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A New National Purpose: Accelerating UK Science in the Age of AI

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Foreword

Artificial intelligence promises to accelerate the pace of scientific discovery and revolutionise how we uncover and use new knowledge. The potential is already clear: DeepMind's AlphaFold, for example, cracked a 50-year challenge in protein-structure prediction, achieving in mere minutes what once took years.

Yet this is just the beginning: future AI systems will become ever more powerful and accessible. Taking advantage of AI's evolving, transformative potential will be essential, not just for achieving scientific leadership, but also for unlocking economic prosperity and addressing critical challenges across health, the climate and security.

The United Kingdom starts from a position of strength. It is home to world-class universities, exceptional scientific talent and strategic assets such as the UK Biobank. It has the third-largest AI sector globally and, in 2024, three of the four Nobel Prizes relating to AI were awarded to Brits.

But the UK cannot rest on its laurels because other countries are moving rapidly. For example, in 2024 the United States committed $12 billion to its Frontiers in Artificial Intelligence for Science, Security, and Technology programme for AI-driven science, and earlier this year it announced a further $500 billion in AI-infrastructure investments.

The political will and dedication needed for the UK to succeed is there. The government's AI Opportunities Action Plan, announced by the prime minister on 13 January 2025, set out a clear vision for establishing the UK as a global AI superpower. The plan makes several references to AI for science, but the government must now take the next step. What is needed is a detailed and actionable plan for ensuring that the UK leads the world in applying AI to the acceleration of scientific discovery.

Several barriers must be overcome. Adoption of AI in the research community remains patchy, with many scientists lacking the training to capitalise on advances in their field. New infrastructure is needed to unlock the potential of AI-enabled science, which requires access to compute and high-quality data sets. Meanwhile, fragmented funding structures make it difficult to support interdisciplinary, AI-driven research – but taking advantage of the Department for Science, Innovation and Technology's overall lead on the policy agendas for AI and R&D means that they can be mutually reinforcing. And, most important for long-term leadership, the UK needs new algorithms for science – and the types of radical organisations that can produce them.

Overcoming these hurdles is a significant but not insurmountable task. The path forward is clear: the UK must adapt its scientific institutions for the age of AI, create opportunities for deep collaboration between research-software engineers, scientists and the private sector, and equip scientists with the skills, tools and data sets they need to thrive. The government's expansion of the AI Research Resource, and introduction of AI Growth Zones and the UK Sovereign AI team, provide a strong foundation, but they must be strategically deployed to areas of scientific excellence.

In previous New National Purpose papers we have stressed the central role of science, technology and innovation in fuelling economic growth, improving social outcomes and ensuring national security in the UK. Building on the momentum generated by the AI Opportunities Action Plan, this paper furthers the New National Purpose agenda by outlining a comprehensive blueprint for putting the UK at the forefront of AI-enabled scientific discovery.

Harnessing AI in research is more than a scientific opportunity: it is an economic and strategic imperative. AI-enhanced R&D can accelerate solutions to major societal challenges, from climate resilience to medical breakthroughs, while also driving productivity and growth in key industries.

As countries increasingly compete based on technological and research capabilities, ensuring AI is fully embedded in UK science will be critical to long-term economic success. The UK has all the ingredients to be a world leader in AI for science, but now is the time to act decisively.

Tony Blair and William Hague

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Executive Summary

The landscape of scientific discovery is undergoing a seismic shift.

AI is not just another new technology; it represents a paradigm shift in science, rewiring the engines of research and shifting progress into overdrive. The nature of discovery is evolving to become more interdisciplinary, data-driven and computationally intensive, requiring new ways of thinking, working and organising. Future-proofing the United Kingdom's R&D ecosystem will require proactive interventions to adapt to the AI era and ensure the country's ability to pioneer the scientific industries of the 21st century.

The recent AI Opportunities Action Plan, led by Matt Clifford, lays out a range of reforms to promote the integration of AI into disparate sectors of UK industry; it also provides an excellent foundation upon which to build. The expansion of the AI Research Resource (AIRR) and the creation of Sovereign AI (SovAI) are huge opportunities for UK science. But their impact will depend on two pivotal factors: the ability of the broader R&D ecosystem to adapt to the demands of the AI era, and how effectively new AI-oriented initiatives are integrated into that evolving ecosystem.

The first of these in particular presents a significant challenge. Despite its considerable strengths – including world-class research institutions, strong computational-science expertise and major assets such as Google DeepMind and the UK Biobank – the UK's performance at the highest levels of AI research remains underwhelming, while the uptake of existing AI tools is uneven. Additionally, the UK faces persistent difficulties in attracting and retaining top talent, and the country's funding structures and research environments are not sufficiently well designed to support interdisciplinary, AI-driven research.

Meeting this moment demands a new approach to research strategy, prioritising bold investments in data, tools and talent, while ensuring that institutions adapt to the demands of the AI era. The legacy of the UK's next phase in science policy – and its research leadership – will be defined by how it approaches this transformation.

But these challenges are also an opportunity. The transition to the AI era should be used as a catalyst for much-needed reforms to the UK's R&D ecosystem, remaking it into something more dynamic and entrepreneurial – and attractive to the next generation of researchers.

This report builds on the momentum generated by the AI Opportunities Action Plan, setting out a comprehensive roadmap to establish the UK as a global leader in AI for science. A successful strategy must address multiple dimensions of AI development and adoption. It should lay the foundations for AI-driven science by creating high-impact scientific data sets, building world-class infrastructure and establishing sustainable talent pipelines. It should accelerate the adoption of existing AI models and tools by equipping researchers with the education, skills and incentives to integrate AI methods into their work. And it should expand capabilities at the cutting edge by enabling the creation of new algorithms for science, and the creation of radical new institutions where UK scientists can pioneer the next wave of transformative breakthroughs. By acting decisively now, the UK can ensure that AI becomes a core pillar of its scientific landscape. This will cement its position at the forefront of global research and unlock new avenues for long-term economic and technological leadership.

Key Recommendations

A strategy to position the UK as a world leader in AI for science must be bold and comprehensive. This report sets out a series of foundational steps, focusing on five enablers: data, software tools, talent, infrastructure and institutions.

BUILD AI-READY SCIENTIFIC DATA

AI-driven discovery depends on the accessibility of high-quality scientific data, yet many of the UK's most valuable research data remain fragmented or inaccessible. Strategic investment in AI-ready data sets is therefore essential to unlock the full potential of AI for science.

- **Create high-quality scientific data sets for training the next generation of revolutionary AI models:** These data sets often require significant national investment and coordination so, as part of its expansion, the AIRR should run data programmes to create or enhance them. These mission-oriented programmes should integrate data acquisition and processing, tool-building and the provision of compute, and should collaborate closely with academia, industry, the SovAI team and Focused Research Organisations.[1]
- **Digitise uncollected scientific data:** The majority of valuable scientific data and experimental information is not published – and much remains inaccessible for AI training or for large-scale analysis. To tap this goldmine, UK Research and Innovation (UKRI) should mandate that all new publicly funded research data be recorded in digital form from 2030. Many UK research institutions are moving in this direction, but decisive input from funding bodies will accelerate the transition to digital-first record-keeping.

DEVELOP SOFTWARE TOOLS FOR AI

Scientific software tools are vital for making data sets ready for training, and for operationalising AI within research workflows. The development, scaling and maintenance of these tools require sustained investment and structural support.

- **Change incentives for tool-building:** There are insufficient incentives for academic researchers to build and share high-quality, reusable tools. UKRI should develop a national recognition framework for scientific software contributions, integrating tool usage and community metrics into key academic processes, such as hiring and contract renewals, grant evaluations and Research Excellence Framework panel guidance.

- **Address the fragmentation and abandonment of tools:** Many valuable AI-related tools are developed with little intention or capacity to scale them for broader use – and consequently frequently become obsolete. UKRI should introduce an adoption-linked tiered funding mechanism to address the lifecycle challenges of AI-enabled or AI-enabling tools, ensuring their scalability, reusability and sustainability.
- **Expand career pathways for research software engineers:** To encourage the maturation of diverse career pathways within the research software ecosystem, UKRI should ensure that flexible, sustainable grants exist for research labs to fund the employment of research software engineers. This funding should be suitable for embedded experts, research studios or external contractors.
- **Support large-scale, mission-oriented AI tool development:** Inspired by the Defence Advanced Research Projects Agency's Grand Challenges, UKRI should establish and fund AI Grand Challenges for scientific tools. This would focus on high-impact use cases that require significant coordination, investment and expertise.

SECURE THE UK'S AI-TALENT PIPELINE

A thriving AI-driven research ecosystem depends on a steady supply of skilled talent. As AI reshapes scientific discovery, researchers must be equipped with the right expertise, institutions must adapt to new ways of working and the UK must become a more attractive destination for top global talent.

- **Reduce visa barriers for AI researchers:** The costs associated with the UK's high-skilled visa have soared in recent years, at the same time as competitor countries have slashed their fees. The UK should introduce a dedicated global AI-talent visa, exempt from the immigration health surcharge, to attract top researchers and engineers.
- **Build non-academic research entities:** Traditional academic and industry labs struggle to accommodate high-agency researchers who wish to work on long-term, high-risk, interdisciplinary projects at the frontier. The UK should establish a mechanism for the creation or designation of disruptive invention labs: high-autonomy spaces operating

at the intersection of AI and various broad scientific disciplines. These should be designed to support risk-taking and long-term AI-driven discovery and invention, offering a new model for public research in the UK based on structural principles akin to those of Google DeepMind.

- **Improve cross-sector mobility:** Few pathways exist for hybrid roles or fluid movement between academia and industry, limiting knowledge transfer and distancing academia from real-world AI advances. To provide greater flexibility for top AI talent to work across these sectors, the government should establish a new AI Industry Fellowship Programme, funding three- to five-year joint appointments between universities and industry partners to allow AI engineers in private-sector R&D teams to hold full- or part-time positions in academia.
- **Enhance AI training for researchers:** Researchers across disciplines must be equipped with basic AI skills, as well as specialised training to leverage cutting-edge AI models within their fields. Training programmes should be substantially enhanced to provide researchers with these skills. This should be the responsibility of higher-education institutions, degree-accrediting bodies, learned societies and other relevant academic and professional bodies, as well as private-sector training providers.

INVEST IN AI RESEARCH INFRASTRUCTURE

AI-driven research relies on advanced computational power and, increasingly, on other types of physical infrastructure, such as automated laboratories.

- **Encourage investment in automation infrastructure:** The concept of AI Growth Zones – as outlined in the AI Opportunities Action Plan – should be expanded beyond compute, to include growth zones aimed at a wider range of AI-enabling research infrastructure. These should be strategically co-located with academic and industrial research hubs.
- **Expand compute access for researchers:** The UK government should ensure that electricity-grid infrastructure is rapidly upgraded to meet the energy demands of AI data centres, while maintaining grid stability and efficiency. The National Energy System Operator should be tasked with

evaluating data centres' energy requirements and their potential for flexible consumption, incorporating these insights into the Strategic Spatial Energy Plan.

REMAKE THE INSTITUTIONS OF UK SCIENCE

Harnessing the power of AI in science requires more than investment in technology: it demands a fundamental shift in how research is funded, coordinated and supported. The UK's institutions must evolve to keep pace with a rapidly changing landscape, ensuring that AI-driven research is not only well resourced but also strategically integrated across disciplines.

- **Modernise and reform UKRI's AI strategy:** The minister of state for science, research and innovation should formally ask the current and incoming UKRI CEOs to make the changes needed for UKRI to play an enhanced role in advancing the UK's position in AI for science. This should include establishing a new central AI function within UKRI to drive forward the frontier of AI research in the UK and the adoption of AI within the UK's research system.
- **Encourage more research funders to invest in AI for science:** All UK research funders should increase the amount they invest in AI-enabled research. This should include establishing dedicated programmes to encourage and facilitate AI adoption in their disciplinary areas, develop talent and skills, and invest in strategic infrastructure and data.
- **Coordinate funding efforts across the R&D ecosystem:** To ensure a platform exists for the cooperation of AI funders across the research community, UK funders should establish a forum for AI-research funders. Chaired by UKRI and drawing on expertise from the AI Security Institute (AISI), this new forum would provide a venue for achieving strategic coherence, sharing knowledge and devising joint actions where needed – especially on interoperability, data sharing, open science principles, research integrity and AI safety. Both the AIRR and SovAI should have representation in this forum.

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The State of Play in AI for Science

As the late Nobel laureate Sydney Brenner famously remarked, “Progress in science depends on new techniques, new discoveries and new ideas, probably in that order.”[2] Over the centuries, disruptive new technologies such as the microscope and the computer have transformed fields beyond recognition, reshaping not only *what* we know, but *how* we come to know it. Artificial intelligence represents the next paradigm-shifting technology, heralding an era of AI-enabled research that will fundamentally alter the pace, scale and nature of discovery.

The profound impact of AI on the pursuit of science is already evident. The 2024 Nobel Prizes in both physics[3] and chemistry[4] were awarded to pioneers of AI-driven research. AI is no longer a peripheral tool, but a central engine of discovery. This new era of research is not defined by a single technology; rather, AI comprises a constellation of related (and evolving) computational and machine learning (ML) techniques.

“AI for science” refers to the application of these techniques to develop better scientific models, automate complex processes or tackle difficult problems that are often data heavy and computationally intensive.[5] In practice, the range of applications for scientific AI models and tools is ever expanding, permeating virtually every aspect of the research ecosystem.

On one hand, advanced AI models are driving groundbreaking discoveries that push the boundaries of scientific knowledge in specific domains. From AlphaFold’s revolutionary breakthrough in protein-structure prediction,[6] to materials discovery,[7] toxicity prediction in drug discovery[8] and predictive modelling in climate science,[9] these domain-specific innovations are redefining what is possible and accelerating the pace at which society’s most pressing challenges can be addressed.

On the other hand, AI is quietly reinventing the research process itself.[10] The AI-assisted scientific workflow will include AI-assisted programming[11] and automated data collection; it will also incorporate large language models (LLMs) to review scientific literature,[12] discuss results, generate hypotheses, speed up the writing process and eventually even suggest conceptual breakthroughs. Ultimately some envisage the emergence of fully autonomous "AI scientists" capable of executing every step of the scientific process, though this vision remains well beyond current frontiers.[13]

For specific examples illustrating the range of ways in which AI might impact the R&D ecosystem, see the annex (available as a downloadable PDF). But for a more comprehensive discussion of AI's potential in research, readers are encouraged to consult recent reports by Google DeepMind,[14] the Royal Society,[15] the European Union[16] and the Organisation for Economic Co-operation and Development.[17] In the remainder of this report, we focus on practical solutions for leveraging AI to enhance the UK's R&D ecosystem.

Most examples of AI for science in this report focus on STEM subjects. But AI can also help social scientists improve society's understanding of how to make government more efficient and how to respond to societal crises. There are some excellent resources available for in-depth explorations of these topics.[18],[19]

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The UK's AI for Science Landscape

AI-enabled science is likely to be a major driver of global economic competitiveness,[20] with some projections estimating that AI-enabled scientific discovery could double the productivity growth rate of advanced economies.[21] Recognising this, the US and EU have already launched major initiatives[22],[23] to embed AI into their scientific-research ecosystems.

For the UK, this moment presents both a challenge and an opportunity. While the country has strong foundations in scientific research, critical structural weaknesses threaten its ability to maintain a competitive edge in the AI era. It must move decisively and build the capabilities to leverage AI in its R&D ecosystem.

Strengths: The UK's Foundations

The UK has several key advantages that position it as a potential leader in AI-driven scientific discovery.

- **Strong scientific base:** The UK is home to some of the world's top universities and research institutions, which consistently produce high-impact research in fundamental sciences. These institutions are also home to cutting-edge AI-enabled laboratories, such as the Digital Chemistry group at Glasgow,[24] and the Materials Innovation Factory in Liverpool.[25]
- **World-leading AI companies:** The UK has the third-largest AI sector globally,[26] and is home to Google DeepMind, one of the world's foremost AI-research labs, as well as pioneering AI-driven science companies such as Isomorphic Labs.
- **Major scientific data sets:** The UK benefits from access to some of the world's largest scientific data sets, notably the UK Biobank.[27]
- **Recent policy momentum:** The UK government has made initial strides in supporting AI-driven research, commissioning the AI Opportunities Action Plan, and subsequently agreeing to the expansion of the AI Research Resource (AIRR).

Challenges: Barriers to Progress

Despite these advantages, the UK has missed out on a number of meaningful opportunities and faces significant hurdles that limit its ability to lead in AI-driven science.

- **Limited competitiveness at the cutting edge of AI research:** The UK's contribution to top-level AI research output is disproportionately driven by Google DeepMind. Without DeepMind, the UK's share of citations in the top 100 AI papers drops from 7.8 per cent to just 1.9 per cent, placing it on a par with Hong Kong.[28]
- **AI-talent drain and weak attraction:** The UK trains the highest number of AI-relevant graduates in Europe,[29] yet it struggles to attract or retain top talent. Many leading AI researchers and teams relocate to the US.[30]
- **Fragmented AI adoption in science:** The integration of AI into research workflows remains highly uneven, and in many fields adoption is minimal. Many UK researchers lack the training to effectively deploy AI in their work.
- **Funding bottlenecks and institutional constraints:** The UK's research-funding landscape is not optimised for enabling cross-disciplinary AI research. Traditional discipline-specific funding structures slow the adoption of AI-enabled methods and projects in many scientific fields, while the UK lacks dedicated mechanisms to support projects that are not well suited to the standard university research model.

A Vision for AI for Science in the UK

Our previous New National Purpose papers have outlined how the UK could develop new strategies to become a leader in the safe and successful development of AI (see *A New National Purpose: AI Promises a World-Leading Future of Britain*), as well as accelerate the pace of science and technology breakthroughs (see *A New National Purpose: Innovation Can Power the Future of Britain*). Now we are setting out the belief that the UK must combine these strengths to become a leader in AI-driven science.

The UK has the raw ingredients to do this. Yet, time and time again, it has missed opportunities to capitalise on breakthroughs at the intersection of science and AI. The loss of DeepMind to Google and the migration of top AI teams to the US barely registered on the radar of policymakers, while the UK's public research bodies largely stood on the sidelines of the deep-learning revolution. These are not isolated missteps but symptoms of a deeper malaise: a lack of sufficient attention and strategic coordination, combined with structural weaknesses in the UK's science and technology ecosystem. To grasp this immense opportunity requires renewed focus, a clear strategy and a bold programme of reforms to existing structures.

While private-sector labs dominate the creation of fundamental AI breakthroughs, the potential for publicly funded research to play a transformative role in the application of AI in science is vast. To unlock this potential, academics must be equipped with the tools, infrastructure and training needed to conduct cutting-edge research in the AI era. Equally critical is putting the right mechanisms in place across the research ecosystem to foster fruitful collaborations – between academia, industry and government – to drive transformative progress.

The rapid evolution of AI capabilities only heightens the stakes. Integrating AI into research is not simply a matter of adopting off-the-shelf tools: it requires deep collaboration between AI specialists and scientists with domain-specific knowledge to create tailored solutions that can solve complex scientific problems. This interplay between disciplines is the crucible for tomorrow's breakthroughs – but without a dynamic exchange of ideas and skills between the public and private sectors it will be far more difficult.

To ensure that public R&D is not left behind, the UK must act decisively. Meeting the challenge will require cultural shifts, institutional reforms and an unwavering commitment from the government, research funders, universities and the broader research community. Failure to adapt will threaten the long-term viability of the UK's research base and undermine its competitiveness in the scientific industries of the 21st century. But seizing the opportunity will deliver lasting benefits: strengthening the research ecosystem, driving innovation and ultimately improving lives.

Through the Action Plan, the government has already demonstrated that it is prepared to act. Sovereign AI (SovAI) and the AIRR initiative represent critical opportunities to revitalise the UK's R&D landscape. If well aligned and integrated into the broader ecosystem, they could catalyse a wave of activity that enhances discovery and strengthens the UK's economic position. SovAI, tasked with striking partnerships, driving commercialisation and scaling new technologies emerging from academia and industry, must select one of its focus areas from the sciences. AIRR programme directors will provide the infrastructure, compute and resources to power cutting-edge AI-driven research. Together, they could form the backbone of a dynamic AI ecosystem.

To succeed, AIRR and SovAI must be flexible and autonomous from the outset, hiring the best people with the right expertise, borrowing from the AISI's model to recruit externally in order to offer salaries that can attract the best talent. They should have streamlined leadership structures that enable quick decision-making and direct access to the highest levels of government. And they should remain open to opportunities beyond their existing project areas to avoid concentrating support on specific remits at the expense of unexpected breakthroughs. SovAI's recent partnership with Anthropic is a positive indicator of things to come, but by investing in embedding AI capabilities across the UK R&D ecosystem, many more partnerships with exciting UK companies could emerge.[31]

The following sections outline recommendations to reimagine the UK's research ecosystem, ensuring that data resources, software building, talent pipelines, research infrastructure and funding structures are aligned with the demands of the AI era.

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Data: The Foundation of AI

As noted in the AI Opportunities Action Plan, data are the lifeblood of modern AI, and this is especially true in the case of AI-driven science. The collation of high-quality scientific data is necessary to train new AI models, which can then be used to derive insights from digitised research data. This report outlines two major challenges in leveraging scientific data for AI.

- **Large-scale data-set creation:** Many of the most strategically valuable data sets, required for training the next generation of AI models, are expensive and labour-intensive to assemble. They also require widespread collaboration, prioritisation and deliberate national investment.
- **The "dark data" problem:** Large volumes of valuable research data remain inaccessible, unstructured or unpublished, limiting AI's ability to derive meaningful insights.

Addressing these challenges will require a combination of policy action, infrastructure investment and strategic coordination between government, academia and industry.

Large-Scale Data-Set Creation: The Next Generation of AI Models

High-quality, well-structured data sets are essential for training AI models that can accelerate scientific discovery. A prime example is DeepMind's AlphaFold, which revolutionised structural biology by leveraging the Protein Data Bank:[32] a meticulously curated, publicly funded data set built over five decades.

Creating the conditions for the next generation of AI models to emerge requires both support for grassroots initiatives within the research community and a deliberate national strategy for assembling strategically valuable data sets. However, assembling large, high-quality scientific data sets can be expensive, requiring sustained investment and technical expertise. It is also time-consuming – demanding extensive annotation and metadata structuring – and requires sustained, high-level collaboration across academia, government and, in many cases, industry, thus requiring central coordination.[33]

Though many data-set assembly initiatives originate within the research community, bringing them to full scale is extremely challenging without government support (though there are many examples of highly successful consortia).[34] Private-sector involvement is also crucial and should be leveraged wherever possible, but many of the most strategically valuable data sets – those with long-term, foundational scientific impact – are too far removed from immediate profit incentives for the market to initiate projects at sufficient scale and quality.[35] When valuable data sets *are* created within industry, they are typically proprietary, limiting their broader scientific and economic utility. Therefore, without targeted intervention, data availability may become the bottleneck keeping researchers from cutting-edge AI applications.

The UK government has recognised the importance of data for AI and is making progress in this area. The National Data Library (NDL)[36] is a welcome initiative aimed at centralising and facilitating access to existing high-impact public-sector data, with the goal of improving public services and providing a resource for researchers. However, the active creation of specific scientific and experimental data sets requires a very different approach.

- **Type of data:** The NDL is likely to focus on UK public-sector data collected from various public bodies, government departments and institutions. This is likely to include NHS data and other health data, but not experimental data derived from scientific research.
- **Mode of operation:** The NDL's primary objective is to enhance the collection, integration, management and utilisation of existing public-sector data, rather than actively creating new data sets. The development of scientific data sets and associated software tools requires deep technical expertise and interdisciplinary teams, outside the current remit of the NDL.

- **Data governance:** Institution-level public-sector data often involve stringent privacy and security measures, particularly concerning personal information or anonymised health data. Many scientific data sets do not carry the same sensitivities, and so conflating these distinct data types within one body could lead to unnecessary regulatory burdens.

As such, the NDL is not the right vehicle for the rapid, mission-driven assembly of national scientific data sets. Instead, we propose leveraging the AIRR – an initiative that is already underway based upon the recommendations of the AI Opportunities Action Plan.

Recommendation: *As part of its planned expansion, AIRR should support at least three dedicated programme directors focused on scientific data-set creation. AIRR data programmes should be tasked with both enhancing pre-existing scientific data sets and creating completely new data sets.*

The planned 20-fold expansion of the AIRR and the addition of mission-focused programme directors to the operating model present a unique opportunity to evolve AIRR's role, such that it includes programmes that bring together compute, data-set creation and software-tool building. The process of initiating such programmes should begin with a data-scoping exercise comprising two aims. First, to determine the state of data digitisation in the various fields of publicly funded science (similar to the data stocktakes recommended by Google DeepMind).[37] Second, to identify the highest-value strategic data sets needed to enable the next generation of revolutionary AI models. This aspect of the audit should be conducted with the collaboration of UKRI, the UK SovAI team and the broader research community to rapidly identify the most valuable projects that align with national priorities.

AIRR's data-programme directors should prioritise the following actions.

- **Launch targeted data-set creation programmes:** The primary aim of AIRR programmes should be to produce high-priority data sets, with each data set inspired by a specific high-impact AI use case. Efforts should span the full lifecycle – from data collection and transformation, to compute and software tool building – so that these data sets and their associated AI models can be effectively operationalised and integrated within scientists' workflow.

- **Establish partnerships across academia, industry and government:** Programmes should establish partnerships with universities, Focused Research Organisations[38] (FROs) and industry partners to co-fund and co-develop data sets. To facilitate this mode of working, programmes should make use of a mix of funding mechanisms to further their aims, including public-private partnerships, open prizes and research grants.
- **Invest in supporting infrastructure:** Data programme directors should provide support for biofoundries, self-driving labs (SDLs) and AI-augmented data-collection centres to accelerate future data-set creation, particularly high-value functional data sets.

GOVERNANCE AND SUSTAINABILITY

AIRR should establish governance frameworks for its data sets that balance openness, security and commercialisation. Programmes could draw on a range of data-access models, while some data sets could be commercialised to sustain AIRR data programmes (similar to the European Bioinformatics Institute), with exemptions for academia, small and medium-sized enterprises (SMEs) and national champions. AIRR should also consider international partnerships for certain high-value data sets, sharing compute and capital costs.

Even where data sets are made freely available, there is a clear national advantage to the UK leading in their creation. As illustrated by the UK government's collaboration with Oxford Nanopore, Genomics England and UK Biobank (with the latter producing the world's first epigenetic map),[39] such programmes draw private investment, concentrate talent, create jobs and drive commercial spinouts. AIRR data programmes would seed crucial interdisciplinary networks and provide a much-needed hub for AI for science in the UK.

Dark Data: The Need for Digitisation

Scientific progress is increasingly enhanced by AI models that extract insights from vast data sets, yet the UK's scientific data landscape remains fragmented, unstructured and underutilised. To leverage AI models to their full potential for enabling scientific research, the UK must take deliberate steps to digitise, standardise and strategically curate its research data. The siloing of data within individual labs is a global problem, but it also presents an opportunity for the UK to establish itself as a leader in this space.

Despite the immense value of scientific data – and the significant investment it represents – most publicly funded research is never published, leaving enormous volumes of raw data uncollected and inaccessible. Beneath many published studies lies an iceberg of dark data: messy experimental results, negative findings, technical and methodological details and unfinished lines of enquiry are often buried in lab books, departmental servers or siloed databases.

This vast but unleveraged data is an untapped goldmine for AI – but only if it is properly digitised and made available for model training and discovery.

Recommendation: *To ensure that the UK remains competitive, UKRI should mandate that all new publicly funded scientific research data be recorded in digital form from 2030.*

Many UK universities and research institutions are already moving in this direction, but decisive input from UKRI will accelerate the transition to digital-first record-keeping. It will also incentivise the research ecosystem (and the market) to build the infrastructure, processes and technologies that will be needed.

THE VALUE OF DARK DATA

Data accessibility varies greatly across disciplines but in many fields, valuable experimental records exist solely in physical lab books, making them inaccessible for AI training and unusable for large-scale analysis. The digitisation of dark data would benefit the research community in four major ways.

First, as scientific publishers are generally interested only in positive (significant) experimental findings, AI models trained only on published data reflect and reinforce publication biases, rather than capturing the full spectrum of scientific inquiry. If an experiment results in null findings 20 times, but just one study reports significant results, AIs will be trained on that lone positive – skewing insights and ignoring valuable, publicly funded negative data. Digitising dark data will therefore be crucial for increasing AI reliabilityin science.

Second, access to both positive and negative experimental results would help prevent redundant research, allowing AI to identify when an experiment has been repeated many times with consistent null results. It would also enable AI to aggregate findings, providing a clearer, more accurate understanding of scientific questions by considering the full body of evidence.

Third, based on the recent success with reasoning models, it may be helpful to provide AIs with training data showing the intermediate process by which conclusions are reached.

Finally, the digitisation of full experimental data (both successes and technical failures) could completely transform research efficiency. AI models with access to such data on a large scale could allow researchers to predict which protocols, reagents and techniques are likely to be optimal in any given context, reducing the waste of time and money.

Strategies to achieve the goal of digital-first experimental data collection by 2030 could include:

- **Requiring digital lab books:** Mandate the use of platforms such as Benchling[40] or equivalent electronic lab notebooks, to make sure that research data are structured and accessible.
- **Automating digitisation:** Support the uptake of AI-driven apps to scan and extract data from physical lab books, or from uploaded photos of lab books, with minimal researcher burden.
- **Incentivising compliance:** Offer funding incentives and technical support to facilitate the transition to digital-first record-keeping.

By embedding digital-first policies into research funding, the UK can create a future-proof foundation for AI-driven discovery.

06 Building the AI-Tooling Ecosystem for UK Science

In addition to high-quality data sets, we need the right software tools – both to assist in the collection and processing of data for training models (first-mile tools) and to apply AI outputs effectively in research workflows (last-mile tools). However, despite their growing importance, the creation and sharing of new AI-enabling scientific software tools remains undervalued and insufficiently supported in academia[41] – a problem highlighted by the Software Sustainability Institute.[42]

Currently, tool-building in academia is highly fragmented. Individual researchers and PhD students often develop tools as side projects, with little formal support and insufficient incentives to refine, scale or maintain them.[43] Many tools are abandoned after publication, while others are redundantly recreated by different groups. Meanwhile, research-software engineers (RSEs) – software engineers working in scientific research – lack a mature and varied ecosystem of attractive career pathways, leading to a lack of integration of top software talent into the academic research process.

Addressing this issue requires a coordinated national effort across some key actions.

- Improve incentives and recognition frameworks in order to remove the structural blocks that prevent scientists from investing time in building high-quality software tools.
- Ensure the interoperability and long-term sustainability of AI tools by addressing the fragmentation and abandonment of software, and provide clear funding pathways from early-stage development through to large-scale adoption.
- Build a national ecosystem for professional research-software development by creating clear, attractive career pathways for RSEs.
- Support large-scale, mission-oriented AI-tool development.

Changing Incentives and Recognition for Tool-Building Scientists

Even though 92 per cent of researchers use scientific software and 69 per cent consider it fundamental to their work,[44] tool development remains undervalued in academic career progression. Scientists are primarily incentivised to publish papers rather than to develop, scale or maintain software tools – only 11 out of 185,000 outputs submitted to the 2021 Research Excellence Framework were in the software category.[45] This can lead to some key issues.

- **A lack of formal recognition for software contributions:** Though researchers are keen to acknowledge the software tools they use, the processes for doing so are unclear,[46] leading to tools being improperly cited (or not cited at all) in scientific papers. This means that they are not sufficiently considered in academic career advancement.
- **Minimal, ad-hoc tool development:** Many researchers build the minimum viable tools to support their own work, but it is not worth their time to perfect and share them widely after publication.
- **Lack of interoperability and usability:** Tools are not designed for broader adoption, leading to redundancy and inefficiencies.

Recommendation: *UKRI should lead the development of a national framework for recognising software contributions. This initiative should integrate tool usage and community metrics into key academic processes, such as hiring, contract renewals, grant evaluations and Research Excellence Framework panel guidance.*

The framework should include a commitment to work with universities, the Software Sustainability Institute and other scientific associations to collectively establish norms and guidelines regarding the types of research software that should be cited. It should also explore how web analytics can complement traditional metrics. This should include a mechanism for recognition of the maintenance or improvement of existing software, which often becomes "invisible" work.[47],[48] Another promising proposal, outlined in a paper published by the Federation of American Scientists,[49] suggests requiring publicly funded research publications to be accompanied by a Software Bill of Materials (SBOM)[50] or a similar document listing all software used in the research.

Importantly, this framework must keep pace with the rapidly developing nature of the field. AI-assisted programming will soon enable more scientists than ever to develop and improve upon software,[51] while the spread of AI models across all research fields will create demand for a huge range of highly specialised tools. It is essential that academic incentive structures do not block researchers from exploiting this opportunity.

Addressing the Fragmentation and Abandonment of Scientific Tools

Many valuable AI-related tools are developed as part of PhD projects or by individual research groups, often without the intention or capacity to scale them for broader use. As a result, these “invisible”[52] tools frequently become obsolete, with other researchers reinventing similar tools instead of building upon existing resources.

Recommendation: *UKRI should introduce an adoption-linked tiered funding mechanism, to address the lifecycle challenges of AI-enabled or AI-enabling tools, ensuring their scalability, reusability and sustainability. This approach could draw inspiration from initiatives such as the Chan Zuckerberg Initiative’s Essential Open-Source Software for Science programme,*[53] *which funds open-source tools to build collaboration and ensure the longevity of critical life-sciences software.*

This proposal aligns with and complements UKRI’s Collaborative Computational Projects,[54] which support sustained, community-driven software development, and the 2021 funding opportunity Software for Research Communities,[55] which focused on adapting or maintaining existing software tools. Funding should support the progression of successful AI tools through three key stages.

- **Early-stage development:** Grants for small-scale funding to support initial development or improvement of existing tools. These should facilitate collaboration with RSEs or other research entities, promote cross-lab partnerships and focus on building tools with scalability and reusability in mind.
- **Scaling up:** Mid-level funding for tools that demonstrate growing adoption and community interest. This stage should prioritise interoperability, multi-institutional collaborations and alignment with FAIR (Findable, Accessible, Interoperable, Reusable)[56] principles, incentivising user-friendly documentation and wider adoption.
- **Long-term sustainability:** Large-scale, renewable funding to maintain and upgrade widely adopted tools. Support should reward projects with proven impact and longevity, as well as effective community engagement, with a clear commitment to long-term maintenance.

It is also important to note that, in many cases, researchers who create valuable AI-assisted or AI-enabling tools have little interest in pursuing support to scale and maintain a public version of their invention. For this reason, UKRI should develop best-practice guidelines for software archiving and promote the use of platforms such as GitHub and Zenodo for long-term accessibility. At the same time, it should introduce mechanisms to reward improvements to existing tools, such as adoption metrics and community-building.

EXPANDING CAREER PATHWAYS FOR RESEARCH SOFTWARE ENGINEERS

Many scientific challenges that could be addressed with AI-enabled (or enabling) tools lie beyond the expertise of discipline-specific researchers, who may only have a limited understanding of AI's potential in their field. Therefore, integrating software engineers into the research process is invaluable, as they augment a lab's discovery potential by enabling new computational techniques, optimising workflows and developing advanced analytical tools.

Despite its increasing importance, the UK's RSE ecosystem is underdeveloped. While organisations such as the Software Sustainability Institute have championed their role, career pathways for RSEs are limited and salaries remain uncompetitive: according to a 2022 survey,[57] just 14 per cent of RSEs earned more than £58,172, with the most common salary bracket being between £32,277 and £43,325 – far below industry standards. As a result, many talented AI developers and software engineers are lost to the private sector, drawn by higher salaries, more varied career opportunities and the chance to work on more dynamic projects.

To harness this untapped potential, the UK should incentivise the development of a rich ecosystem of programmes and research entities that bring scientists and software engineers together. This would facilitate collaboration, accelerate AI adoption in research and create compelling career opportunities for RSEs to contribute to public-sector research.

Recommendation: *To expand career pathways within research software, UKRI should ensure that flexible, sustainable grants exist that allow research labs to fund the employment of RSEs. This funding should be suitable for research studios, embedded experts and external contractors.*

We have identified three potential models to integrate RSEs into the research landscape. The first two already exist in the UK ecosystem but should be scaled up, while the third could emerge under the right conditions.

- **Research studios:** These autonomous operational units sit within university departments, ensuring deep collaboration between RSEs and scientists and, unlike traditional IT departments, sit within academic environments, working closely with multiple research labs to develop software tools and solutions tailored to researchers' needs. A successful example is the Neuroinformatic Unit at University College London, which builds open-source software for neuroscience and ML.[58]
- **Embedded experts:** Individual software engineers can be seconded from industry or public-sector organisations and embedded within research labs for a given period to assist in AI-driven projects. An example of this

model is the recent collaboration between the Advanced Research and Invention Agency (ARIA) and Pillar VC, where top AI talent will be embedded for one year within 30 leading UK research labs.[59]

- **Technical contracting firms:** Drawing inspiration from the model of Bolt Beranek and Newman – the pioneering ARPANET contractor of the 21st century[60] – agencies such as ARIA and AIRR could commission external software groups to build high-value tools. For RSEs, this model is an attractive alternative to academia, as external firms can choose cutting-edge, high-impact projects while maintaining autonomy and avoiding excessive bureaucracy. Crucially, these firms would have greater flexibility in remuneration, offering the potential for significantly higher salaries than those typically available in academic-research roles.[61]

Supporting the Large-Scale, Mission-Oriented Development of AI Tools

While small-scale development of academic tools is critical, some AI tools require extensive development, sustained funding and large-scale collaboration – and that is beyond what traditional research grants can support. In recognition of this, mission-oriented tool development should be embedded within our proposed AIRR data programmes, ensuring that high-quality tools are built alongside strategic data sets. These programmes should receive adequate funding to leverage technical contracting firms in developing mission-specific scientific tools.

However, not all high-impact AI tools will fall within the remit of these programmes, nor align with an ARIA opportunity space.

Recommendation: *Inspired by DARPA's Grand Challenges,*[62] *UKRI should establish and fund AI Grand Challenges for scientific tools, focusing on high-impact use cases that require significant coordination, investment and expertise.*

Such schemes are already being trialled in other countries. For example, the US National Science Foundation's Cyberinfrastructure for Sustained Scientific Innovation[63] funds software development to address specific scientific challenges. One such initiative, DeepChem,[64] provides pre-built ML models for researchers across disciplines, supporting applications from drug discovery to materials design.

Similar measures will strengthen the UK's capacity to build cutting-edge tools, creating a vibrant ecosystem where software engineers and scientists collaborate to drive breakthroughs in AI-powered research.

07

Honing the UK's AI-Talent Pipeline

The most crucial asset in any scientific endeavour is talent. If the UK is to lead in AI-driven science, it must ensure that it has the right people with the right skills to capitalise on the historic opportunity that AI affords. The country has a strong foundation, benefiting from world-class universities and producing more AI-relevant graduates than any other European nation[65] (though smaller countries outpace the UK on a per-capita basis).[66] However, structural weaknesses threaten to undermine this advantage, requiring focus on three interrelated areas.

- **Retaining AI-talent:** The UK faces fierce global competition, with key individuals and teams relocating overseas, particularly to the US.[67] They are often drawn by higher salaries, opportunities to work on exciting problems and more flexible career pathways.
- **Bridging the AI-skills gap in research:** Many scientists lack the skills or confidence to use AI effectively, and surveys indicate that they have concerns around AI companies' use of their data.[68]
- **Strengthening collaboration between academia and industry:** Industry plays a huge role in AI innovation, yet weak links between academia and industry make it difficult for researchers to transition between the two sectors or collaborate effectively.[69]

The government has acknowledged these challenges, concurring with the AI Opportunities Action Plan's proposals for a skills-gap assessment, talent-attraction efforts and industry-relevant training, and the important role of Skills England.[70],[71] However, a bold, clear plan is needed to support AI pioneers and build an AI-enabled research workforce.

Attracting Top Global AI Talent

The UK's immigration system for high-skilled workers remains a formidable barrier to securing world-class AI talent – a concern raised by the House of Lords Science and Technology Committee, policymakers and university leaders.[72] AI engineers and researchers are among the most sought-after professionals globally, with many countries actively reshaping their visa policies to attract them. Visa reform is essential for the UK to find its place at the forefront of the current AI-enabled scientific revolution.

While we welcome the AI Opportunities Action Plan's proposals to introduce a flagship AI-scholarship programme and expand the Turing Fellowship scheme, these measures alone will not be sufficient to secure all the types of talent that the UK needs. It is crucial that core issues with the UK's high-skilled visa are addressed.

Recommendation: *The government should establish a new, dedicated AI Talent Visa to allow top AI professionals to work in the UK, whether in industry or academia. This visa should be exempt from the immigration health surcharge, and should allow flexibility for recipients to change roles, establish spinout companies, and move between academia and industry.*

The AI Talent Visa would enable world-class researchers and engineers to contribute directly to the UK's scientific ecosystem, strengthening its position in high-value research and innovation. Since 2021, research-visa costs have increased by 40 per cent after being adjusted for inflation, reaching £5,891.[73] Meanwhile, France has slashed its visa costs by 95 per cent – a move that propelled it to second place in Europe for its share of AI talent. Researchers entering the UK through the Global Talent visa, which is intended to attract world-class researchers, incur 1,272 per cent higher costs than they would entering comparable countries using equivalent schemes.[74]

Despite the government's positive rhetoric on attracting AI talent, indications suggest that upcoming visa reforms may focus on process improvements rather than substantive fee reductions – and this would be a critical misstep.[75],[76],[77] The UK cannot afford to view AI-talent policy through the lens of immigration control and lose out to countries that have recognised it as a strategic priority. Instead, it must be treated as an economic and technological imperative, ensuring that the scientists, engineers and entrepreneurs who will build the scientific industries of tomorrow do so in the UK.

Retaining Top AI Talent, Teams and Projects

Attracting top talent alone is not enough: the UK must also provide a domestic environment in which AI innovators can build transformative technologies, enduring careers and pioneering new research entities. Yet here we find cause for concern. Some of the most exciting AI researchers emerging in recent years have left the UK to build their visions elsewhere – most often in the US, where ambitious new AI research labs, such as non-profit Future House, have been launched outside traditional academia.[78] Without decisive action, the UK risks becoming a training ground for talent that ultimately flourishes abroad.

BUILDING DISRUPTIVE RESEARCH ENTITIES OUTSIDE ACADEMIA

Global leaders in AI for science have no shortage of options, building their new projects, labs or institutes in environments that allow them the greatest freedom. Many of AI's most revolutionary advancements – including transformers, LLMs and AlphaFold – have emerged from labs that are funded by the largest technology companies. These labs share many structural similarities with some of the most successful research organisations of the 20th century, such as Bell Labs and Xerox PARC. They prioritise autonomy, cultivate dynamic interdisciplinary teams and pursue mission-driven projects while providing researchers with the long-term funding necessary to push the boundaries of discovery.

The UK's most successful AI-research entity, Google DeepMind, exemplifies this model. In recent years, a number of scientific institutions have emerged, mostly based in the US, with the aim of learning lessons from such unconventional labs to foster disruptive progress.[79]

By contrast, academic structures are not designed to empower young talent to launch ambitious research programmes at the intersection of science and technology, and short-term pressures to publish papers and secure grants stifle long-term, high-risk research. Standard industry labs have their own constraints, as they are tied to short-term commercial goals and so rarely invest in tackling foundational scientific questions.

This presents the UK with an exciting opportunity: to learn from the most successful environments to pioneer a new research model that does not exist in the publicly funded ecosystem.[80]

Recommendation: *The UK should establish a mechanism for the creation or designation of disruptive invention labs: high-autonomy spaces operating at the intersection of AI and various broad scientific disciplines. These labs should be designed to support risk-taking and long-term, AI-driven discovery and invention – offering a new model for public research in the UK based on structural principles akin to those of Google DeepMind.*

The UK has already taken encouraging steps to diversify its R&D ecosystem with the establishment of the revolutionary funding agency ARIA in 2022,[81] together with the planned expansion of the AIRR to include mission-oriented programmes, the creation of UK SovAI to support "national champion" AI companies[82] and the announcement of Bind Research, the first UK-based FRO.[83]

However, what is missing is an entity dedicated to supporting new research labs designed for the AI era, enabling the UK to compete with elite US entities such as the Arc Institute, FutureHouse and OpenAI. Previous TBI papers, such as *A New National Purpose: AI Promises a World-Leading Future of Britain*, have called for such an entity, which would provide significant long-term core funding for AI-enabled research labs, and with them the autonomy for driven AI pioneers to conduct groundbreaking work outside the constraints of traditional academia.

The establishment of such an entity would create a new centre of gravity for AI-driven science in the UK and would ensure that the world's most ambitious AI researchers see the country as the place to build the future.

CROSS-SECTOR MOBILITY: MAKING INDUSTRY-TO-ACADEMIA TRANSITIONS EASIER

Researchers with strong AI skills are in high demand and often leave academia for higher salaries and better resources in industry. However, many would prefer to remain engaged in fundamental scientific research – a feat that can be very difficult under the current system. There are few pathways for hybrid roles or fluid movement between the two sectors, and so researchers who leave academia rarely return, cutting off collaboration and slowing the transfer of knowledge between the sectors.

Recommendation: *To provide greater flexibility for the best AI talent to work across academia and industry, the government should establish a new AI Industry Fellowship Programme, funding three- to five-year joint appointments between universities and industry partners. The programme should accommodate both part- and full-time research to attract leading talent from industry, while encouraging part-time teaching where possible. This would enable AI engineers in private-sector R&D teams to contribute to scientific research while maintaining links to industry, mirroring successful models such as the Royal Society's Industry Fellowship*[84] *and similar schemes in Germany and the US.*

Industry plays a leading role in advancing AI for science,[85] so feeding expertise back to academia would ensure that academic research remains relevant to real-world AI advances. Greater permeability would also facilitate the sharing of skills, tools and techniques between the two sectors.[86] By embracing a more fluid AI ecosystem that enables high-agency researchers to chart their own course, the UK can not only attract world-class talent but also ensure that it stays and builds the future of AI-enabled science in the UK.

Enhancing AI Training for Researchers

AI is transforming almost every aspect of the scientific process, but many researchers lack the foundational AI competencies needed to integrate AI into their work and harness its benefits. It is imperative that researchers across disciplines are equipped with both basic AI literacy and training tailored to leverage cutting-edge ML models or automation tools within specific fields. Moreover, researchers must become discerning consumers of AI products and services, capable of critically assessing and integrating these tools into their workflows.

Recommendation: *Training programmes for scientists should be significantly enhanced to provide researchers with the requisite knowledge and skills to adopt AI technologies pertinent to their research domains. This should be the responsibility of higher-education institutions, degree-accrediting bodies, learned societies, other relevant academic and professional bodies, and private-sector training providers. The process should be informed by, and inform, the government's AI-skills audit.*

Strategies to enhance the training of academic researchers in AI for science could include the following.

- **Integrating AI literacy and best practices through curriculum development:** Professional associations, learned societies and other relevant bodies should review and update the accreditation criteria for scientific degrees to include foundational AI-related content. This integration would mirror existing requirements, such as the Royal Society of Biology's prescription of a foundation in statistics and mathematics in a biological context,[87] establishing AI literacy as a fundamental component of academic programmes.
- **Providing training that uses collaboration between industry and academia to leverage cutting-edge AI models in research:** In line with our AI Industry Fellowships proposal, universities could establish knowledge-exchange pathways to bring in AI practitioners from the private sector for part-time, academic-adjacent roles, ensuring that academic programmes remain aligned with the latest advancements in AI. These practitioners could conduct workshops, modules of undergraduate courses, or bootcamps for staff, students and technicians, fostering a practical understanding of domain-specific, advanced-AI applications.
- **Using postgraduate and postdoctoral industry placements for upskilling:** Expanding existing industry-placement programmes to include AI startups would provide late-stage postgraduate and postdoctoral researchers with opportunities to apply their domain knowledge in exchange for the chance to work in cutting-edge AI

companies. This mutually beneficial arrangement could be supported through funding from Innovate UK, to incentivise companies to take part in the scheme.

By expanding training, enabling hybrid careers and supporting disruptive AI-driven research labs, the UK can build a dynamic scientific AI ecosystem, ensuring that world-class talent thrives.

08

Building the Physical Infrastructure for AI-Driven Science

AI has already revolutionised the research landscape, but it is only going to become more crucial as capabilities and levels of adoption improve. Much of this continued progress will be dependent upon advances in robotics to automate and optimise many aspects of scientific discovery, as well as stable access to compute. It is essential that the UK invests in the necessary infrastructure to support the current and future needs of AI-driven research.

This includes not only access to advanced compute, but also cutting-edge research facilities designed to harness AI's full potential, such as biofoundries[88] and SDLs.[89] Together, these AI-powered research environments – henceforth referred to as automated laboratories – can provide step changes in scientific capacity, streamlining critical processes and enabling breakthroughs at an unprecedented pace.

Automated-Lab Infrastructure

AI-powered automated laboratories can support scientists in many aspects of the discovery process – rapidly and accurately performing repetitive tasks and generating high-quality data sets and materials – thus freeing up researchers to focus on more creative tasks.

However, significant barriers constrain the UK's ability to build these sorts of supporting labs: restrictive planning regulations and high land costs. The demand for space in research hubs such as Cambridge far outstrips supply.[90] It is estimated that for every €1 billion of venture-capital investment, 46,000 square metres of additional life-sciences space is required.[91] The UK must develop a mechanism to bust through these blockages, incentivising the private sector to build out data centres and next-generation labs.

Recommendation: *The concept of AI Growth Zones – as outlined in the AI Opportunities Action Plan – should be expanded beyond compute, to include growth zones aimed at a wider range of AI-enabling research infrastructure. These should be strategically co-located with academic and industrial research hubs.*

The types of infrastructure that should be supported by such AI growth zones could include self-driving labs: AI and robotics-powered experimental facilities that automate lab workflows (particularly repetitive ones), perform high-throughput experiments and generate high-quality data sets, including functional data sets. Biofoundries are another contender: facilities that integrate robotics and AI to automate the design and fabrication of biological materials and systems. Biofoundries can provide researchers with tailor-made materials (such as genetic constructs or microbes) more quickly and cheaply than would otherwise be possible.

The UK private sector boasts some companies with world-class capabilities in automation, such as Automata, which has automated 91 per cent of end-to-end lab workflows.[92] However, publicly funded research institutions remain behind the curve. Apart from a handful of state-of-the-art labs, UK research institutions remain underdeveloped in robotic automation.

To bridge this gap, the government could consider matched funding mechanisms to de-risk private-sector investment in AI-for-science infrastructure. The UK Research Partnership Investment Fund has demonstrated success in this area, unlocking investment for high-impact facilities such as the Materials Innovation Factory in Liverpool: a world-class research hub for advanced materials discovery.[93] Targeted funding for SDLs and AI-driven lab automation could generate similar returns.

International models demonstrate the power of investing in such infrastructure. The Acceleration Consortium at the University of Toronto is leading the way in SDL infrastructure, with facilities designed for remote access, allowing multiple institutions to make use of cutting-edge AI-driven labs.[94]

Compute

As AI adoption accelerates across research and industry, the demand for computing power is surging. The planned 20-fold expansion of the AIRR and the introduction of Growth Zones to support data-centre deployment are important steps forward. Ensuring that these resources are strategically allocated and accessible – particularly for researchers and SMEs – will be critical. The government should provide clarity on how AIRR usage will be prioritised to maximise its impact, and the Department for Science, Innovation and Technology (DSIT) must maintain oversight of the allocation process and its outcomes.

Expanding access to compute is vital. Most compute resources in the UK are at capacity, while investment has stagnated. As highlighted in our paper *State of Compute Access 2024: How to Navigate the New Power Paradox*, the UK has only a 1.3 per cent share of global compute capacity, and does not have a single system in the top 25 of the TOP500 Supercomputers list. Increasing the volume of compute is necessary but will not be sufficient. Investments must be strategic and coordinated, taking both power requirements and access models into consideration.

The energy implications of AI Growth Zones require careful consideration. Reliable, clean power will be essential for the UK's long-term competitiveness in this sector, necessitating close alignment between energy-system planning and AI-infrastructure development.

Recommendation: *The UK government should ensure that electricity-grid infrastructure is rapidly upgraded to meet the energy demands of AI data centres, while maintaining grid stability and efficiency. The National Energy System Operator (NESO) should be tasked with evaluating data centres' energy requirements and their potential for flexible consumption, incorporating these insights into the Strategic Spatial Energy Plan. Additionally, reforms to electricity-market structures should be considered to incentivise AI data-centre investment in locations that align with the national energy strategy.*

AI-driven expansion of data centres presents a critical challenge to the electricity grid, requiring proactive planning rather than reactive infrastructure expansion. NESO, in collaboration with transmission and distribution operators, should identify and prioritise areas with sufficient grid capacity to minimise connection delays. AI data centres should also be encouraged to co-locate with renewable energy sources, and to adopt flexible consumption models that align with intermittent generation. The government's AI Energy Council should coordinate efforts between AI developers, energy firms and regulators to ensure that AI's energy footprint contributes to – rather than destabilises – the UK's clean-energy goals. Additionally, leveraging AI for grid management and optimisation should be explored to enhance efficiency and reliability, ensuring that AI-driven growth does not outpace infrastructure readiness.

The AI Opportunities Action Plan also advised that the government should resolve the question of the Edinburgh exascale investment, which was withdrawn in August 2024.[95] It is our view that any exascale system should be designed and deployed to serve AI use cases first, with standard high-performance computing applications as a secondary benefit. The government should be able to steer the use of compute investments towards the highest impact AI applications, whether in research or industry.

By focusing on the foundations of AI-driven science – from talent development and infrastructure to fostering collaboration and strategic investment – the UK has an opportunity to build a research ecosystem that thrives in the AI era.

09

Remaking the Institutions of UK Science

AI capabilities have exploded over the past five years and this rapid revolution has taken much of the research world by surprise. While universities and publicly funded institutions have historically led in the development of many paradigm-shifting breakthroughs that transformed research itself, the majority of the most transformative developments in AI so far have originated outside these traditional institutions.[96] This raises pressing questions about the readiness of the UK's publicly funded institutions to compete at the frontier of AI research and to adapt to its rapidly evolving capabilities.

At the heart of this challenge lies the role of research funders, who must drive progress by identifying opportunities and incentivising change. This means reprioritising funding for foundational AI and AI-enabled research, coordinating and concentrating efforts on highly strategic AI research areas and fostering collaboration across disciplines, as well as between industry and academia. Funding should be used as a lever to incentivise researchers to adopt new AI techniques, and to support them in doing so safely and responsibly.

Enhancing UK Research and Innovation's Role

As the UK's largest public research funder, UKRI has a critical, central responsibility to drive the transition of the UK's research ecosystem into the AI era. UKRI and its research councils are responsible for implementing key recommendations of the government's AI Opportunities Action Plan, including the expansion of the AIRR. This remit represents an opportunity for an important enhancement of UKRI's role, reflecting an increased sense of ambition from DSIT ministers.

But to support an AI-enabled scientific ecosystem – especially if it is to take on additional responsibilities – UKRI must adapt. This urgent necessity, along with the upcoming appointment of a new CEO, presents an opportunity for much needed reform.

The independent review of UKRI, led by David Grant, highlighted serious issues in governance, accountability and organisational efficiency.[97] UKRI's investment strategy for AI must also be improved if it is to play an enhanced role in driving forward AI for science. The Alan Turing Institute, the UK's flagship AI research body, has faced ongoing criticism regarding its strategy[98] and judgement,[99] while the Technology Missions Fund – intended to support AI and other high-tech fields – was rolled out too hastily, leading to suboptimal investments that do not advance the UK's position in these technology areas. While the societal issues around AI safety will require continued discussion and debate, the £31 million invested in "responsible AI" has done little to shift the dial on the practical issues around the development and adoption of AI by academia or business. Without focused investment in technical research that can drive rapid and safe development and adoption, the UK risks falling behind the curve. UKRI therefore needs to take urgent action in a number of areas to ensure it is ready for the role it will need to play.

- **Increased internal coordination:** AI's adoption within research is an issue that transcends disciplinary silos. Despite some positive efforts to increase interdisciplinarity,[100] UKRI's existing quasi-federated structure is holding back effective collaboration. Clearer collaboration between UKRI's councils is needed to avoid duplication and ensure that scarce resources can be prioritised for the highest-impact activity.
- **Increased agency:** To accelerate the adoption of AI in their domains, research council executive chairs will need to take tough decisions regarding what to fund and what not to fund. They must be empowered to hold the line.

- **Increased expertise:** UKRI needs a much stronger connection with the technological frontier in order to pivot its investments towards areas that are genuinely impactful. It should refresh its pool of technical experts and bring in those working at the cutting edge, including those operating in the private sector.
- **Increased speed without increased haste:** Coordination should not be an impediment to getting things done quickly. Approval processes should be streamlined – particularly those associated with business cases, which take an average of 17 months to conclude.[101]
- **Increased experimentation with AI:** UKRI needs to evolve its policy position on AI to encourage experimentation; its prohibitive stance on the use of generative AI in funding applications signals a conservative approach.[102] More promising has been the Economic and Social Research Council's support for AI-driven evidence synthesis for policymakers.[103]

We see a huge opportunity for renewal in each of these areas. The imminent appointment of a new CEO at UKRI represents a turning point for the organisation; it is a moment that both UKRI and DSIT should seize.

Recommendation: *The minister of state for science, research and innovation should formally ask the current and incoming UKRI CEOs to make the changes needed for UKRI to play an enhanced role in advancing the UK's position in AI for science. This should include establishing a new central AI function within UKRI to drive forward both the frontier of AI in the UK and its adoption within the UK's research system.*

The UKRI central AI function will have a formal mandate from DSIT, strengthened and taken forward in full by the new CEO, to undertake a range of reforms across the organisation – and this will enable UKRI to play the enhanced role that we have laid out. Led by a senior responsible owner – an individual with a high degree of technical expertise who can work on this agenda full time – the new central AI function will be responsible for breaking down internal silos, undertaking prioritisation of resources and increasing UKRI's technical capacity and capability on AI.

The UKRI central AI function will need to be agile to keep pace with, and inform, fast-moving developments in technology and policy. It should have the licence to design and implement new flexible funding mechanisms to support the most promising projects, people and institutions, and to leverage increased investment from organisations within the private and philanthropic sectors, including the Wellcome Trust,[104] Renaissance Philanthropy[105] and Chan Zuckerberg Initiative.[106]

The function should also have clear visibility within government to ensure it links up effectively with the government's wider AI agenda, including formal links to UK SovAI, the AI Opportunities Unit and the Government Office for Science.

In time this function could be a model for how UKRI establishes cross-cutting themes more generally. UKRI's potential lies in its ability to integrate strategically across domains, with divisions between disciplines becoming less prominent and relevant. UKRI's internal governance could ultimately reflect that transition, with existing councils being replaced by a smaller number of strategic priorities integrated across the organisation. This approach should be the north star for UKRI in the post-AI era.

The Role of Research Funders

In the short to medium term, this government reform initiative for UKRI will be critical. But over the longer term, the entire UK research-funding ecosystem must play its part in bringing forward a new era of AI-driven science. The UK has a rich array of funding organisations: government funders such as the National Institute for Health and Care Research and Advanced Research and Invention Agency (ARIA); charity funders such as Cancer Research UK and the British Heart Foundation; and philanthropic foundations such as Wellcome. All these organisations have a role to play in driving up the application of AI within their disciplinary areas. This should be seen by all funders as a strategic priority.

Recommendation: *All UK research funders should increase their investment in AI-enabled research. This should include the establishment of dedicated programmes to encourage and facilitate AI adoption in their disciplinary areas, develop talent and skills, and invest in strategic infrastructure and data.*

Getting on board with this agenda will require funders to overcome multiple interconnected challenges. They will need to make high-stakes funding decisions in a fast-moving technological landscape, navigate the growing knowledge gap[107] between academia and industry (while ensuring it does not widen) and build trust within a community that is potentially sceptical towards AI. Funders also need to navigate issues of AI safety and security, which requires a deep understanding of the technical capabilities of state-of-the-art models. This will all need to happen in tandem with upholding the integrity of funding processes, given the explosion in the use of generative-AI tools.[108]

We see an opportunity for the wider community of research funders to collaborate on navigating the AI-for-science agenda. This should include a particular emphasis on understanding the shifts in AI-enabled research, sharing expertise, understanding safety and security risks, developing good practice, and ensuring diverse and complementary funding approaches.

Recommendation: *To ensure the existence of a platform for the coordination of AI funding across the research community, UK funders should establish a new forum for AI research funders. Chaired by UKRI, and drawing on expertise from the AISI, this new forum would provide a venue for achieving strategic coherence across funders, sharing knowledge and devising joint actions where needed – especially on interoperability, data sharing, open-science principles, research integrity and AI safety. Both AIRR and UK SovAI should have representatives in this forum.*

We propose that the forum undertakes work in the following areas.

- **Defining shared funding standards:** This would focus on data collection, curation, preservation and access, as well as the use of software and tools.

- **Streamlining collaboration with industry:** The idea would be to form a collective request of private-sector AI companies in order to maximise the impact (and minimise the burden) of their participation in the likes of funding calls and project assessments.
- **Embedding open-science principles:** The emphasis would be on data and AI methods, given the “black box” nature of AI models,[109] with open-source practices duly rewarded.[110]
- **Sharing knowledge:** In particular, this would centre around the technical opportunities and limitations of AI for research, while also navigating the safety and security risks (in coordination with the AISI) that may arise from some AI applications.
- **Pooling resources for shared initiatives:** It will be important to identify areas where joint action could increase impact – such as the establishment of new institutions or setting up funding awards and prizes – while also working to prevent duplication. This could also include initiatives pertaining to responsible and safe AI, the impact of AI on research integrity and work around data sharing.
- **Aligning risk appetites:** Key would be any “big bet” investments made across multiple funders.

This is a unique opportunity for the UK’s scientific institutions to adapt for the age of AI, and they must do so.

10

Trends, Risks and Implications

At this early stage, the transformative potential of AI in science is only beginning to come into focus, and its precise trajectory remains unpredictable. This report has focused on strategies for the UK government to accelerate the integration of AI into our research ecosystem. Success in this endeavour will bring immense opportunities but also challenges and potential risks.

In this chapter we explore these issues, first discussing emerging risks to public health and national security that may arise from new AI capabilities and outputs, second outlining concerns regarding the quality and processes of AI-enabled research. Finally, we will explore the broader implications of widespread AI adoption on the R&D ecosystem and wider society.

Safe Practices in the Application of Research

The ability to use AI to rapidly advance scientific discovery and invention introduces significant dual-use risks.[111] For example, the same technologies used to design and synthesise life-saving therapeutic molecules could also enable the creation of chemical weapons or engineered pathogens.

Addressing this and other security risks will require technical and policy interventions. Advances in biosecurity safeguards, such as upgrades to DNA-sequencing controls, could mitigate the risk, particularly through the input of AI experts acting in a manner analogous to “ethical hackers” to stress-test safeguards.[112] It should also be remembered that AI offers many opportunities to strengthen biosecurity and support better public health, including the development of new vaccines or therapies to combat emerging global threats.[113]

The AISI[114] plays an important role in model evaluation, working in collaboration with the wider national-security community, researchers, private companies[115] and the international network of like-minded institutes to assess risk, both pre- and post-deployment.[116] Model-evaluation methods will need to evolve alongside the technology itself to remain effective.[117],[118] The TBI paper *A New National Purpose: Leading the Biotech Revolution* outlines a comprehensive biosecurity strategy for the AI age, including the establishment of a dedicated body to monitor and mitigate biosecurity risks in emerging AI models.

Implications for the Processes and Quality of Scientific Research

Beyond security concerns related to the outputs of AI, the broad integration of AI into scientific research raises complex issues around the processes and quality of scientific research, including reliability, reproducibility and automation bias. If left unmanaged, these issues could undermine trust in AI-enabled discoveries, or indeed the integrity of the scientific process itself.

AI models are prone to errors stemming from limitations in training data[119] or model architecture (such as tendencies to hallucinate),[120] and are vulnerable to corruption through intentional or unintentional data poisoning.[121] Such issues can corrupt scientific understanding. To enhance reliability, it is essential that training data sets are high quality, comprehensive and as unbiased as possible. Digitising all research data – including negative results – could help mitigate bias towards positive findings and significantly expand training data for scientific knowledge. But most critical is simply that scientists stay vigilant about the limitations of AI models and treat AI outputs as starting points rather than conclusions, rigorously verifying findings experimentally.

As AI is deployed more widely, human oversight and accountability will remain critical in order to guard against the risk of automation bias:[122] the tendency to over-rely on AI systems and AI-generated outputs.[123] Though the extent of the phenomenon is debated, researchers may defer to AI outputs even when results contradict intuition or domain-specific knowledge. To counter this, a culture of healthy scepticism must be fostered, ensuring that researchers can fully leverage this transformative technology while maintaining the confidence to critically assess and challenge AI outputs.

It is also plausible that the reproducibility crisis in science could be exacerbated by AI's "black box" nature[124] and by a lack of transparency around methods, code and data.[125] But when considering reproducibility, AI may prove to be at least as beneficial as it is detrimental.

Highly accurate AI-enabled experimental automation (such as exists in SDLs) could aid reproducibility by standardising experimental processes and reducing human error. These systems enable precise control over experimental parameters while simultaneously collecting and analysing data, making it possible to exactly repeat experiments and track errors.[126] For these reasons, updating the UK's research infrastructure could both accelerate discovery and increase reproducibility.[127] AI also offers tools to improve quality and spot errors at the research-publication stage. For example, AI tools can detect statistical[128] or mathematical[129] mistakes, and some academic journals have adopted AI to detect flaws in submitted papers,[130] including suspicious images and figures.[131]

The proliferation of AI tools may exacerbate another negative trend relating to the communication of scientific research: the decoupling of scientific production from meaningful progress. By drastically lowering the cost of producing papers, AI risks amplifying a system already overwhelmed by output, where publication itself has become the goal, and the sheer volume of papers far exceeds the community's capacity to properly absorb and evaluate them. This could force a long-overdue shift in how the research ecosystem identifies and rewards intellectual value, moving away from an emphasis on paper metrics and towards measures that reflect genuine scientific impact.[132]

Beyond concerns related to scientific communication, AI compels us to consider the very essence of scientific discovery. Will increasingly AI-driven research lead to the homogenisation of scientific output,[133] reducing real creativity and serendipity? Or will it enable researchers to turn their minds towards high-level problems, freed from scientific drudgery by automation?[134] Will it inadvertently steer science towards predictable, data-rich areas at the expense of speculative or unconventional fields? Some worry that the "black box" nature of AI may reduce understanding of fundamental principles.[135] Researchers have limited scope to interpret AI-driven results and justify them rigorously, but if AI-derived results are productive and useful, might researchers forget the importance of the “why” behind scientific phenomena? In this view, over-reliance on AI could lead to the “end of theory” itself,[136] where science moves away from hypothesis-driven inquiry towards purely data-driven approaches.

These questions do not have simple answers, but they underscore the need for ongoing dialogue and research. UKRI’s new Metascience AI early-career fellowships are a welcome step.[137] We also believe that our proposed UKRI Forum for AI Researchers should play a role in facilitating the research community’s approach to maintaining research integrity in an AI-driven R&D ecosystem.

Implications for Society and the R&D Ecosystem

The integration of AI into the UK R&D ecosystem will inevitably reshape the social structures of science, with implications for all researchers at all levels, as well as society more broadly.

As AI and automation take over routine aspects of the scientific process, researchers may get back time to focus on higher-level theory, specialist training and project management. However, facilitating this shift might require structural changes to the academic landscape. Traditional career pathways, such as the postdoctoral pipeline and principal-investigator model, may need to evolve to reflect the reduced demand for some roles and the emergence of others.

The resource-intensive nature of AI-driven research[138] also raises concerns about the balance of power in scientific discovery. As AI models demand greater compute resources and access to vast data sets, scientific discovery and invention may shift further towards well-resourced private-sector entities.[139] While private-sector leadership in innovation can be a strength, there is a risk that short-term commercial incentives could increasingly shape the research agenda at the expense of fundamental scientific research, which is essential when it comes to laying the groundwork for the clinical and commercial breakthroughs of tomorrow. Safeguarding this foundation requires a robust public sector capable of leading in exploratory research that pushes the boundaries of knowledge.[140]

AI-driven shifts in power dynamics and access to resources are not confined to the public/private dichotomy, but may also exacerbate national, regional and global inequalities. Countries and institutions with the infrastructure to support large-scale AI research are likely to dominate key fields, potentially creating barriers to entry and competition (see *State of Compute Access 2024: How to Navigate the New Power Paradox*). Addressing this disparity requires collaborative strategies (both within the UK's ecosystem and internationally) to ensure access to key data sets, technologies and compute for new entrants, and policies should be aimed at preventing restrictive practices that could stifle innovation. In the best-case scenario, where such resources are accessible to a diverse range of players, AI can function as a great leveller, making it easier and cheaper for researchers worldwide to pursue groundbreaking discoveries.[141]

While this paper has focused on AI for science use cases in STEM subjects, AI will also help social scientists to research important societal questions.[142] In addition, developing and implementing AI systems that solve real-world challenges often requires social-science expertise (assessing AI's limitations as part of larger sociotechnical systems, for instance).[143]

One example comes from the Predicting Fertility data challenge organised by the University of Groningen and the Open Data Infrastructure for Social Science and Economic Innovations in the Netherlands, in which a team led by Matthew Salganik used an innovative AI approach to predict when, where and to whom children will be born, using surveys and population registries.[144] The UK can make its many and world-leading social-science departments a source of competitive advantage in the digital age by incentivising more cross-disciplinary collaboration like this.

Beyond systemic and societal concerns, models with increasing capabilities are likely to prompt questions on an individual level: what does it mean to be a scientist in the age of AI? Some worry that the joy of discovery could be diminished if AI provides answers too readily, leaving human scientists as mere biological aides to *in silico* researchers. Yet just as AlphaZero has elevated the games of Go and chess to new creative heights, enabling players to reach unprecedented levels of mastery, AI can expand scientists' horizons, allowing them to explore previously uncharted territory.

The questions we face now, from ensuring safety to maintaining scientific integrity, are not peripheral, they are foundational. The success of AI-driven science in the UK depends on facing these challenges head on and integrating solutions into a bold and purposeful vision for the future.

Readers who wish to read more comprehensive discussions of these issues – as well as of possible solutions – should read the recent reports from the Royal Society[145] and Google DeepMind.[146]

11

Conclusion

This is perhaps the most exciting time in history to be a researcher. AI is not just another tool: it signals the dawn of a new era of discovery, accelerating the pace of progress in ways once unimaginable. Scientific revolutions of the past were defined by those who moved first – the countries that built, nurtured and empowered talent, and that created spaces where new ideas could flourish. The UK must decide whether it has the will to lead this global transformation and define the future of AI-driven science.

The breakthroughs that lie ahead will challenge people's understanding of the world. AI will illuminate patterns hidden in nature, simulate realities that cannot yet be observed and propose solutions to problems not yet conceived. But these capabilities will not emerge in a vacuum. They will be built on the foundations we lay today.

For all the promise, there are risks in standing still. The pace of AI innovation will not slow to accommodate outdated structures, siloed institutions or bureaucratic inertia. The UK's deep scientific heritage, world-class universities and globally competitive AI sector give it a head start, but potential is not enough. The UK must reimagine its pursuit of science with the ambition and urgency that this moment demands.

History has shown that transformative technologies reward those who act boldly. The AI Opportunities Action Plan has provided a starting point. If the UK invests and organises wisely today, it can establish itself as a global leader in AI-driven discovery, shaping the next century of scientific progress. The challenge is vast – but so is the opportunity. The UK's greatest scientific achievements still lie ahead.

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For more information on current and future applications of AI in science, see the annex (available as a downloadable PDF).

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