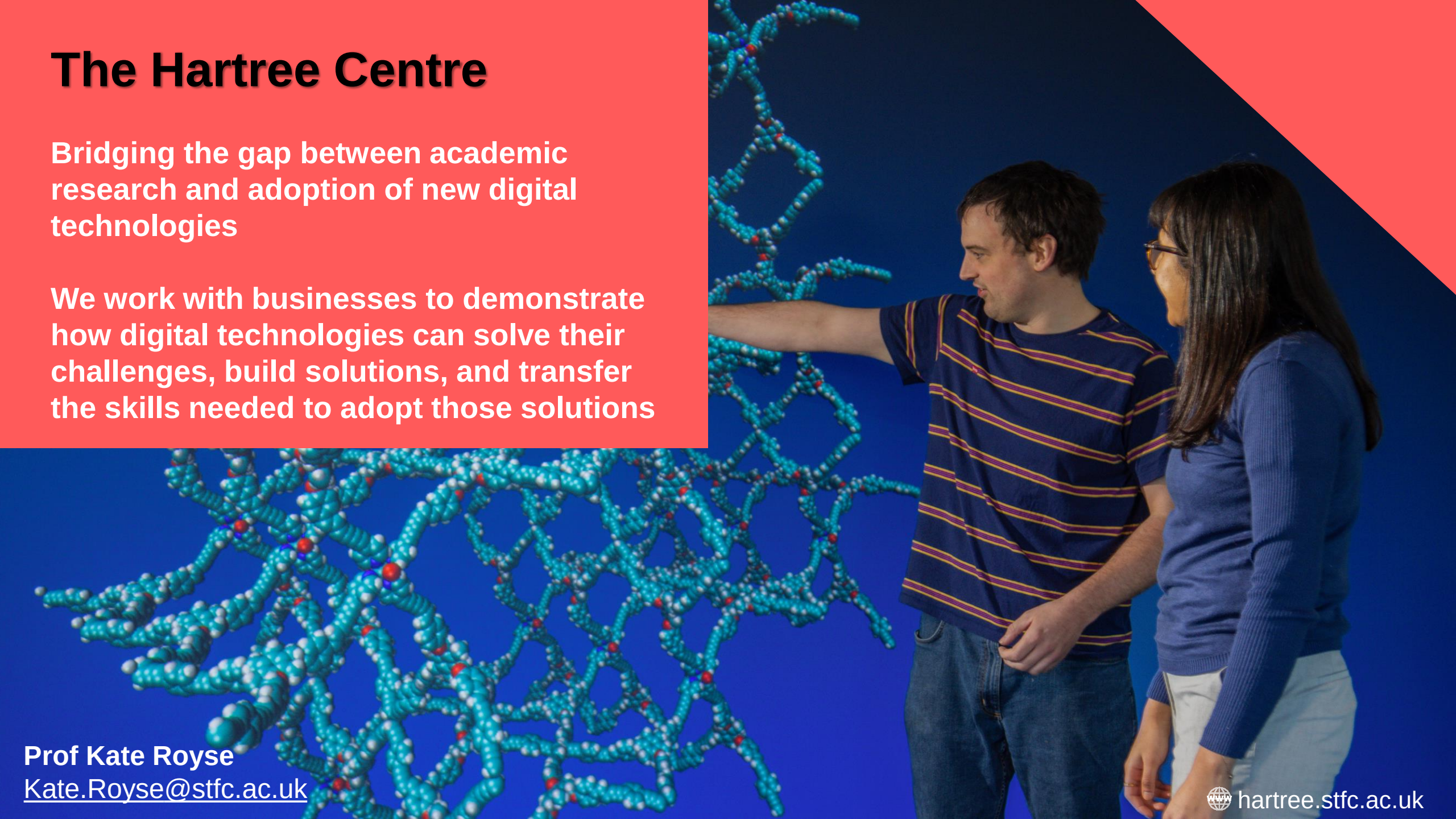
The Hartree Centre

Bridging the gap between academic research and adoption of new digital technologies

We work with businesses to demonstrate how digital technologies can solve their challenges, build solutions, and transfer the skills needed to adopt those solutions



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The Scientific Method Has Been Humanity's Best Model for Discovery. It Has Evolved Over Time and Has Entered a New Paradigm of Discovery.

1st Paradigm

Empirical Science

Observations
Experimentation

Pre-Renaissance

2nd Paradigm

Theoretical Science

Scientific laws
Physics
Biology
Chemistry

~1600s

3rd Paradigm

Computational Science

Simulations Molecular dynamics Mechanistic models

~1950

4th Paradigm

Big data-driven Science

Big data
Machine learning
Patterns
Anomalies
Visualization

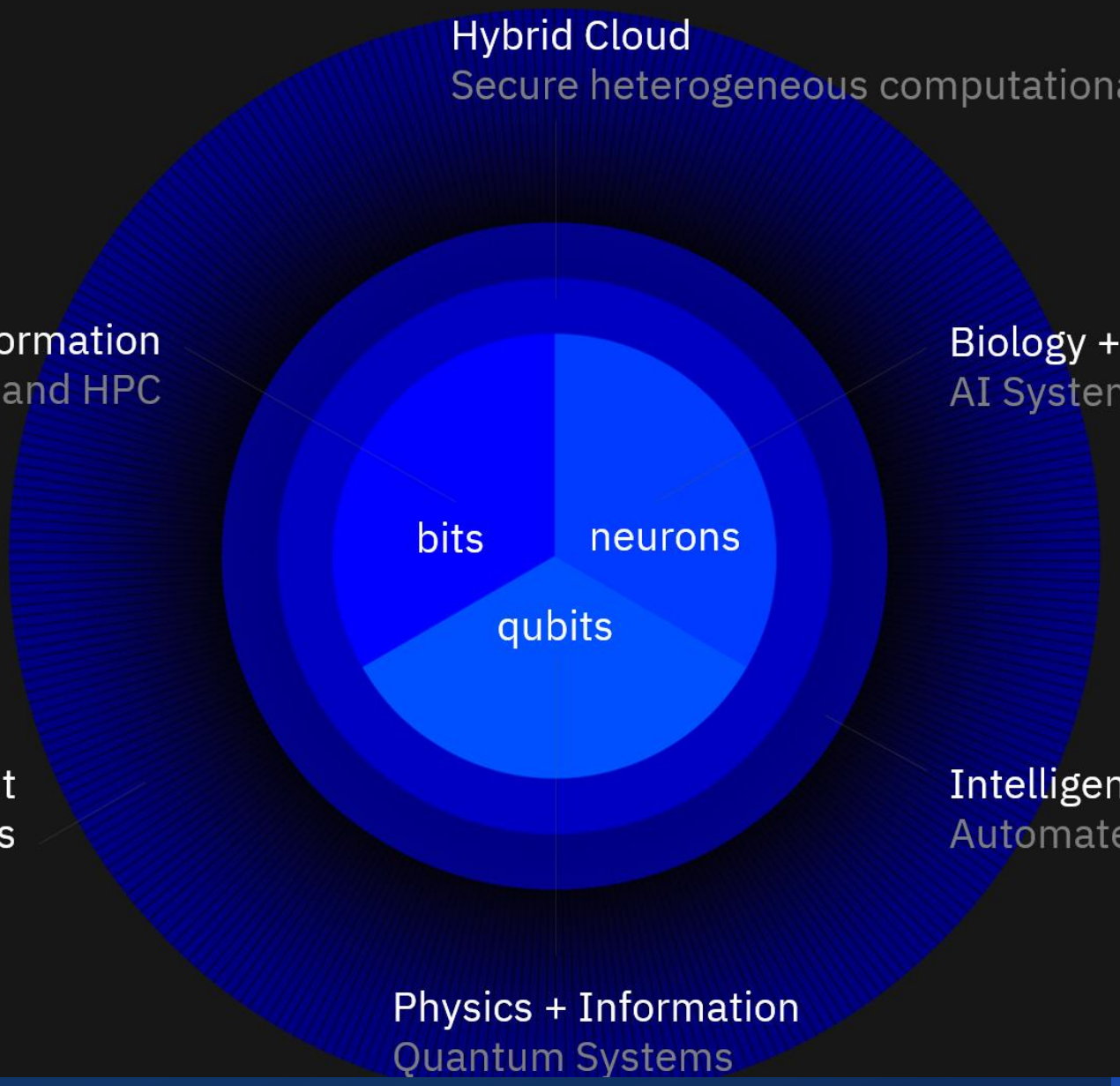
~2000

Accelerated Discovery

Scientific knowledge at scale
AI generated hypotheses
Autonomous testing

2020

The future of computing



Convergence
HPC, AI & QC

- The next wave of technology disruption will not be from a single technology, but through **a converged ecosystem of composable technological innovations, validated through application on real-world, disruptive, challenges**

The UK seeks to become a global AI superpower

Data science and AI are changing the world but the potential for AI in innovation is still not being fully realized

- UK scores highly on “talent” metrics in exercises such as the Global AI Index , but a lower score in Digital infrastructure and commercial exploitation of research outputs
- Increase demand for AI-HPC and QC requires the UK to Scale up its Digital research infrastructure for AI. Access to compute in the UK at a national and regional level is much lower than in comparator countries
- Access to computing systems with GPUs is a priority to meet needs of AI community
- One key barrier to adoption is significant gaps in training and knowledge, with fast paced developments in tools and techniques there is a need for continuous professional development
- The adoption of AI will depend on the development and implementation of standards and processes for collating, organizing and sharing data for AI, in line with the FAIR (Findability, Accessibility, Interoperability, and Reusability) principles

Innovate Globally, Empower Locally

The Industry Adoption challenge

	2000	2018	2019	2020	2021	2022
All private sector	3,467	5,668	5,868	5,981	5,591	5,509
All SME (0-249)	3,460	5,660	5,860	5,973	5,583	5,501
All small (0-49)	3,433	5,625	5,825	5,937	5,548	5,465
All employers (1+)	1,111	1,389	1,410	1,413	1,416	1,448
Non-employers	2,356	4,278	4,458	4,568	4,175	4,061
Micro (1 to 9)	914	1,137	1,155	1,157	1,162	1,187
Small (10 to 49)	163	210	211	212	211	217
Medium (50 to 249)	27	35	36	36	36	36
Large (250+)	7	8	8	8	8	8

Table: Estimated number of businesses (in thousands) in the UK private sector by employment size-band , start of 2000, and 2018 to 2022 (Source: ONS Gross Domestic Product, 2020)

99.8% SMEs

99.3% Small SMEs

74% Non-employers

Challenges faced by SMEs in adopting AI

While the potential benefits of AI adoption for SMEs are evident, there are key challenges that need to be addressed to ensure the integration is smooth and effective:

Skills and knowledge

SMEs need to upskill existing staff and recruit new expertise to effectively integrate and benefit from AI technologies

Funds to invest

Access to resources and funding is a common barrier for SMEs looking to adopt AI technologies

Organizational readiness

Adapting to AI requires change management and resource allocation

Ethical and regulatory considerations

Navigating ethical and regulatory complexities of AI adoption

Support for SMEs

Public- private partnerships, like the collaboration between the Hartree Centre and IBM (HNCDI) or through investment schemes e.g. Innovate UK Bridge AI programme (where Hartree is a delivery partner), can provide financial support, access to advanced technologies and expert guidance for SMEs looking to adopt AI technologies

Upskilling and training programs

Providing training and support to upskill existing staff and enable effective use of AI technologies

Access to advanced technologies

Offering SMEs access to advanced AI tools and infrastructure

Financial support

Providing funding and resources to support AI adoption

What's needed for Technical Innovators

- **It is hard for small volume hardware innovators to break into the market due to lack of opportunities for validating their value on industrial problems.**
  - **development of composable digital ecosystem, where hardware innovations can be seamlessly integrated into existing solutions and workflows for first in kind development**
- Access to opportunities to validate and scale with real world problems

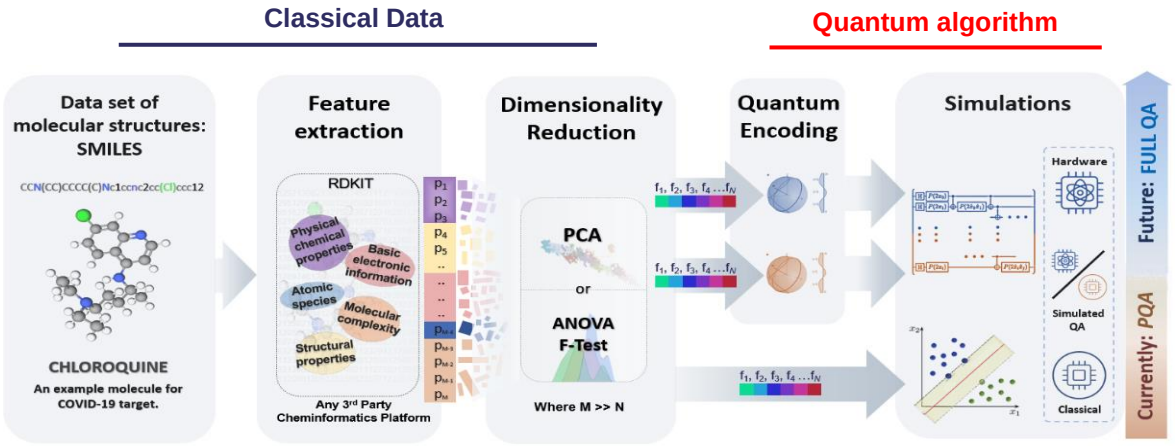
- **Opportunities to create value through technology can be missed if the technology developers do not understand the application domain**
  - **Co-locating technologists with application (domain) specialists enables the distribution of knowledge, and encourages creative uses for technology**
- Access to experts who can respond to challenges articulated through the domain and identify impact for emerging technology

Quantum Computing and Drug Discovery

Hybrid classical quantum application to identify novel potential drug candidates in virtual databases of molecules

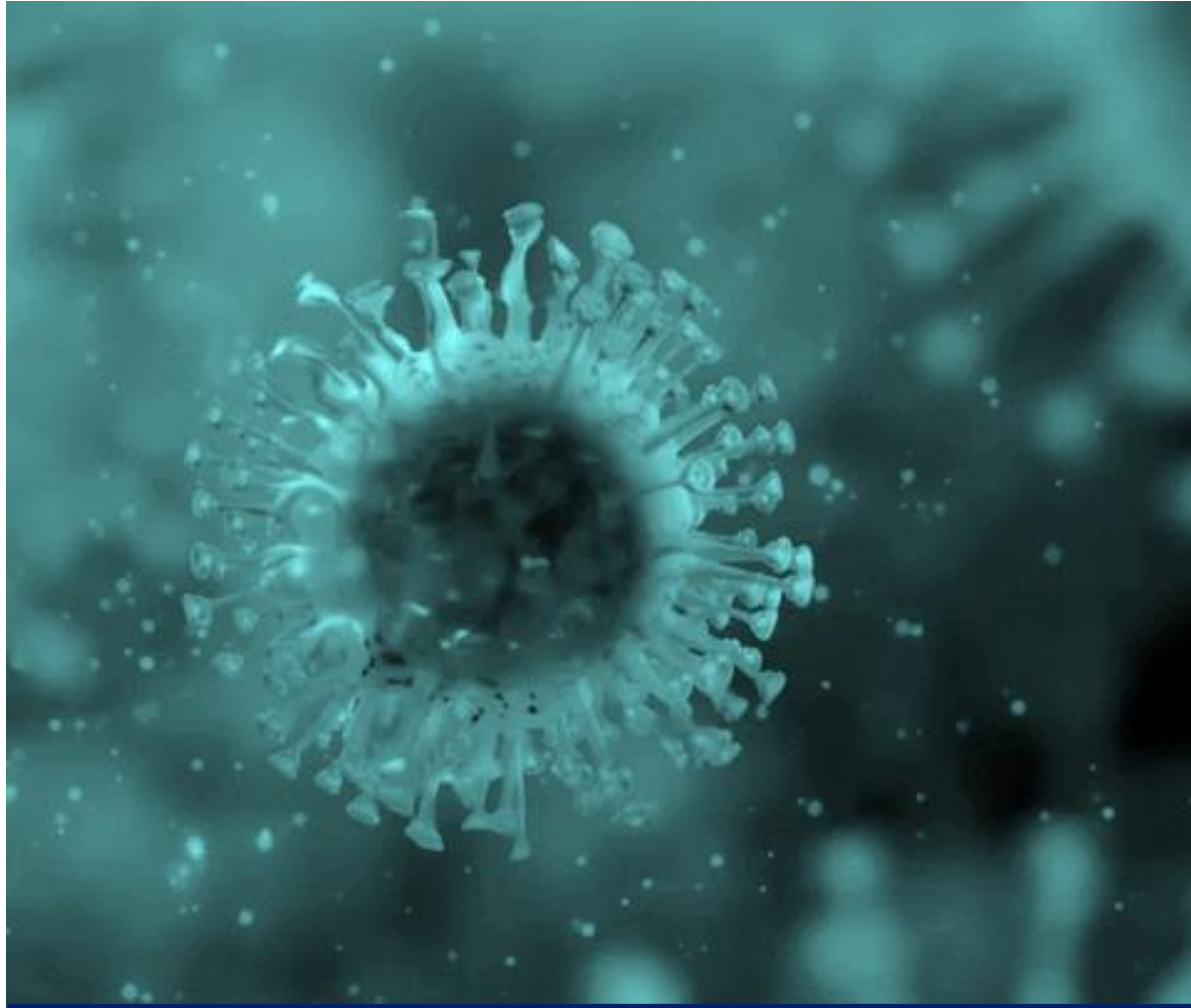
Up to 20% more accurate

"Its amazing to live in times where quantum computing is making slow transfer from the realm of purely theoretical divagations to the realm of commercial applications"
-Code Poets



Science and Technology Facilities Council
Hartree Centre

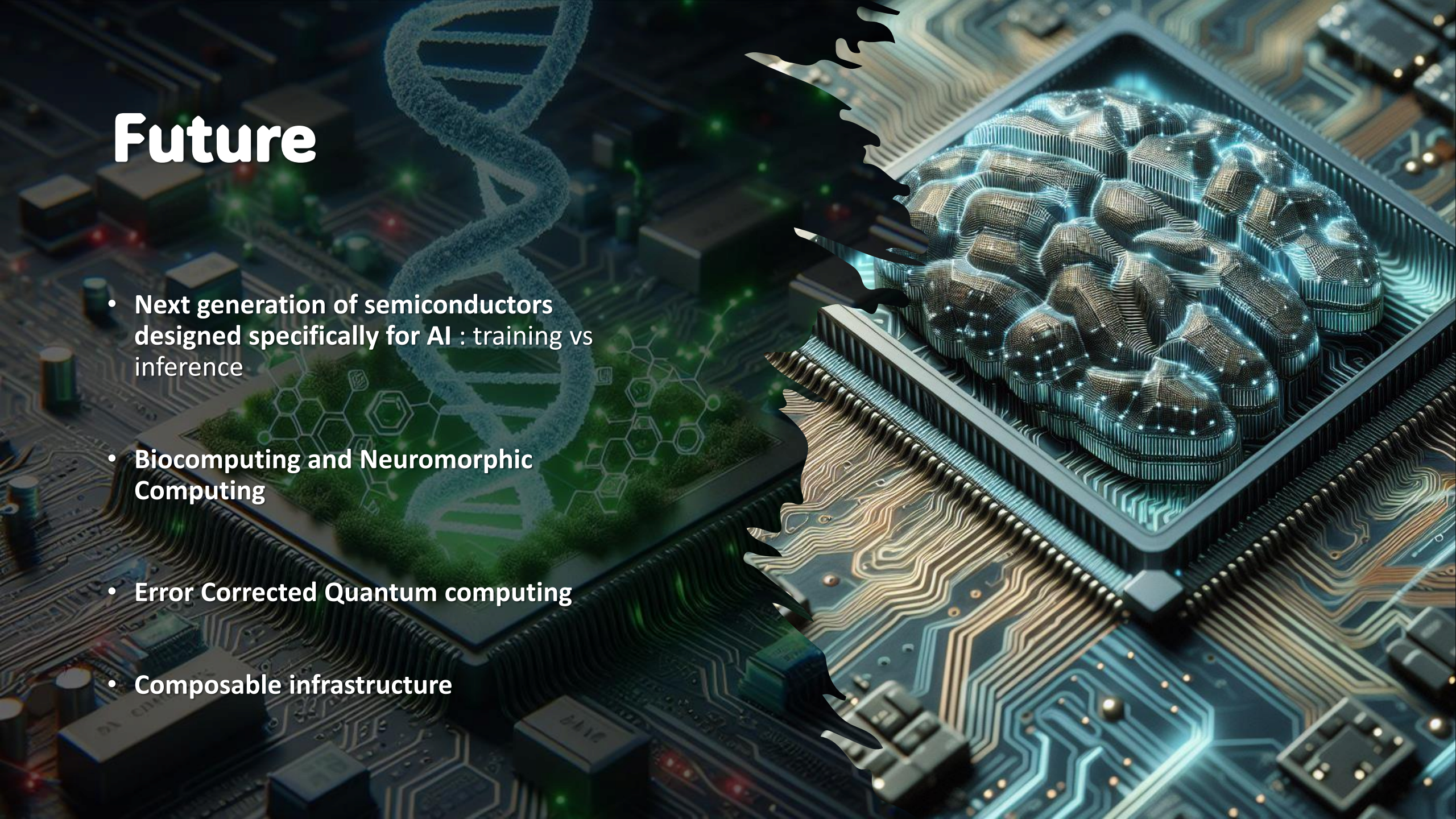
IBM



Can quantum computing enhance computational workflows for drug discovery?

Future

- **Next generation of semiconductors designed specifically for AI** : training vs inference
- **Biocomputing and Neuromorphic Computing**
- **Error Corrected Quantum computing**
- **Composable infrastructure**



In Summary

Compute is the bedrock of modern life, akin to electricity, rail travel, and the internet.

The next decade promises even more astonishing advances, and the UK’s readiness to seize these opportunities will determine its position as a Science and Technology Superpower.

The **Hartree Centre** continues to contribute significantly to emerging digital technologies, including quantum computing. Its commitment to supporting businesses and enhancing productivity underscores the importance of forward-looking compute strategies.

the future of compute isn’t just about machines—it’s about empowering people, driving innovation, and shaping a brighter tomorrow.