

£27mIn for Supercomputing Services Drive Scientific Breakthroughs in UK



More scientific breakthroughs from UK researchers, notably in the fields of artificial intelligence (AI) and drug design, can be expected with the launch of state-of-the-art supercomputing services.

The "Seven High Performance Computing (HPC)" services will be supported by a £27 million investment from the Engineering and Physical Sciences Research Council (EPSRC), part of UK Research and Innovation (UKRI).

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The funding, announced on 24 February, will provide new state-of-the-art computing hardware across a wide range of different technologies. Moreover, the investment will help much in developing research computing skills, including boosting the careers of Research Software Engineers, across the UK.

"Computation is becoming an ever-more important scientific tool, be it for analysing large data sets generated from experimental work or modelling situations which can't be replicated in experiments," said EPSRC Executive Chair Professor Dame Lynn Gladden.

With the HPC services, <u>researchers will have access to the tools they need to make breakthroughs</u> in a wide range of fields that impact on people's lives. Such ground-breaking endeavours, Professor Gladden notes, include the use of advanced computational drug design for therapeutics targeting a large variety of health conditions.

The seven HPC services are:

Cambridge Service for Data Driven Discovery (CSD3): This University of Cambridge-led project comprises one of the most powerful academic supercomputers in the UK specially designed to combine large scale data intensive simulation and AI science within a single computer system. It will accelerate research across a wide range of engineering and physical science themes, including health informatics, medical imaging and bio-simulation, and AI and machine learning.

The Materials and Molecular Modelling Hub: Led by University College London, the MMM Hub provides high performance computing capacity for researchers to carry out ground-breaking research on the properties of new and existing materials, and EPSRC's new funding (£4.5 million) will build on the hub's capability. Researchers will study, for example, how changes to the recycling of metals can reduce the environmental damage caused by metal extraction.

GW4 Tier-2 HPC Centre for Advanced Architectures (Isambard 2): The GW4 Alliance comprises the Universities of Bath, Bristol, Cardiff and Exeter, and is hosted by the Met Office. Isambard 2 will provide the latest technology that is expected to be used in some of the first supercomputers capable of a billion billion calculations per second, called Exascale supercomputers. The current Isambard system has been used to investigate potential drugs to treat osteoporosis and simulate Parkinson's disease at the molecular level. Isambard 2 will enable researchers to expand this further with the potential for scientific breakthroughs.

Kelvin-2: This service, led by Queen's University Belfast and Ulster University, will provide access to an enhanced computing facility focused on Al-based research. It will accelerate ground-breaking work initially in several specialist areas such as neurotechnology and computational neuroscience, including work on brain-computer interfaces and heterogeneous catalysis.

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Joint Academic Data Science Endeavour–2 (JADE 2): Spearheading this service is the University of Oxford, with support from other UK's leading academic institutions. The JADE 2 service, hosted at STFC's Hartree Centre, will provide a state-of-the-art GPU (Graphics Processing Unit) computing facility for research into Al/machine learning and molecular dynamics, a computer simulation method for analysing the physical movements of particles that make up molecules.

Cirrus Phase II: Preparing for Heterogeneity at Exascale: This service, led by The Edinburgh Parallel Computing Centre at the University of Edinburgh, will expand the capabilities of the Cirrus service by adding specialised GPUs to the current system. Cirrus has already supported different projects such as modelling protein shape for better drug design. The new GPUs will provide a high-performance platform for Al training and research.

Northern Intensive Computing Environment (NICE): The service is led by <u>Durham University as part of the N8 Research Partnership.</u> NICE will use the same technology that runs leading supercomputers in the world. The technology has been chosen with the aim of combining experimental, modelling and machine learning approaches, bringing these communities together to address new challenges. This approach will enable scientists to, for example, advance the imaging techniques necessary to produce the next generation of x-ray instruments.

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