


The UKRI logo consists of the letters 'UK' stacked above 'RI' in a white, bold, sans-serif font, set against a dark blue square background.

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The background features a complex, abstract pattern of glowing, multi-colored lines (green, blue, yellow, and red) that appear to be flowing and swirling, creating a sense of dynamic energy and movement. A large, solid blue triangle is positioned on the right side of the image, partially overlapping the glowing lines.

Welcome

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Industrial Use of High-Performance Computing and Artificial Intelligence

Dr. Ubaid Ali Qadri

Team Lead – Multi-Fidelity Design & Twinning



Agenda

1 Why does it matter?

2 What does "industry" need?

3 What are we doing?

4 Case studies





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Why does it matter?



Why does it matter?

- It is a common belief that improved computing power boosts progress, productivity, and brings about economic benefits.

“Compute has the potential to unlock productivity as sectors across the economy make better and more extensive use of data analysis, simulation and AI technologies.”

Future of Compute Review

Why does it matter?

- Is there evidence that more computing power actually produces benefits?

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Financial ROI Projects

	Average of Revenue \$ per HPC \$ Invested	Average of Profit or Cost Saving \$ per HPC \$ Invested
Total	\$509.3	\$47.2

Note: This study analyzed ROI for 26 academic projects, 6 government projects, and 143 industry projects.

Source: Hyperion Research, 2022

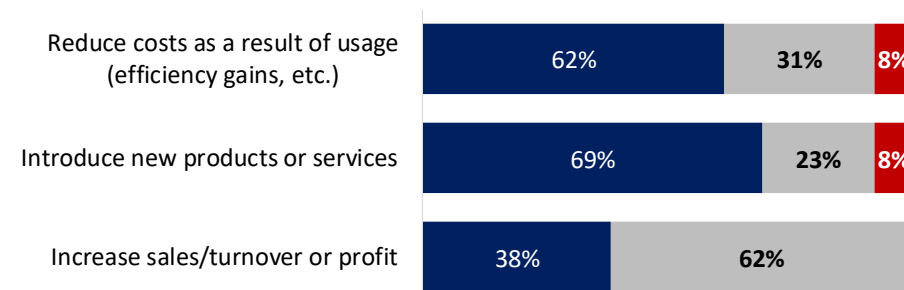
The Economic and Societal Benefits of Linux Supercomputers, April 2022, Hyperion Research



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The Impact of EPSRC's investments in High Performance Computing infrastructure, Nov 2019, London Economics

Figure 32 Figure 33 'Has access to / usage of EPSRC's HPCs helped your organisation to ...?'



■ Yes ■ Don't know / not applicable ■ No

Note: Based on 13 responses from industry. Source: London Economics survey of users of HPC capabilities

Why does it matter?

- Is there evidence that more computing power actually produces benefits?

THE IMPORTANCE OF (EXPONENTIALLY MORE) COMPUTING POWER

Neil C. Thompson^{1*}, Shuning Ge², Gabriel F. Manso³

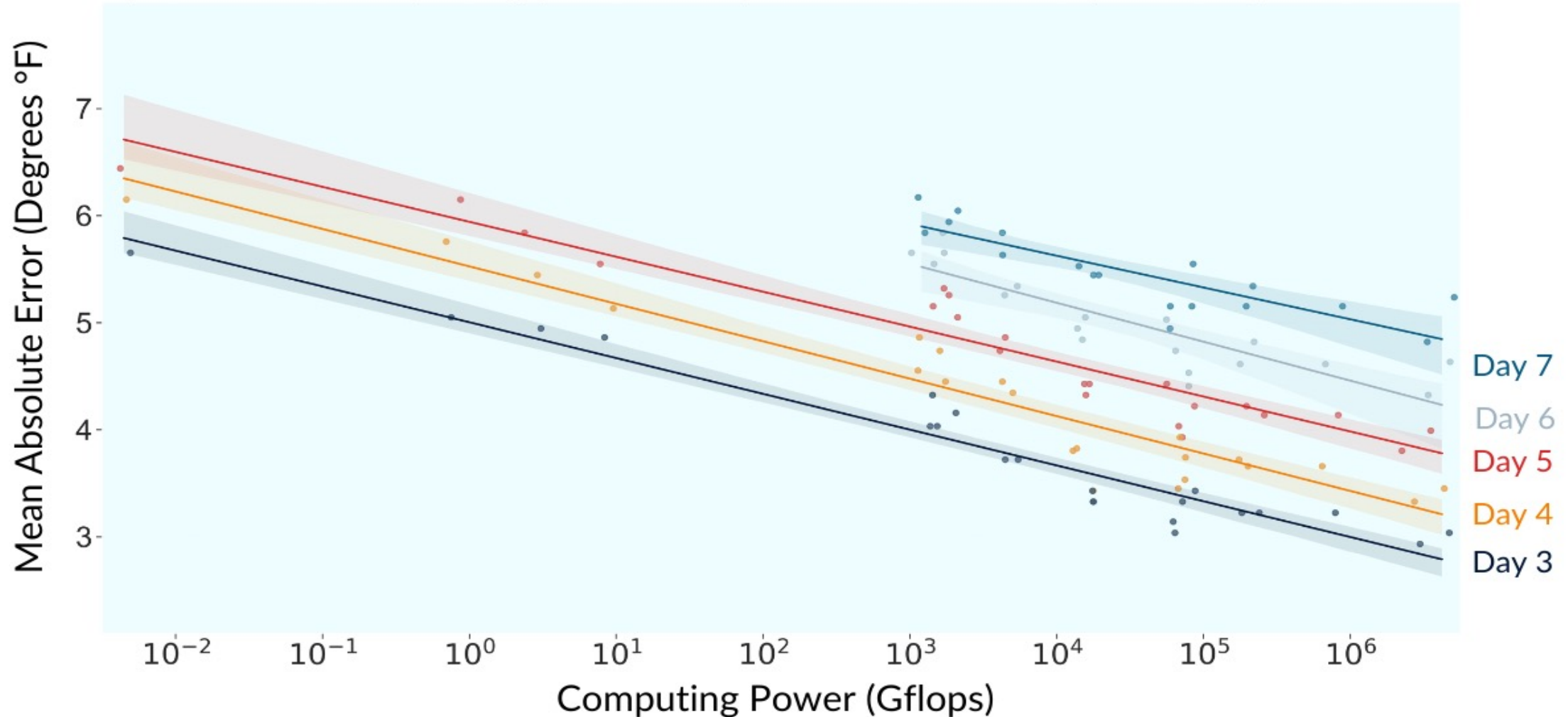
¹MIT Computer Science and A.I. Lab,
MIT Initiative on the Digital Economy, Cambridge, MA USA

²MIT, Cambridge MA, USA

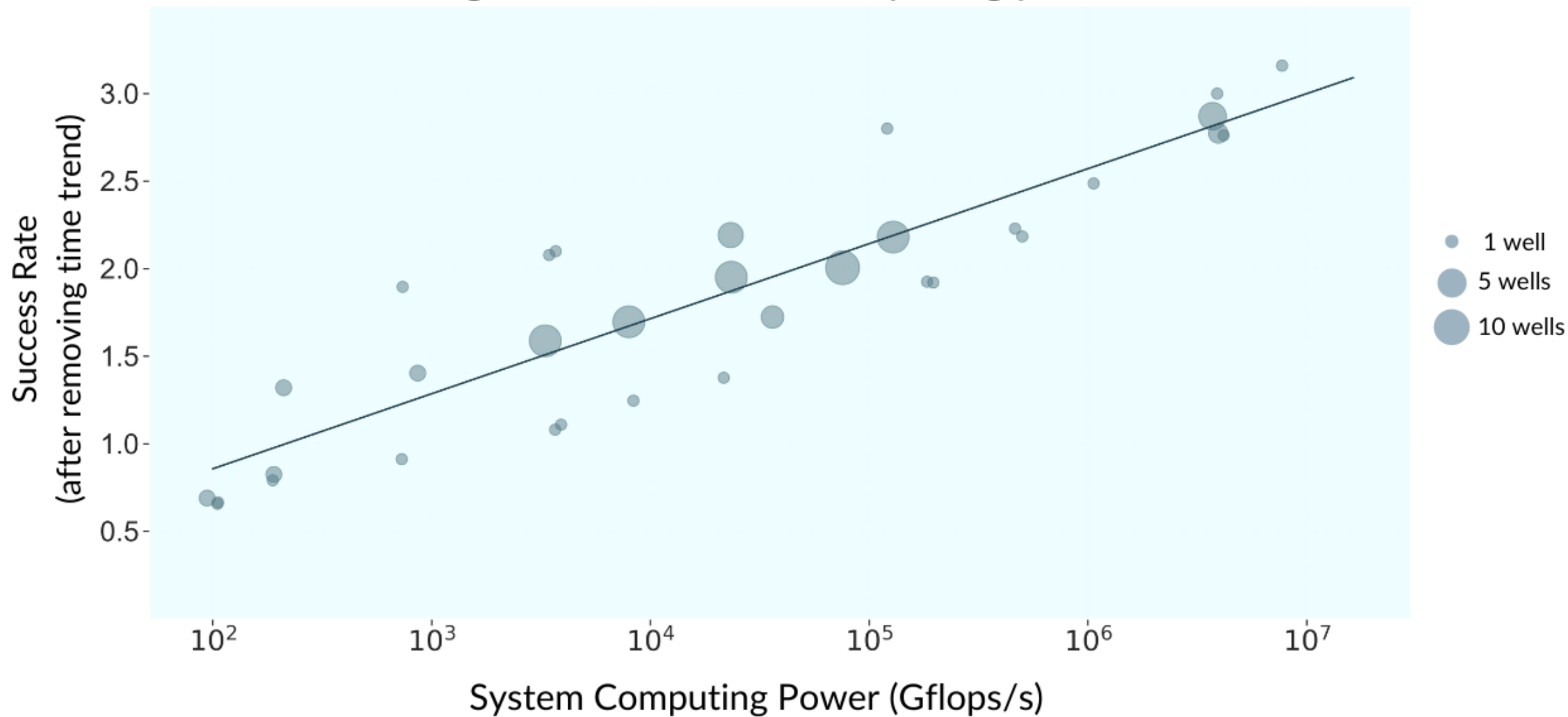
³FGA, University of Brasilia, Brasilia, Brazil

*To whom correspondence should be addressed; E-mail: neil_t@mit.edu.

c) Growth in computing power and performance in temperature prediction



b) Drilling success rate and computing power at BP



Why does it matter?

- What about AI?

Impact of AI in the innovation process can have more significant effect than impact of AI on final good productions.

Economic impacts of AI-augmented R&D

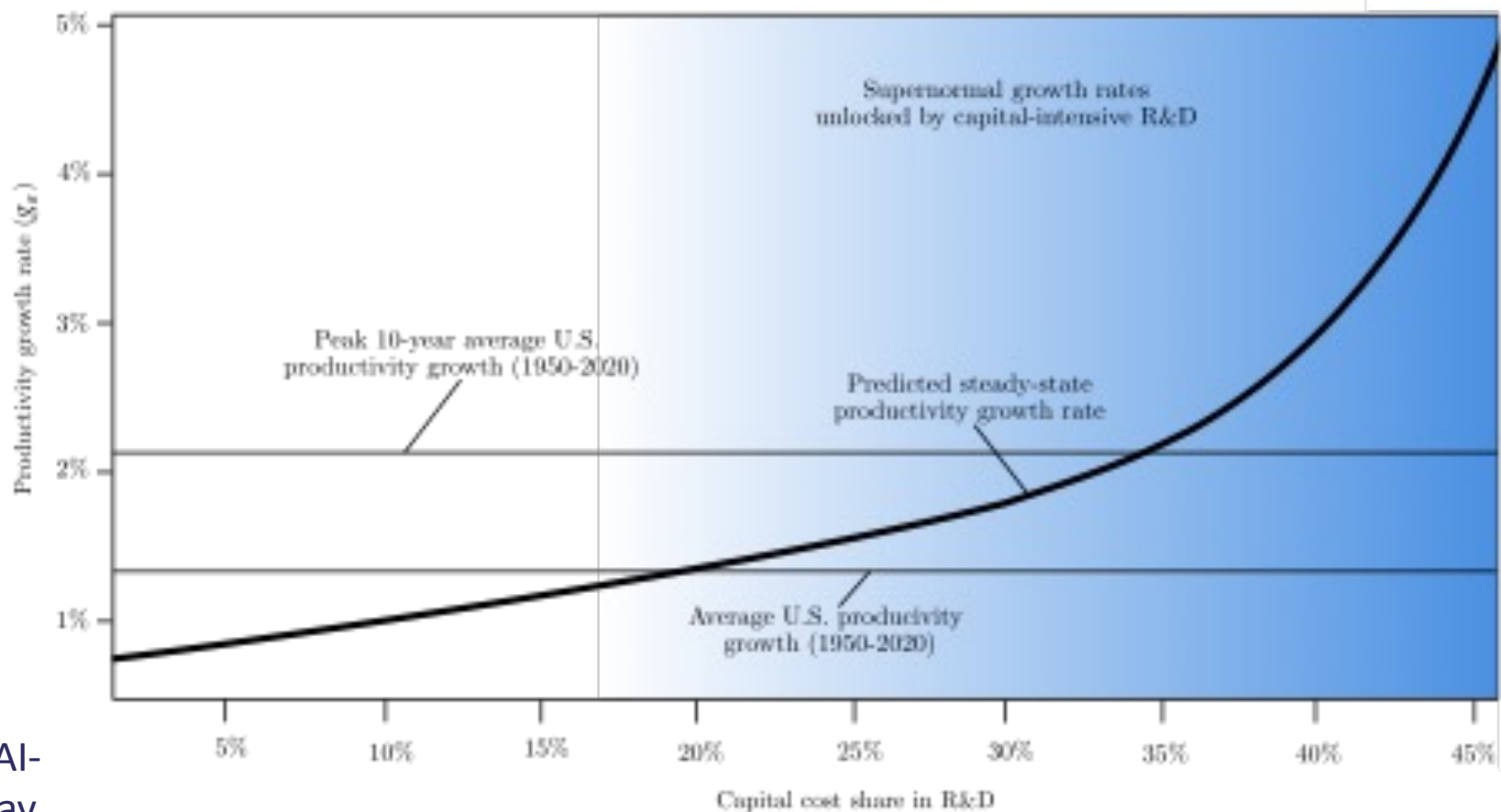
Tamay Besiroglu*
MIT FutureTech

Nicholas Emery-Xu*
UCLA Dept. of Economics, MIT FutureTech

Neil Thompson†
MIT FutureTech

Abstract

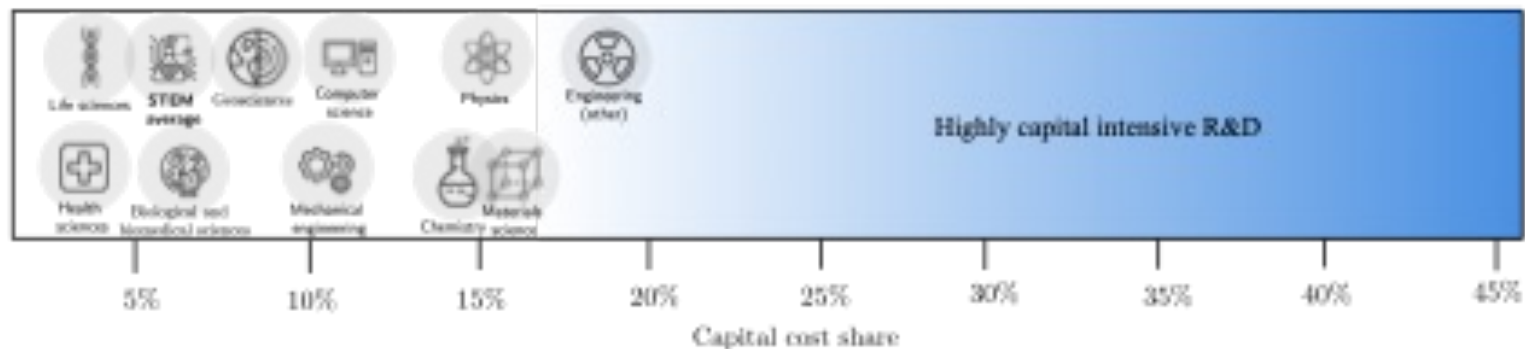
1a Predicted steady-state productivity growth rate and R&D capital intensity



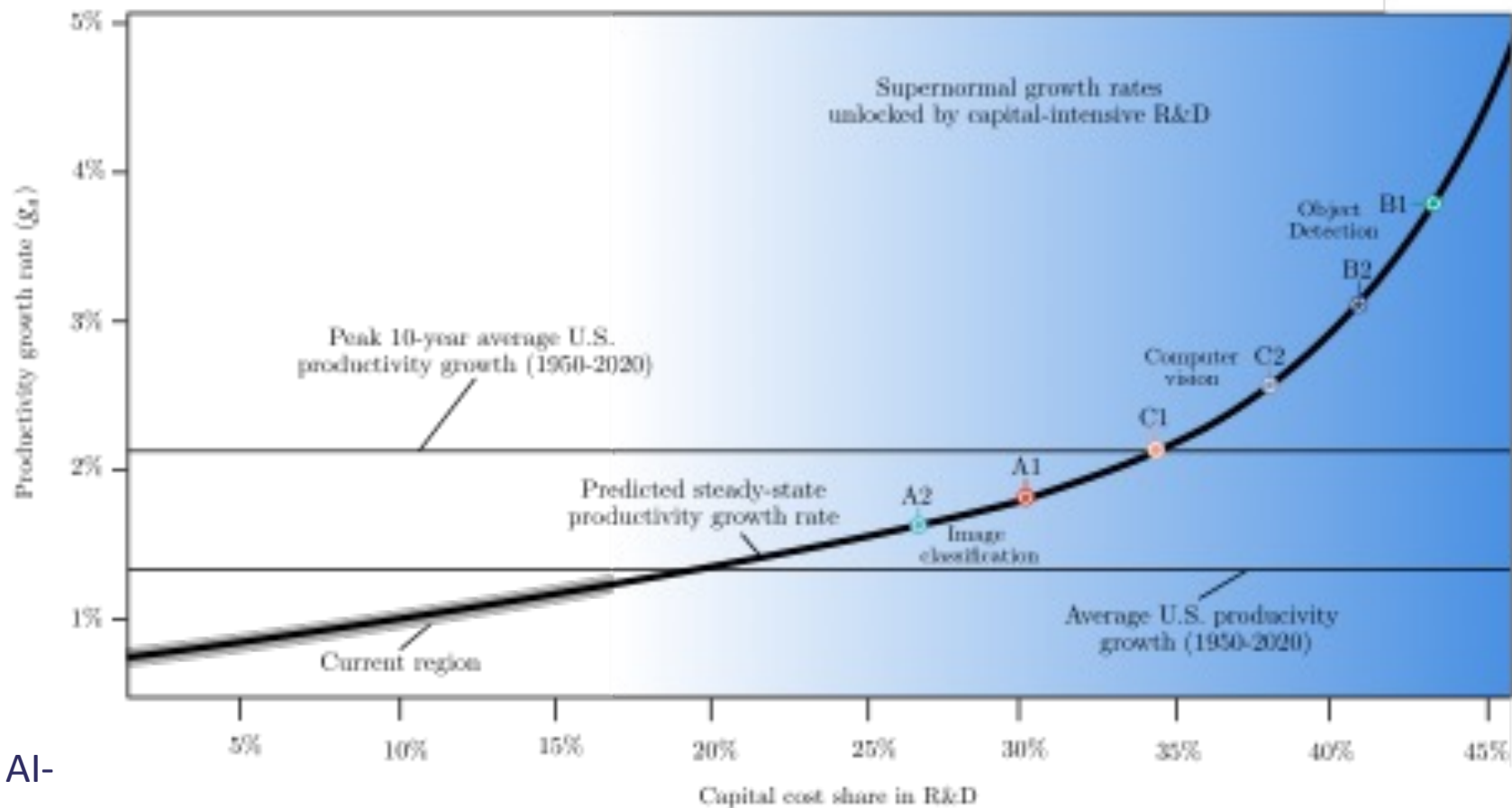
“Economic impacts of AI-augmented R&D”

Tamay Besiroglu, Nicholas Emery-Xu, Neil Thompson

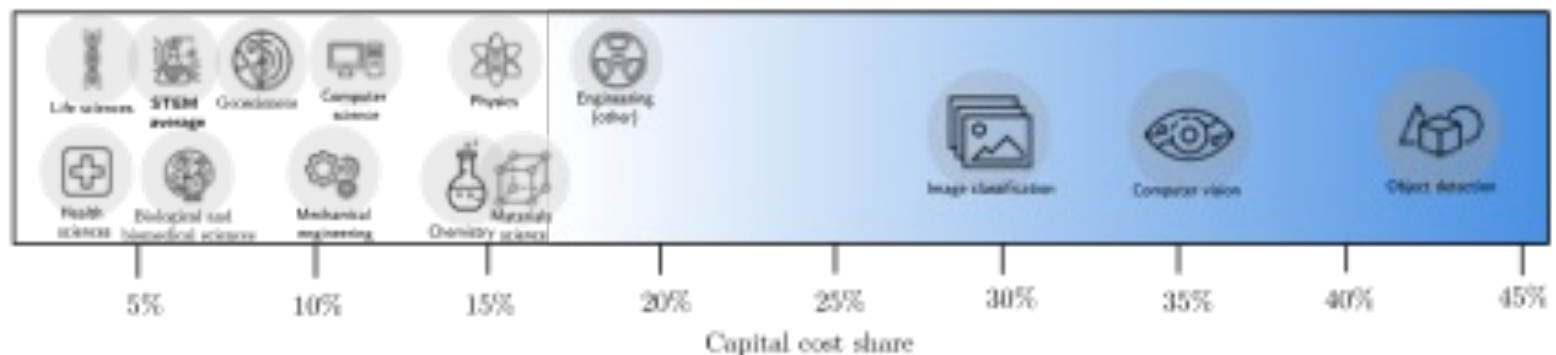
1b Observed capital intensity across R&D fields in the US



5a Predicted steady-state productivity growth rate and R&D capital intensity



5b Observed capital intensity across R&D fields in the US



“Economic impacts of AI-augmented R&D” Tamay Besiroglu, Nicholas Emery-Xu, Neil Thompson

Why does it matter?

- The use of HPC and AI has demonstrable impact on “good outcomes” in traditional sectors.
- HPC and AI can produce permanent increase in productivity due to their positive impact on the innovation process and idea generation.



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What does industry need?

What is holding us back?



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Users of compute

PIONEERS

Cutting-edge computational research

World-leading science, research, development and innovation

Sectors include



TIERS 0 and 1

Specific needs



ESTABLISHED USERS

Large-scale modelling, simulations and data science

Use in a particular research domain

Sectors include



TIERS 1 and 2

Private facilities

Specific needs



EMERGING USERS

Small-scale modelling and simulations

Use in traditionally non-compute-intensive disciplines

Sectors include



TIER 3

Commercial cloud

Specific needs



AI USERS

All scale AI training and AI-based research

Use in AI training and inference

Sectors include



ALL TIERS

Private facilities
Commercial cloud

Specific needs

At least **3,000** top-specification accelerators



Future of Compute Review, 2023



What are the needs?

Awareness

Accessibility

Applicability

Agility

Accelerators

- We don't know much about compute or AI, what do we do?
- How will it help us?



What are the needs?

Awareness

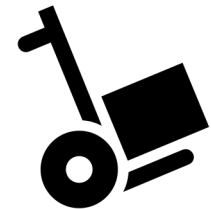
Accessibility

Applicability

Agility

Accelerators

- We don't have the compute power, what do we do?
- We don't have money to pay for them or people to use them, what do we do?
- We don't want to be coding, will your solutions work for us?



What are the needs?

Awareness

Accessibility

Applicability

Agility

Accelerators

- Will these technologies work for our problem?
- Will the solutions that we get be trustworthy, reliable and robust?



What are the needs?

Awareness

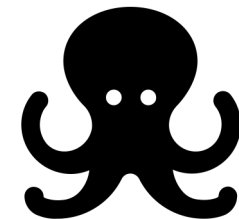
Accessibility

Applicability

Agility

Accelerators

- We use different platforms for different purposes, would we be able to integrate our workflows?
- We don't want to be locked in, can we move anytime?



What are the needs?

Awareness

Accessibility

Applicability

Agility

Accelerators

- Our software needs to be able to run on GPUs, can you help us?
- Our ML needs lots of GPUs, can you help us?



What are the needs?





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What are we doing?

Where do we fit in?



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What is the Hartree Centre?

- World-leading supercomputing, data analytics, AI and quantum computing technologies
- 120+ scientists, technologists and business professionals in bespoke teams working on challenge-led projects
- UK Government funded to boost productivity and innovation for industry and public sector organisations of all sizes
- Part of the Science and Technology Facilities Council in UK Research and Innovation
- Working with an international network of research communities and technology partners



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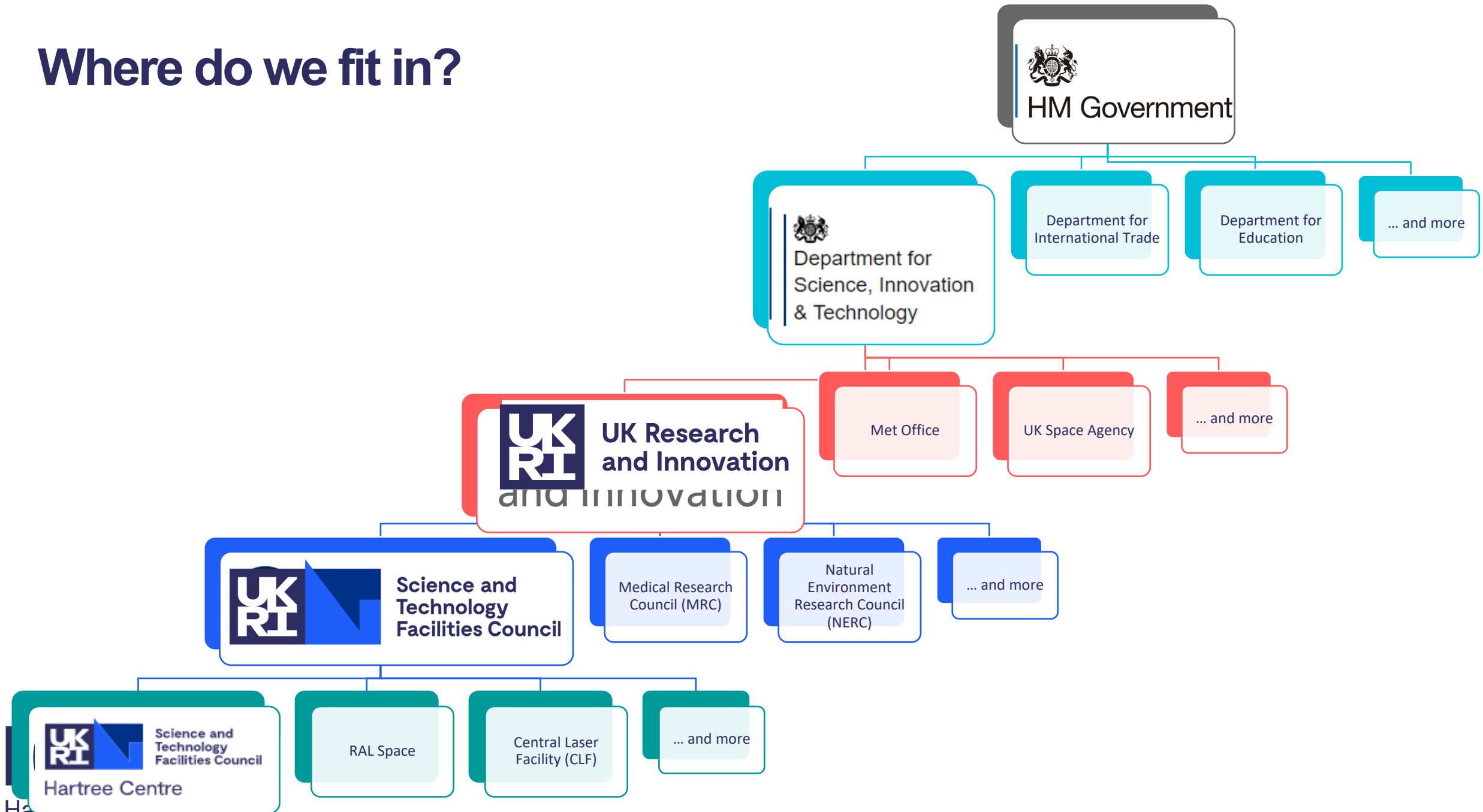


What is our mission?

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



Where do we fit in?



Our platforms and facilities

Scafell Pike

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/JADE-2 – Oxford University

Tier 2 Regional Deep Learning Supercomputer

NVIDIA DGX SuperPOD™ architecture

Atos Bull 63x DGX nodes

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

Cloud Facilities – On-Premise

- RedHat OpenShift (self-service)
- OpenStack VM provisioned
- AMD CPU/GPU, Nvidia A100, Alveo U200

Cloud Facilities – Public Cloud

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



Hartree National Centre for Digital Innovation (HNCDI)

- Five year collaborative partnership with IBM Research
£172M UK Govt investment + £38M IBM in-kind
- Enabling businesses and public sector organisations to adopt AI and quantum computing
- A dynamic and supportive expert environment for **UK organisations of all sizes** to explore the latest technologies, develop proofs-of-concept and apply them to industry and public sector challenges for **productivity, innovation and economic growth.**
- Helping navigate the possibilities, de-risk investment into new technologies and discover the next step



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Tackling industry challenges

Skills

Tackling gaps within your organisation and widening the talent pool



EXPLAIN

Technical Capability

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



EXPLORE

Application

Developing and implementing practical solutions within your business



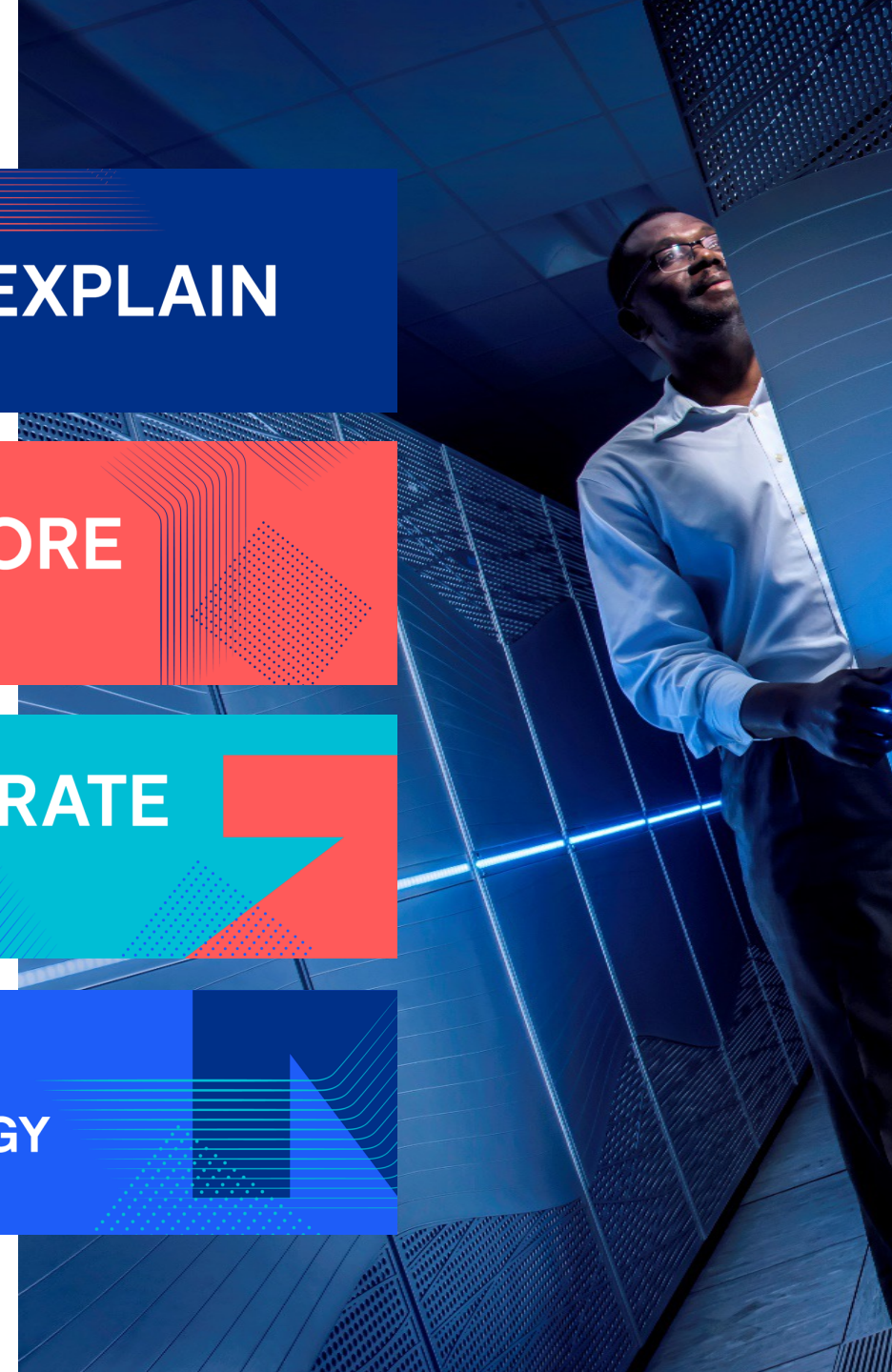
EXCELERATE

Resilience

Knowing how to prepare for and when to invest in the right emerging technologies (e.g. quantum computing)



EMERGING TECHNOLOGY



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

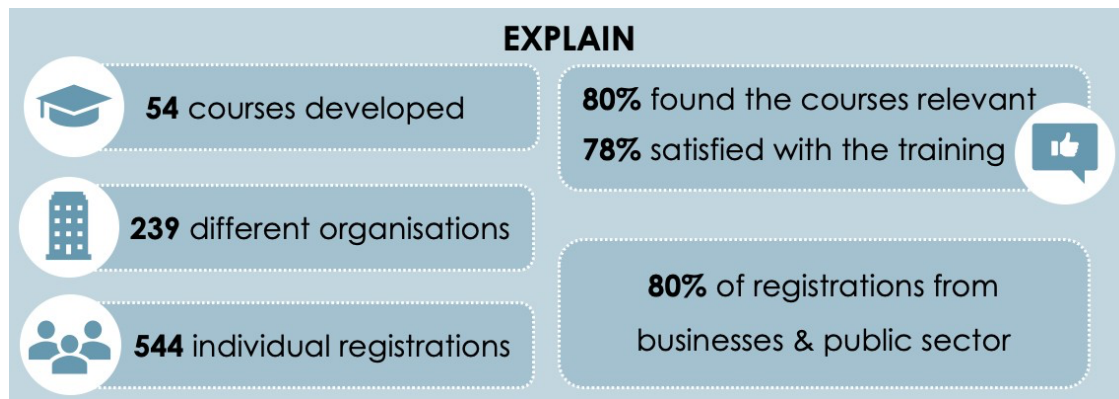
– Training and skills

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



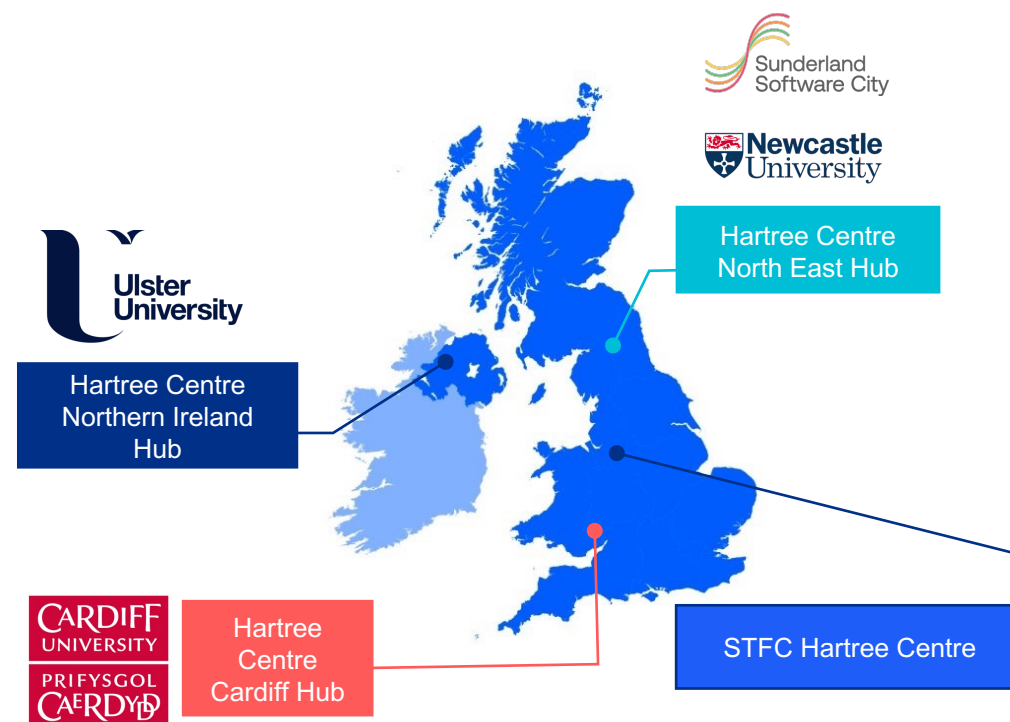
Training and engagement

HNCDI Progress Report June 2021-Dec 2022



HNCDI Explain

- Free at the point of access courses in HPC, data science, AI, full stack, cloud computing.
- Access anytime with scheduled access to technical experts.



HNCDI SME Engagement Hubs

- Engaging with local networks to increase the adoption of technologies
- Upskills SMEs locally through short projects and training.



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Case studies

How has Hartree contributed?



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Case study

Valve design for hydrogen transport

For a company with decades of experience developing valves, using simulations and virtual design enabled refinement and understanding.

“The Hartree Centre has allowed us to use specialist techniques to refine our designs to a level that otherwise would have been beyond our reach.”

– Nick Howards, Oliver Hydrovalves



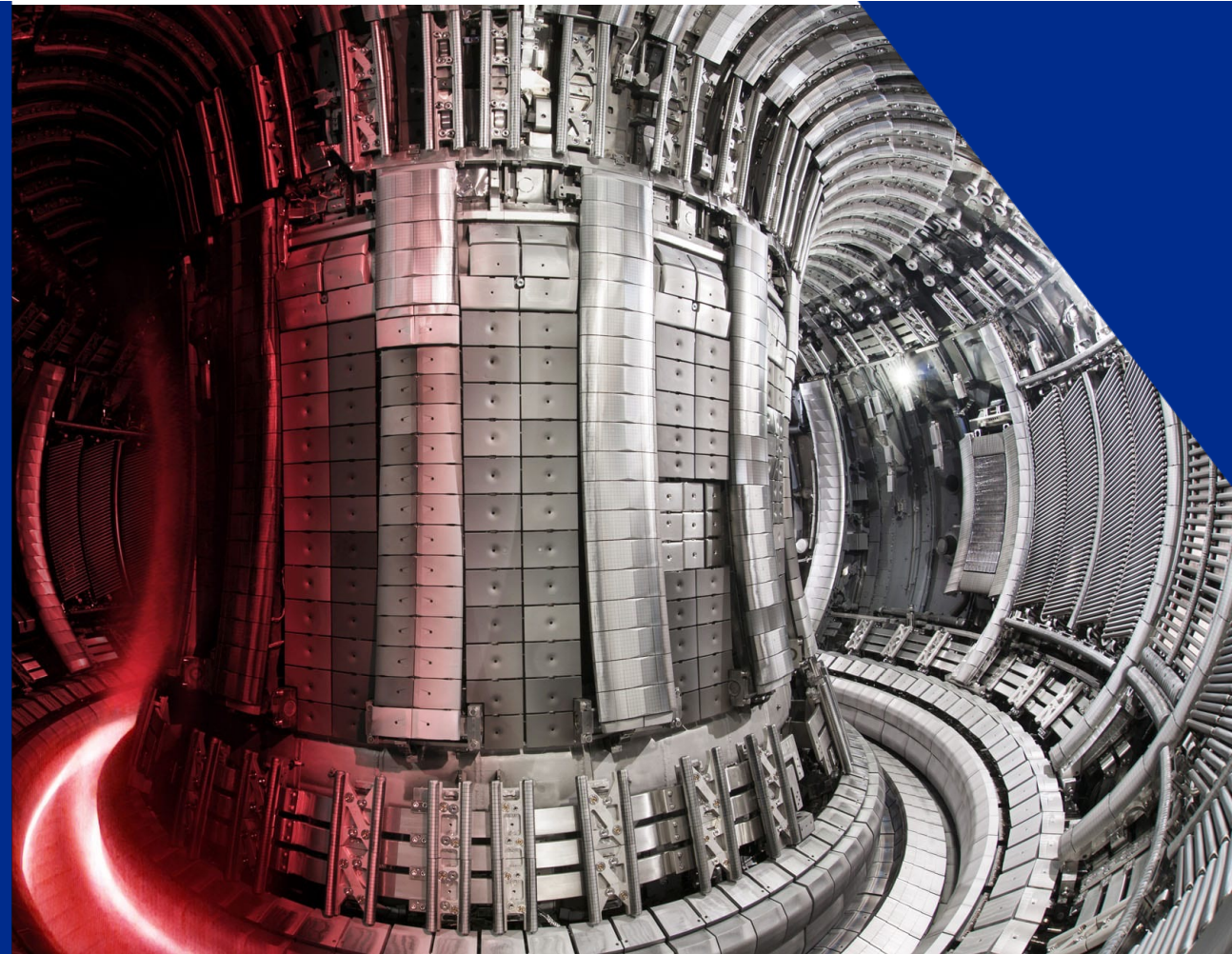
Case study

Accelerating materials discovery

- Computational materials discovery to make high-fidelity predictions of suitable properties is demanding.
- Hartree-MaDE (Materials Discovery Engine) is a tool that simplifies and automates this process

“Working with The Hartree enabled us to efficiently explore an extremely complex area of ceramic material discovery for a niche application where currently available options are far from ideal.”

- Richard White, Lucideon



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LUCIDEON

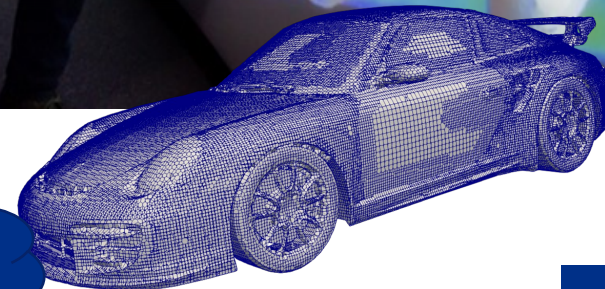
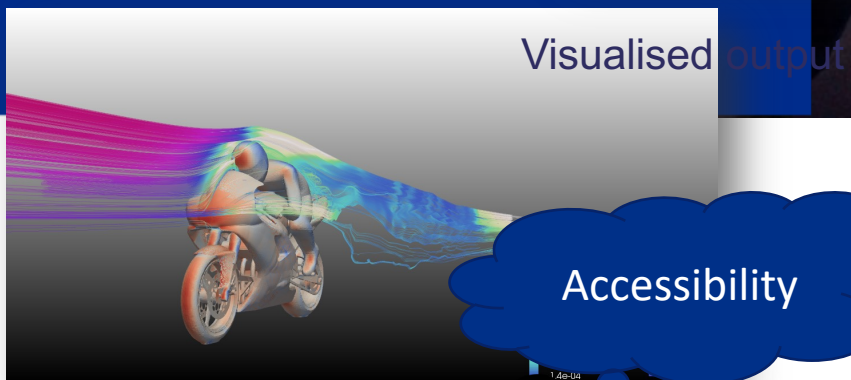
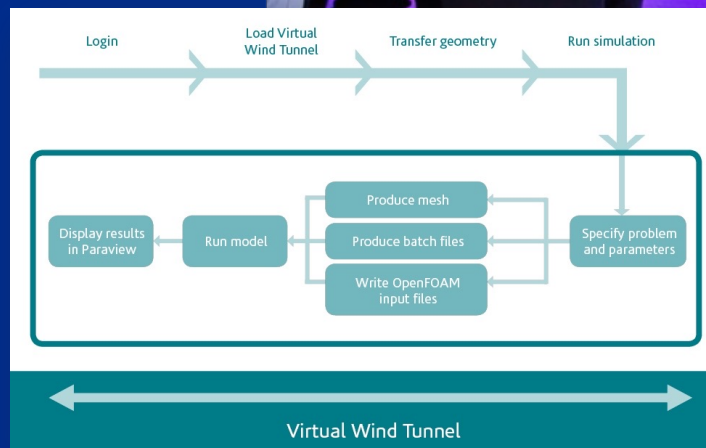
Collaborative R&D

Case study

Virtual Wind Tunnel

Saving time and money for automotive and aerospace design

- Builds the wind tunnel environment
- Automate the domain decomposition
- Produce an automatic mesh from a 3D model file (.obj / .stl)
- Automatically configure the CFD engine
- Submit the job onto Scafell Pike (Hartree Centre flagship HPC platform)



Accessibility

Collaborative R&D

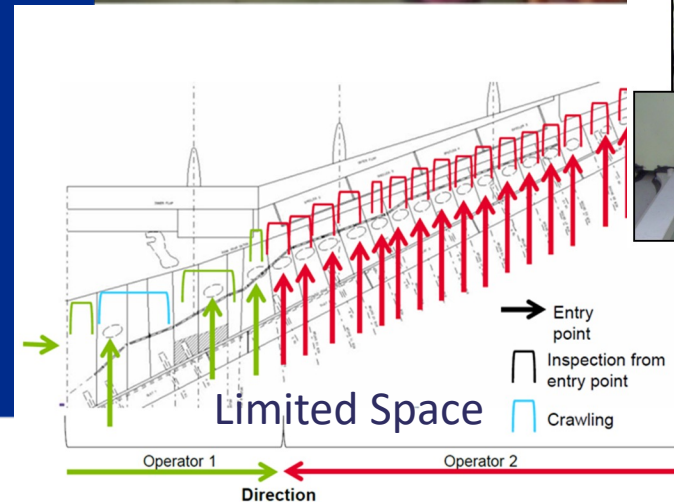


Case study

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

Virtual design of fusion reactors

Develop framework for harnessing the power of HPC for design of future fusion reactors

- Reduced order modelling
- Identifying libraries and algorithms for multi-physics coupling and exascale computing
- Dealing with large data and efficient data management processes
- New hardware and visualisation capabilities



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Press release

UKAEA and Hartree Centre join forces to accelerate fusion energy research using advanced computing

New Centre of Excellence in Extreme Scale Computing in Fusion to be located at STFC's Hartree Centre



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UK Atomic
Energy
Authority

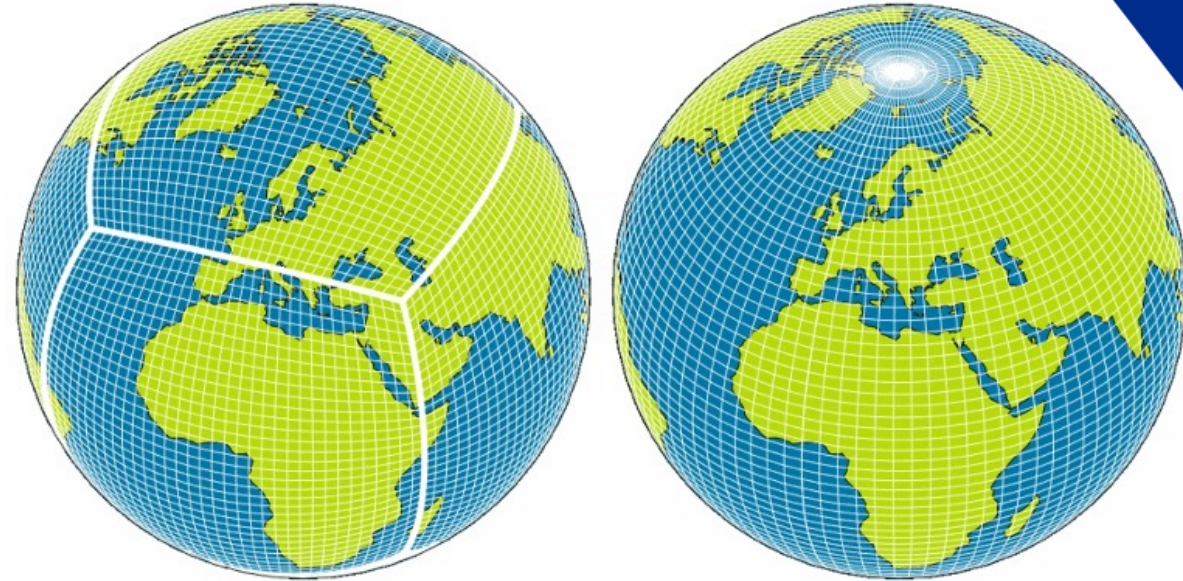
Collaborative R&D

Case study

Enabling separation of concerns in next generation weather models.

The Hartree Centre created Pclone, a tool which auto-generates the code needed for the Met Office's next-generation weather model to run on different HPC architectures.

- Frees scientific developer from worrying about parallelism and optimisation
- Allows the HPC expert to optimise an entire scientific code for a particular architecture using Python scripting



Applicability

Agility



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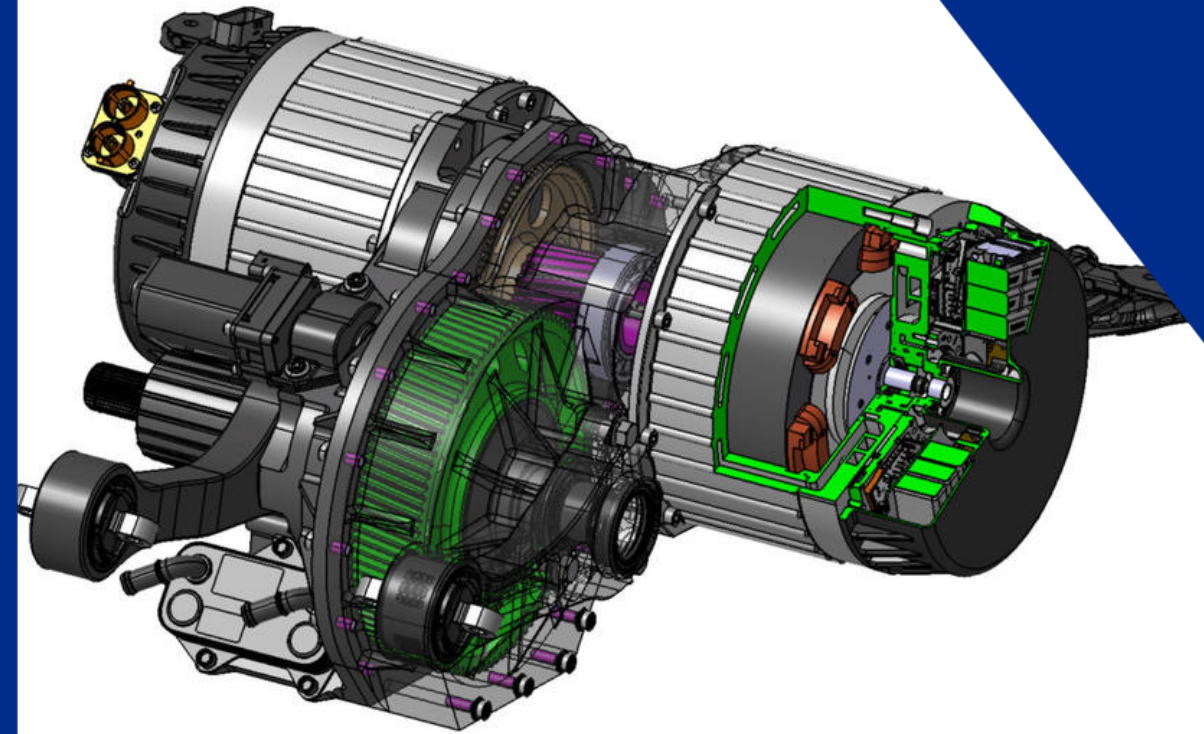


Case study

OCTOPUS – Towards a digital twin of an electric vehicle powertrain

Develop an efficient digital solution for virtual design of the gearbox.

- Identify what we want the model to be used for
- Identify what physics needs to be captured to get the answers we want
- Develop a multi-physics GPU-accelerated simulation toolkit based on smoothed particle hydrodynamics



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





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Thank you

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