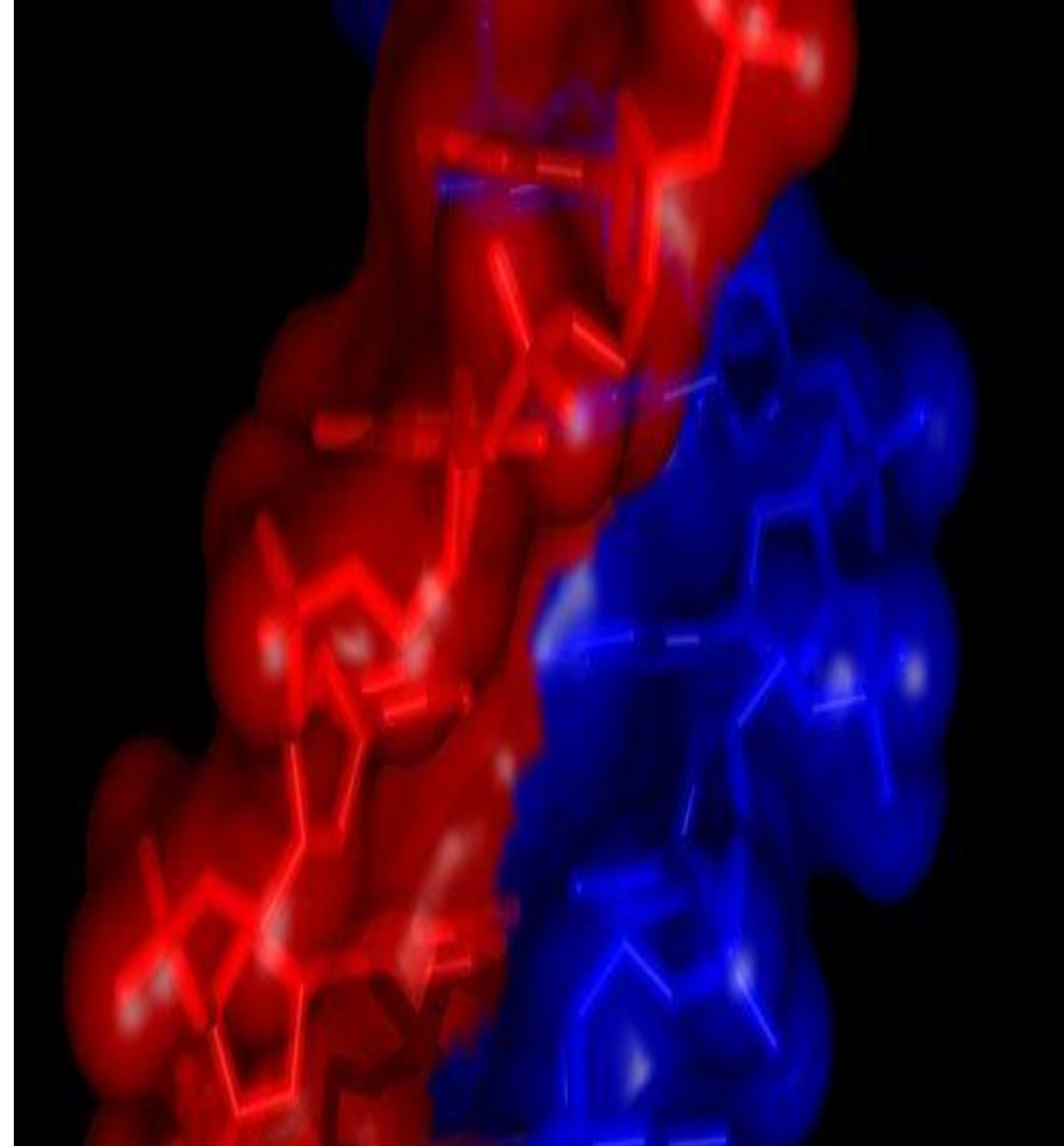


## Case Study

*We worked with Syngenta – a leading agricultural and biotechnology company – to design bioinformatics tools for high throughput screening of candidate compounds.*

Assessing the toxic potential of a molecule is an essential element in drug discovery.

Data from their research was coupled with machine learning pipelines to generate in silico predictive models that could classify potential toxicity using gene expression profiles from cell lines treated for a range of candidate compounds.



# Case study

## Computer aided formulation

Faster development process for products like shampoo, reducing testing

*“The Hartree Centre’s high performance computing capabilities help us achieve better design solutions for our consumers, delivered by more efficient, cost-effective and sustainable processes.”*

– Paul Howells, Unilever



# Case study

## Code optimisation for aerospace engines

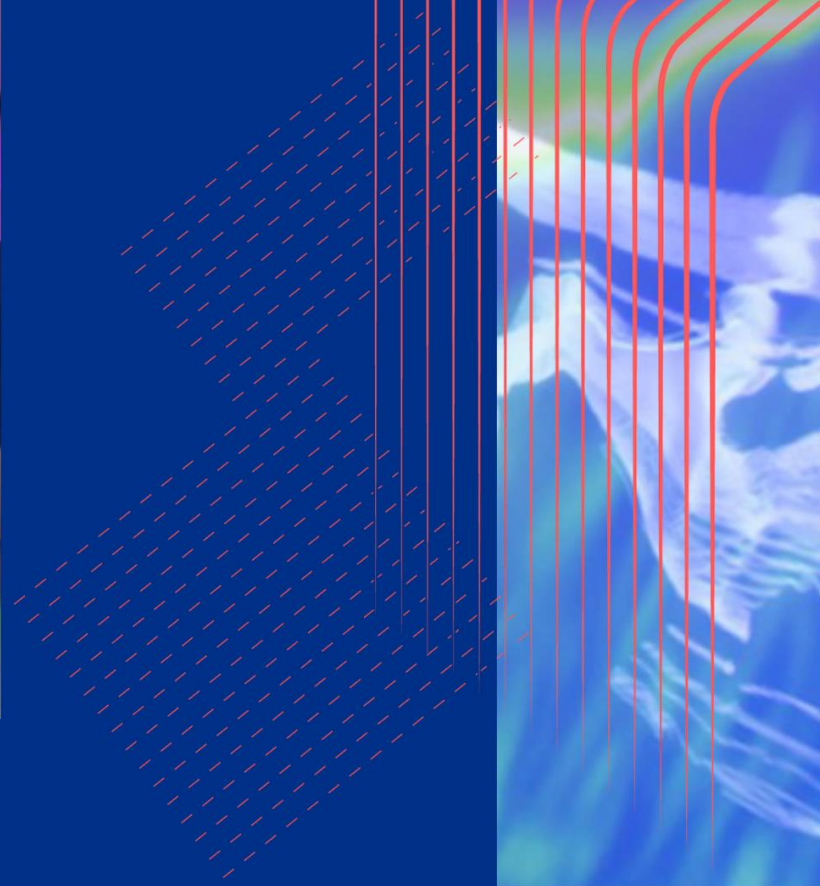
Codes for modelling component design made to run ~ 40% faster

*“Working with the Hartree Centre, we have quickly made significant improvements to our code, delivering faster turnaround and more capability to our engineers.”*

– Matthew Street, Rolls-Royce



Collaborative R&D



# HARTREE NATIONAL CENTRE FOR DIGITAL INNOVATION



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# Hartree National Centre for Digital Innovation (HNCDI)

A new Hartree collaborative programme with IBM Research. £210m investment - £172m UK Govt investment + £38m IBM in-kind

- Enable **businesses** and **public sector organisations** to adopt digital innovations, such as AI and quantum computing, by providing a dynamic and supportive expert environment.
- Provide an environment where **UK organisations of all sizes** can explore the latest technologies, develop proofs-of-concept and apply them to industry and public sector challenges for **productivity, innovation** and economic growth.
- Help organisations navigate the possibilities, and **de-risk investment**, of new technologies.
- Support organisations in planning and taking their next steps in their **digital transformation** journey



Hartree Centre



# HNCDI work streams - Tackling industry challenges

## Skills

Tackling gaps within organisations and widening the digital talent pool



### EXPLAIN

55 Training Course

## Technical Capability

Exploring and evaluating data-driven AI technologies to help enhance productivity



### EXPLORE

18 Person mths over 9mths

## Application

Developing and implementing practical solutions within organisations



### EXCELERATE

42 Person mths over 14mths

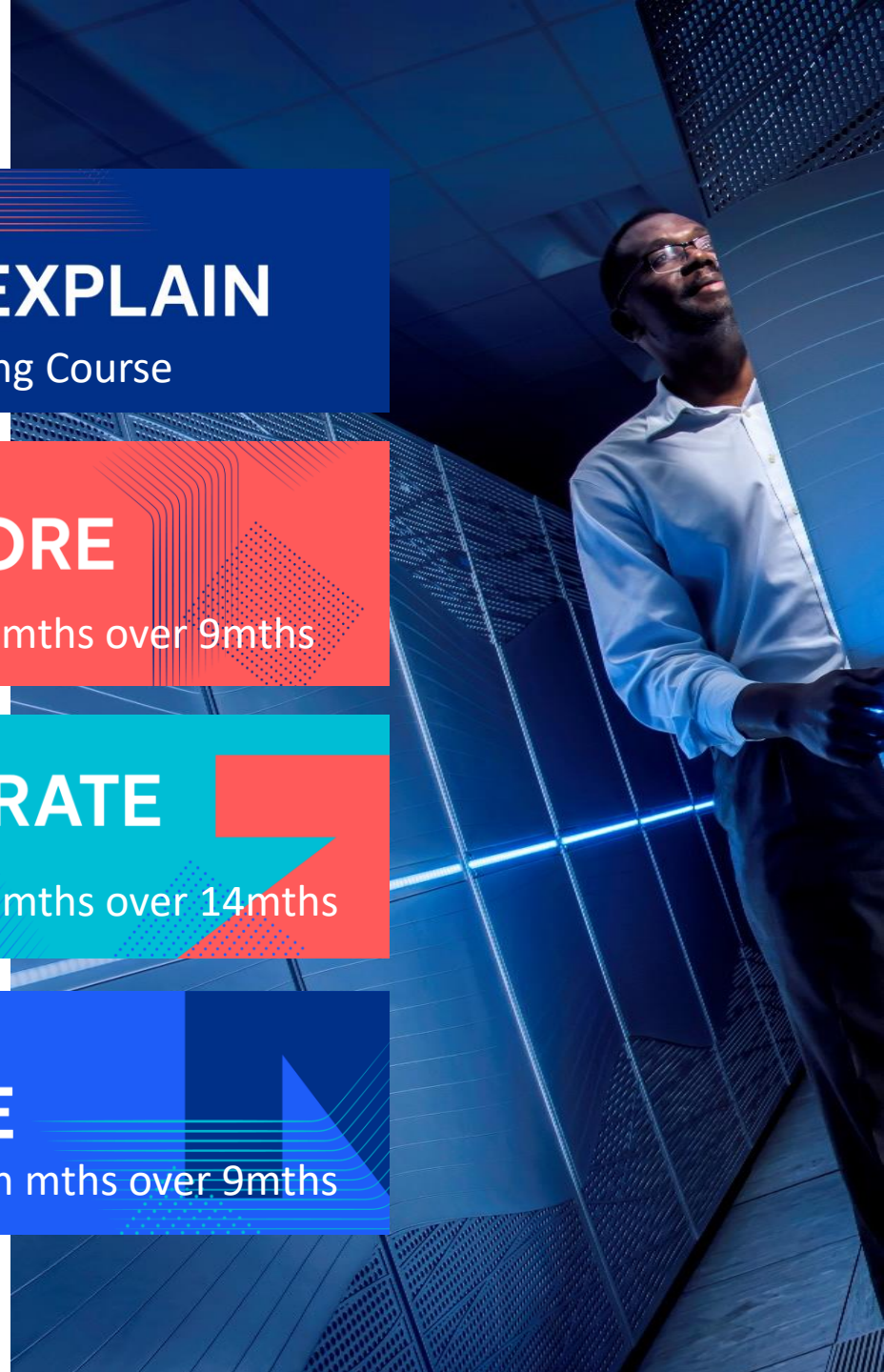
## Resilience

Enabling organisations to understand when to invest in the right emerging technologies (e.g. quantum computing)



### EMERGE

18 Person mths over 9mths



# How to engage with us

## Collaborative R&D Projects

- **Commercial**
  - High priority projects for Hartree resource allocation
  - Short lead-time – project scoping & project start dates
- **Grant funded**
  - Assistance with grant applications
  - Longer lead-time – project scoping, multi-stage application processes & project start dates
  - No guarantee of funding – delaying project start dates



# Where to start

- **Clear challenge statement**
  - Set the scene – where are you, what have you done already and what are the desired outcomes
  - Outline how this work has the potential to impact your company
  - Quantify any potential changes to productivity
  - Access to the appropriate data – quantity and high quality
- **Collaborative project work**
  - Deliver project outcomes
  - Knowledge transfer





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# Thank you

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