The evolving AI ecosystem, and its effect on business adoption

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Abstract

We will introduce the role of STFC Hartree Centre, part of the UK Research and Innovation family, in helping to unlock the potential of advanced digital technologies to create real-world impact. By equipping UK industry with the necessary knowledge, skills and compute, we help derisk business adoption of AI, big data, supercomputing, quantum computing and cloud technologies. To demonstrate the translation of AI research into business adoption, we will go through a few examples from the work we have done.

One of which is the use of generative adversarial networks (GANs), originally designed for marketing and media, for quality engineering and maintenance, and even accelerated fluid dynamics for turbulence control. We contrast with other object detection and classification approaches.

Taking a deeper dive into how gen AI and “classical” machine learning are being used in consort, we also explore enhancements in the process of novel material engineering. In this example, we will look at Metal Organic Frameworks (MOFs) for carbon capture.

Chemical engineering is also being transformed by automation. We will explain how we use AI to generate phase diagrams, enabling the prediction of phase behavior based on the chemical structures of surfactants, which are widely used in formulations within the fast-moving consumer goods industry. This advancement reduces the time and resources required to develop new products.

We will also discuss our fusion computing lab project with UK Atomic Energy Authority (UKAEA) and various partners, which acts as a test bed for the development of emerging AI approaches which will bring new design and control capabilities, which will be introduced.

We also discuss briefly the different facets of the AI landscape, including a variety of access programmes, a summary of infrastructure, and recent policy positions.

1. Introduction to UKRI STFC Hartree Centre and Wider Ecosystem

We introduce the role of the STFC Hartree Centre, part of the UK Research and Innovation family with a mission to derisk business adoption of AI, big data, supercomputing, quantum computing and cloud technologies and to equip UK industry with the knowledge, skills and compute needed to fully unlock the potential of advanced digital technologies. As a national centre, we provide both facilities and expertise to enable projects where these technologies converge.

We will briefly highlight the relationship to Alan Turing Institute, Digital Catapult, wider Catapult network, organisations like Make UK, Tech UK, other activities within EPSRC such as the AI Hubs and Centres of Doctoral Training, and more recently ARIA seeking to pursue a few high-risk, high-reward challenges.

2. Real world uses of Generative Adversarial Networks

We describe how generative adversarial networks originally designed to marketing and media [1] have the flexibility to be used in quality engineering and maintenance – in this case by providing a capability for foreign object detection with a highly unbalanced set of data to work with. This is contrasted with other object detection and classification approaches. We highlight how these are also useful in the context of accelerating fluid dynamics and turbulence control in consort with other macroscale simulation techniques. StyleGAN allows to separate and control coarse, middle and fine details. This can be used to achieve super-resolution and anomaly detection tasks given a target image using the anomaly GAN approach [2].

3. ML for material property prediction

We take a deeper dive into how gen AI and “classical” machine learning are being used in consort using novel material engineering as a basis by designing the structures of new Metal Organic Frameworks (MOFs) for carbon capture. MOFs are porous crystals comprised of metal clusters joined by organic linker molecules to form a 3D scaffolding with a very large surface area to mass ratios. They are cheap to produce; a surface area of 40 football pitches can be obtained per £1 at typical production costs. A MOF with a surface that CO_2 binds to easily would be a very powerful carbon capture material. With tens of thousands of combinations of possible metal clusters and linker molecules, there are trillions of MOFs that could be manufactured. However, only a small fraction of these can absorb CO_2. This ‘needle in a haystack’ search problem

makes it unlikely that a good carbon capture material will be designed in the classical R&D cycle where substances are manufactured and tested 'by hand' because time and resources may run out before a good material is found. Our GFLOWNET [3] based AI is comparatively cheap (~£1000) to train and deploy. This can be contrasted with the well documented high costs incurred in training some better known generative AIs. After two days it generated 15 MOFs that had greater predicted CO_2 uptake than any simulated uptake we have seen in the ~100,000 crystals which are published in academic literature. Our work is open-source and it is straightforward to adapt to perform similar tasks on other chemistry and materials problems.[4]

We also examine how chemical engineering is being transformed by automating the creation of phase diagrams, which are used to determine the performance of surfactants. These surfactants determine the properties of a wide range of fast-moving consumer goods (FMCGs), a billion-pound industry that plays a significant role in the UK economy. Replacements for the chemical building blocks of surfactants are frequently needed, due to environmental legislation and consumer concerns over health and environmental impact. We trained an AI to predict phase behaviour from chemical structures, decreasing the time and resources required to develop new formulations, and crucially, massively reducing time to market for these products in a sector where this is essential.

4. Future AI topics

The Fusion Computing Laboratory is a partnership launched between UK Atomic Energy Authority (UKAEA) and STFC Hartree Centre. Now extended to other partners, it is using supercomputing, AI, and data analytics to accelerate the design and development of fusion power plants. Aiming to create the first digital twin of a fusion power plant, this initiative enables parallel testing and rapid optimisation, overcoming significant technical and financial barriers. We will showcase some of the technological areas being developed and how we foresee these being adopted by the wider community.

5. The evolving landscape for AI

We offer opinion on the recently published AI opportunities action plan [5], and pick out the key themes from that report which are likely to define the government's mission led approach to innovation. We summarise recent investments in infrastructure. We will describe funding routes such as the Hartree National Centre for Digital Innovation, Analysis for Innovators, BridgeAI, Smart Manufacturing Data Hub (SMDH), and broader UKRI

initiatives to access the main centres of excellence in AI innovation such as the wider Made Smarter programme, Digital Catapult, wider Catapult network, organisations like Make UK, Tech UK, other activities within EPSRC such as the AI Hubs and Centres of Doctoral Training, and more recently ARIA seeking to pursue a few high risk, high reward challenges.

6. References

[1] https://www.nvidia.com/en-gb/glossary/generative-ai/ (retrieved 5/3/25)

[2] https://arxiv.org/pdf/1906.11632 (retrieved 5/3/25)

[3] https://arxiv.org/abs/2111.09266 (retrieved 5/3/25)

[4] https://pubs.rsc.org/en/content/articlelanding/2024/dd/d4dd00020j (retrieved 5/3/25)

[5]https://assets.publishing.service.gov.uk/media/67851771f0528401055d2329/ai_opportunities_action_plan.pdf (retrieved 5/3/25)