THE IMPACT OF NATIONAL HIGH PERFORMANCE COMPUTING

An analysis of the impacts and outputs of investment in national HPC

Dr. Edward Clarke
Dr. Iain Larmour

August 2016
Executive Summary:

High Performance Computing (HPC) is now accepted as a key enabling technology for scientific and industrial research; the phrase ‘To Out-Compute is to Out-Compete’ having been coined in the early 2000’s and reinforced since by European, Chinese, Japanese and American initiatives in this area. The UK has maintained a strong position in HPC, but increasing requirements for evermore powerful compute resource risk the UK position and ability to compute and compete.

High performance computing is a ubiquitous and essential tool for science. It enables new discoveries, drives innovation and allows new insights into existing scientific challenges. HPC can be exploited in many ways to advance scientific understanding and deliver industrial competitiveness. Examples include understanding the quantum mechanical properties of polymers to simulate nucleic acids and proteins, with biomedical application; modelling air flow in jet engines to avoid building expensive and time-consuming engineering prototypes; and modelling the environment to understand risks on many scales, from tectonics to storms.

The competitiveness of the UK depends on our ability to enhance the computational ecosystem needed to progress the science and engineering upon which our nation depends. That ecosystem will include many other important types of computing, from the high-throughput computing necessary to manage data output from experiments that range from genomics to the Large Hadron Collider, to the data intensive computing platforms necessary to mine data for business, and the operational computing necessary for defence and weather forecasting. However, in many important areas of science and engineering, it is only an internationally competitive high performance computer that can provide the necessary horsepower to deliver enough calculations fast enough. The UK is now falling behind Poland, South Korea and Australia.

The scientific achievements and outputs described in this report can only be maintained if the UK commits to making long-term, strategic and sustained investments in HPC. We stand on a knife-edge if we are to be successful and build on our computing accomplishments. A programme of strategic and sustained investment is necessary to avoid the loss of scientific talent, to enable new scientific areas to flourish and ensure the UK maintains its position as a recognised centre of excellence. We cannot afford to stand still while both computing technology and scientific discovery drive forward.

Such an infrastructure includes not only computer hardware at Tier 1 (national) and Tier 2 (regional) levels, but also integrated data analysis systems, with appropriate storage capacity, data management systems, and software – along with continued development of all these components. These need to be smarter, and more integrated, nationally and internationally, and across science and industry. It will also require skilled people, who themselves will contribute to the competitiveness of the UK.

The science, impacts and benefits presented in this report are a small representative sample of the power of HPC to drive our nation forward. Our vision is that a sustained programme of targeted and timely investment in HPC will provide maximum return and generate scientific and economic benefit for our society. It will enable research that will directly address the economic, societal, scientific and environmental challenges faced by our nation, sustain numerous areas of scientific enquiry, provide critical underpinning to industry, and be necessary to position ourselves for a long-term and sustainable future.
Contents

PART I – SETTING THE SCENE ................................................................................................................. 4
1.1. Commitment to Compute ............................................................................................................... 4
1.2 A Universal Tool for Scientific Research ....................................................................................... 5
1.3 National e-Infrastructure for 2020 ............................................................................................... 7
1.4 Collaboration, Interoperability and Sustainability ..................................................................... 9
1.5 HPC for 2020 .............................................................................................................................. 10
1.6 Regional Centres ......................................................................................................................... 12
1.7 Continuity and Competitiveness ............................................................................................... 17
1.8 Technology Challenges and Opportunities .................................................................................. 18
1.9 People and Productivity ............................................................................................................... 21

PART II - A PROSPEROUS NATION ..................................................................................................... 25
2.1 EPSRC and NERC Science ........................................................................................................... 25
2.2 – One Nation, Many Views ........................................................................................................... 26
2.3 NERC – Business of the Environment ....................................................................................... 27
   2.3.1 Benefiting from Natural Resources ..................................................................................... 28
   2.3.2 Resilience to Environmental Hazards .................................................................................. 28
   2.3.3 Managing Environmental Change ..................................................................................... 29
   2.3.4 Discovery Science .............................................................................................................. 30

PART III – ONE NATION ..................................................................................................................... 31
3.1 A Productive Nation ..................................................................................................................... 32
3.2 A Connected Nation ................................................................................................................... 36
3.3 A Resilient Nation ....................................................................................................................... 39
3.4 A Healthy Nation ......................................................................................................................... 42
3.5 A Sustainable Nation .................................................................................................................. 45
3.6 A Globally Responsible Nation .................................................................................................. 47

Acknowledgements: Grateful thanks to all who contributed to the production of this report. In particular, the Science Board for their expert advice, input and guidance (Richard Kenway, Matt Probert, Jason Reese, Beth Wingate, Stephen Mobbs and Bryan Lawrence), the Regional HPC Centres and the EPSRC/NERC consortia for case studies and photos and all who contributed evidence to the consultation. Special thanks to colleagues at EPSRC for case study input and editing.

Eddie Clarke, Swindon, September 2016.
PART I – SETTING THE SCENE

1.1. Commitment to Compute

Imagine that you had access to a powerful, universal tool that could tackle any task with ease and, like TV’s Dr Who’s ‘Sonic Screwdriver’, could adapt to any purpose. That’s what supercomputers do for science.

Popular culture aside, and despite what you read in the papers, supercomputers are not built to beat humans at chess or describe how toast always lands butter-side down. HPC machines are primarily built to calculate!

These workhorses of computing power lie quietly in secure locations around the UK and perform a thousand trillion calculations per second, every hour of every day. Designed over many years and built for maximum efficiency, they diligently crunch through massively complex scientific problems that will enable advances to improve our lives, from health to engineering, from advanced materials to advanced mathematics. They are the end product of extensive research and the best the computing industry has to offer for maximum efficiency and speed. These machines have the power to change the world a trillion calculations at a time. They can predict how a jet engine will perform; they will show us quantum effects between atoms not visible by any other means, and they can warn us of impending natural disasters – HPC has the power to change the world.

The Power to Change the World

a) Air flow inside a jet engine, coloured by temperature (Ivan Langella, University of Cambridge) b) Polymers interlinking with clay sheets using quantum mechanics (Hugh Martin, University College London) c) Global mantle convection including plate tectonics at the surface (Fabio Crameri, University College London)
1.2 A Universal Tool for Scientific Research

It has long been recognised that successful nations are driven by engineering and technology and that the research endeavour contains three essential, interlinked strands; experimental, theoretical and computational research. We are in the middle of a revolution in the research endeavour: over the last few years, computational and data analytic approaches have become ubiquitous, and are now the ‘third and fourth legs’ of scientific enquiry, alongside experiment and theory. These approaches are essential for the creation, sharing, saving and exploitation of knowledge. More than 100,000 researchers are reliant on the UK’s e-infrastructure, and this number is growing. The development of a sustainable and cutting edge e-infrastructure eco-system is therefore vital to support excellent and innovative research across a wide range of disciplines and industrial sectors and to develop the next generation of computational and data scientists.

The coupling and interaction between these strands of activity mean that High Performance Computing has had a direct and indirect influence on every aspect of our 21st century lives. New research areas that cross traditional discipline boundaries are emerging, enabled by this technology (e.g. the ability to link diverse genetic, health, social and environmental data to better understand and prevent chronic disease); and the analytical and computational tools and techniques are being newly applied to research domains such as history and the arts. ‘Whole system’ approaches and analysis, be it engines or human bodies, are at the forefront of the demand for greater e-infrastructure resources.

A Powerful Tool for Research

Case Study 1 – Software Developments to improve neurosurgery

- Scientists are developing software to model blood flow within the cranium, the part of the skull that encloses the brain, using a model of the patient’s blood vessels generated by an MRI scan.
- We can now identify blood pressures near points of weakness, such as aneurysms, allowing increased understanding and better treatment of conditions.
- The software has undergone extensive development and performance improvement to utilise the full power of the National HPC service, ARCHER, to allow the “Circle of Willis” (a network of blood vessels in the brain) to be studied for the very first time.
- This work, supported by EPSRC, is being led by a team from University College London in collaboration with Allinea Software.

---

To enable cutting edge research it is vital to have the appropriate infrastructure in place because today’s world-leading science on large machines is a product of years of research on innovative, but smaller, university-based computer resources. There is a flow of science, talent and expertise which, nascent on local university compute resources, grows to maturity on the larger scale national systems. We need both the infrastructure and test-beds to support and nurture this delicate ecosystem of computing.

These processor technologies and architectures will be candidates for the national machines of the future. This will be even more important in the next decade as there is a paradigm shift in computing on the horizon and the UK needs to have resources and infrastructure in place to take advantage of the change.

In 2011, the then BIS Minister for Universities and Science, David Willetts, commissioned Professor Dominic Tildesley to write a report on how an e-infrastructure could be created to support the paradigm shift in the scientific process that was being observed.² This led to an additional £145M of capital investment in e-infrastructure and has enabled the UK to exploit the wide ranging benefits of computational research.

The resulting developments in e-infrastructure since the 2011 Tildesley report have included new data intensive computing hardware for the mining of knowledge, high performance computing hardware for modelling and simulation and the development of new software algorithms in both areas. New and extended networks link researchers to hardware and data, and all these investments contributed to the development of skills in E-science.

---


---

**A Powerful Tool for Research**

*Case Study – Extreme Weather Forecasting with Extreme Computing*

- Weather-related natural disasters have led to the loss of thousands of lives and billions of pounds of damage each year.

- The European Centre for Medium-Range Weather Forecasts (ECMWF) can complete their 10-day forecasts in less than an hour and provide accurate forecasts around the world.

- They correctly predicted, 7 days early, that Hurricane Sandy would strike the East Coast of the US, while most other models predicted a move out to sea. This gave essential early warning to government and the general public.

- ECMWF has used the power of the national HPC resource to increase the speed of their modelling by 20%. This allows a real improvement in warning time and forecast quality.
1.3 National e-Infrastructure for 2020

The Research Councils, in partnership with the research community, have worked extensively to implement the recommendations in the Tildesley report. To ensure the world leading position that this initial investment produced is not lost, RCUK have worked together with Innovate UK, Jisc and the Met Office in 2014 to develop a roadmap that sets out the requirements of all research communities. The roadmap highlighted the integration of elements for the most effective deployment; where hardware (the compute infrastructure) is only one part; connectivity to other facilities, capability in skilled people and a managed, integrated approach across agencies and government are also vital.

Research Council and UK government investments since 2011/12 as a result of the Tildesley report have enabled updates and upgrades to the UK’s computing and data infrastructures, and has established a range of complementary e-infrastructure capabilities: from cutting edge High Performance Computing Services (ARCHER and DiRAC, predominately utilised by the physical science research communities), to secure, data intensive computing facilities, capable of managing increasingly complex and often sensitive, personal data (ESRC Big Data Network, the Farr Institute of Health Informatics and MRC Medical Bioinformatics Awards), to research centres such as the Hartree Centre, and the Alan Turing Institute. We must act to support, maintain and grow this important infrastructure.

This document primarily concentrates on the HPC component of that infrastructure, but Figure 1 shows a functional view of the wider e-infrastructure landscape, outlining the key components.

Figure 1- A functional view of the UK e-infrastructure landscape - high performance computing is configured differently for requirements that range from operational to research; data intensive computing is configured to support the research and industrial communities, and high throughput computing is sometimes specialised and sometimes generic (using the public cloud). All is underpinned by software research and development (in both projects and long-term infrastructure programmes), and exploits high-speed networking to link both the users and the components.
The key message is that the national e-infrastructure needs to serve a range of very different needs – high performance computing, data intensive computing, high throughput computing, and software research, maintenance, and development – for a range of communities, from research in science and industry, to operational numerical weather prediction and defence. In order to support that infrastructure, we need a throughput of trained people with comprehensive skills in software development and engineering. Without the skilled people to utilise and develop the potential of the hardware, there is no science and the hardware will lie redundant.

As shown, the landscape is a series of interconnections. No single element works in isolation but rather, through partnerships, form part of the UK’s national e-infrastructure landscape. Tier 2 (regional) architectures are researched and tested today in preparation to become the Tier 1 (national) technology of tomorrow. Important structures such as PRACE and Cloud computing, while forming part of the landscape, have external interfaces to the wider international and commercial communities.

**GungHo**

Gung Ho: Is a joint project between Imperial College, London and the Universities of Exeter, Bath, Reading, Manchester, Warwick and Leeds, the Met Office and STFC Laboratories to research and develop new world-leading mathematical algorithms that that will allow Met Office models to have maximum amount of reality in a simulation and with time-to-solutions of an hour or less. This will help to ‘future-proof’ the codes on new computational infrastructure to prepare for the coming shift in computer architectures.

It will keep the UK on the forefront of HPC for mathematics and computing in climate and weather prediction. The project has a 10-year lead time from the original development of algorithms to its use in an operational setting. This is a common time-scale for developing software as the hardware changes, allowing the Met Office to be prepared for the next computing architecture shift.

The model will be targeted at Met Office operational forecasting as well as climate prediction by the Hadley Centre and NERC-funded climate researchers around the UK.

ARCHER is being used to demonstrate that new algorithms, developed in the project, are both accurate and achieve high performance on relevant HPC architectures - crucial if Met Office is to be competitive on next generation architectures.

*The figure shows a test case from the Dynamical Core Intercomparison Project (DCMIP), run with 24576 horizontal cells and 60 vertical layers, on 96 computer cores.*
Over the last five years EPSRC has invested approximately £9 million per annum in software. This has covered the spectrum from new algorithm development at the leading edge of research applications through software development to code maintenance and programmes of continuous improvement.

This also includes training, and community support activities, such as networking and public outreach as well as initiatives such as the 'Women in HPC' initiative. (Page 22.)

The current portfolio of activities has supported a thriving community of computational scientists who are recognised internationally via the £7m ‘Research Software Engineer’ programme of support. These individuals work together with scientists to develop better codes and enable more productive science. (See Section 1.9, page 21.)

Our aim is for the UK to have an integrated e-infrastructure: one that is run and managed as a whole without silos, and the usage of the infrastructure will be optimised and maximised, leading to the best value for money from government investments. We aspire for the UK to be world-leading in how we do this integration. We aim:

• To maintain our world leading computational and data-intensive research by providing increased capacity and capability across the e-infrastructure ecosystem

• To nurture a cadre of highly-skilled data and computationally literate individuals whose influence extends beyond academia.

• To increase the ease of access to e-infrastructure resources for users from all sectors

• To support the expansion of use of this new technology to new research communities

• To progress towards an integrated e-infrastructure by developing the tools and techniques to support it (access and security; data storage and access) and by finding opportunities for co-location, sharing and aggregation

The UK has made significant inroads to the recommendations to provide and support a well-connected e-infrastructure, but without a long-term, coherent and joined-up approach to the problem, investments cannot realise their full potential.

1.4 Collaboration, Interoperability and Sustainability

The RCUK e-Infrastructure group proactively coordinates e-Infrastructure activities across the Research Councils, Innovate UK, Jisc and Met Office. We have successfully worked together and have made progress towards better integration and collaboration.

Some examples of its work include the production of an RCUK e-infrastructure roadmap for the BIS E-Infrastructure Leadership Council, an integrated financial forward look, guidance for researchers on e-infrastructure security and access management good practice, and jointly funding a pilot project to develop access management tools which will be key enabling technologies for integration across the ecosystem.
The group has also commissioned a series of collaborative reports from the community (e.g. on cloud, data, access management); and an annual survey has been carried out for the last three years, to gain a picture of the people and hardware that go to make up the UK’s e-infrastructure ecosystem.

We are therefore in a good position to take advantage of this culture of collaboration, make the next step and use further capital investment to drive further integration.

The benefits of such an integrated e-infrastructure are:

- Increased productivity by driving resource usage to the maximum, thus increasing research outputs and quality, and reducing time to results.

- Easy for users from all sectors (academia, industry, NHS, etc.) to find resources, access training and use them.

- Enabling interdisciplinary research and collaborative working in shared digital environments.

- A more stimulating environment for research software engineers and technologists, supporting the proper development of a career path and aiding in their retention in the UK.

- Resources for technology development – test beds and early adoption of new technologies. This allows strong engagement with the e-infrastructure vendor industry.

- Knowledge transfer is much easier and the spread of best practice is encouraged.

- Co-localisation of resources in energy-efficient centres.

- Enabling integration with similar services in other countries, thus supporting global scientific collaborations.

1.5 HPC for 2020

The UK is rapidly falling behind in terms of raw HPC compute power and this is affecting our ability to achieve impact, retain raw talent and ensure the continuation of essential research. However, the UK leads the world in many areas of advanced science and it is essential that this lead is not lost for the lack of the right tools to deliver the next generation of scientific breakthroughs. Investment in the most up-to-date HPC provision will ensure the UK extends this world-leading position.

The scientific advances of tomorrow will require an even greater compute capacity. There is a race to develop the first ‘exascale’ computer, giving unrivalled access to computing power. At the same time, there is a drive to reduce the power consumption of HPC and make power savings while increasing computing throughput.

By 2020, we will be two or three generations of future processor technologies down the line and these technologies will enable even greater complex problems to be solved. We will be able to model whole systems, whether these are engineering based (whole jet engine modelling, for example), biological (modelling human body and processes) or environmental (earth systems).
The research done today will inform and shape the research of tomorrow; research does not happen in isolation – it is a continuous flow of ideas, people and knowledge which builds on previous breakthroughs. In the same way, the technology and processors still on the drawing board today will become the tools of tomorrow’s research. Software developments made today will enable greater scientific productivity and insight in 2020. A long-term vision for research and investment is required in HPC today in order to enable tomorrow’s breakthroughs to succeed.

International agreements and collaborations attract international users to the UK (based on previous machines, we might expect 45% of their users to be involved in international collaborations). With the current machines, this internationalisation of cutting-edge HPC also means that UK researchers can gain access to some of the largest machines in the world (Tier-0 machines in Figure 2) e.g. TITAN at Oak Ridge National Lab in the US. Through the Partnership for Advanced Computing in Europe (PRACE), UK researchers have gained 8.4% of the available Tier-0 resources and they have generated cutting-edge science on the biggest High Performance Computers in Europe. However, this represents only a fraction of the compute power that the UK science communities require, and is dependent on the UK having suitable machines for partnership and development.

The increasing power of HPC systems is opening up new opportunities for modelling the more complex problems that face us. If the UK is to take advantage of this, we will require a step-change in computing power to deliver a science-driven programme of research in the UK that is economically and scientifically sound. ARCHER and DiRAC currently provide the highest capability research HPC machines in the UK, delivering both the capacity horsepower to deliver leading edge science, and the capability to develop next generation codes.

However, both are relatively old now, and are nearing the end of their lives as internationally competitive machines. As at November 2015, the ARCHER supercomputer in the UK has fallen to 40th position in the world’s top 500 machines, and the UK is now falling behind Poland, South Korea and Australia.

Along with the Tier-0 and Tier-1 resources, progress requires training machines, entry-level capacity machines such as those in the Universities and regions, and both experimental and customised machines. In the next decade both experimental and customised machines will become more important as the relatively homogeneous computing landscape of the last two decades fragment into a much more complicated future of very different computing architectures.

---

The research community will need access to a range of machines to develop appropriate software and prepare for the future – and at the same time maintain and extend customised data intensive computing environments such as JASMIN, used by the environmental science community to support the exploitation of the high-end simulations produced on Tier-0 and Tier-1 systems as well as integrate data from earth observation satellites on behalf of the UK and European Space Agencies (UKSA and ESA).

### Customised Data Intensive Computing – Analysis of Faults on JASMIN

- Earth observation data is voluminous (just one radar on the Sentinel 1 satellite generates petabytes of data per year – a petabyte being roughly equivalent to 2000 years of MP3 music).
- The JASMIN data intensive supercomputer was deployed in 2011, and was customised to support the storage and analysis of this Sentinel data and many other environmental datasets.
- One such analysis is the development of earthquake monitoring systems by the University of Leeds that can use the Sentinel 1 surface deformation data to measure surface deformation with millimetre accuracy.
- Other JASMIN usages include supporting the delivery of the modelling data to the scientific community which underpins the Intergovernmental Panel for Climate Change (IPCC) assessment reports; real time tracer transport modelling to forecast where research aircraft should fly to get the best measurements; and supporting the UK space research and industrial communities in exploiting the Copernicus climate change initiative.

### 1.6 Regional Centres

As well as evidence from UK-based HPC services, it is internationally recognised that access to HPC enhances the technical efficiency of research outputs.4

As seen in Section 1.5, the HPC ecosystem in the UK consists of Tier-1, Tier-2 and Tier-3 (local university resources). The Tier-1 resources, which provide the current highest capability research HPC machines, are ARCHER and DiRAC. These machines provide the capacity to deliver leading edge science and the capability to develop next generation codes. UK researchers can also access Tier-0

---

4 [http://www.theregister.co.uk/2015/03/25/does_your_university_need_hpc_it_depends_on_disciplines/](http://www.theregister.co.uk/2015/03/25/does_your_university_need_hpc_it_depends_on_disciplines/)
resources through PRACE. Along with the Tier-0 and Tier-1 resources, the UK computational science community requires training machines, entry-level capacity machines such as those in the Universities and at Tier-2 level, and both experimental and customised machines.

Case Study: HPC Stepping Stones – Wind and Tidal Turbine Design

- To understand the energy yield of wind turbines you need to understand the wind flow past the blades and the loading that can occur on the material.
- New wind turbine designs make use of moveable wings which complicates the required modelling.
- EPSRC has supported researchers from Lancaster University to develop novel software to model these complex wind turbines.
- They have used the N8 Regional HPC centre to test and model features of the code allowing faster publication and international collaborations to be formed.
- Work on the Regional HPC Centre was vital in supporting the successful application for time on the National Supercomputer ARCHER.

A globally competitive supercomputer has been available to researchers in the UK for many years. However, the gulf in capability from a small university system to the National Service has acted as a barrier for some researchers and communities from realising the full benefits of the national supercomputer. This capability gap was recognised and in 2012 EPSRC invested £11million to establish a network of Regional HPC centres. Sitting between university provision and the national service, these regional HPC centres provide a seamless transition for users to develop their skills, software and research to enable them to fully exploit the biggest research computer in the UK.

Requirements for computational resources can be defined as either capacity or capability computing. Capacity computing is sufficient for the high throughput of a large number of simulations, each of which addresses a relatively small problem size. It can be provided using the distributed computer infrastructure at departmental and university level, access to which will be enabled by the emerging e-Infrastructure. Capability computing on the other hand is needed for simulations that address much larger problem sizes. Such simulations, which require high communication bandwidth and low latency times, can only be achieved in a viable timescale by a high performance computing system at national level and not by using a distributed computing architecture. These systems must be world-class for the UK to maintain its international position for those research areas that need access to capability computing.

The scientific impact of the Tier-2 facilities has already been significant, with each facility featuring in an average of more than 100 grant applications totalling nearly £50m and its use acknowledged in at least 280 publications. The remit covered by these facilities span a wide range of scientific disciplines from life sciences to earth sciences and engineering.

The Tier-2(T2) level of HPC provision is fundamental because it provides a diversity of computing architectures, which are driven by science needs and are not met by the national facilities or universities. This is because the National HPC Service must meet the needs of the whole UK community and so cannot specialise in specific novel architectures or novel requirements. The
different types of computing requirements provided by Tier-2 include high-throughput and GPU computing and are supported by local expertise in these areas.

The T2 layer also provides easy access through a light touch review process for users, a rapid turnaround in experiments and allows small compute runs to be carried out which are not suitable on a national machine. It also enables researchers to carry out proof of concept studies which can in turn help users to migrate to the National Facility ARCHER.

**Case Study: ARCHIE-WeSt Regional Centre - Developing State-of-the-art Desalination Processes using Molecular Dynamics**

Water scarcity is a major and increasing problem in both developing and developed countries. The United Nations estimate that by 2050 four billion people in 48 countries will lack sufficient water.

As 97 percent of the water on the planet is saltwater, large-scale technologies to make seawater, or other contaminated water, drinkable are therefore urgently needed.

Until recently, the tools to understand and model the molecular processes just did not exist. However, these tools are currently being developed at the University of Strathclyde and are underpinned by the ARCHIE-WeSt High Performance Computer to design next generation membranes.

These new nano-materials will deliver clean water for future generations with a smaller energy footprint. This will be achieved through molecular engineering to exploit nanoscale fluid phenomena in order to generate ultra-efficient membrane designs, which will essentially function as molecular sieves.

The Tier-2 centres are available to multidisciplinary researchers from across the UK. An important feature of the T2 level is that it provides local access, training and support for users. Therefore, the centres have the ability to broaden access to researchers new to HPC for example certain science communities or universities that do not have access to local resources.

After the EPSRC’s initial investment in this layer of HPC in 2012, this infrastructure now needs to be refreshed and reinvigorated to ensure that it continues to be fit-for-purpose in the rapidly changing e-infrastructure landscape over the next 4-5 years. Tier-2 HPC forms a vital part of an integrated e-infrastructure landscape. The continuation of a sustainable and cutting edge e-infrastructure ecosystem is vital in allowing EPSRC to deliver its Strategic Goals and support excellent and innovative science and engineering research.
During 2016, EPSRC invested over £20m in a new layer of Tier 2 HPC provision, including novel architectures, regional support and a world-leading ARM-based testbed in partnership with a commercial HPC provider.

A coherent strategy for developing and delivering the UK’s next Tier-2 HPC ecosystem is essential in driving forward advancements in computational science in the UK because it provides the diversity of architectures and easy access routes needed to do a diverse range of science. Tier-2 HPC is an essential component of an integrated e-infrastructure landscape, and is vital for maximising the benefits obtained from both national and local facilities. It enables integration both vertically from Tier-3 to Tier-1 and horizontally, between other Tier-2 centres.

Our vision is to work towards a diverse and flexible UK Tier-2 HPC provision with the capability and capacity to meet the scientific needs of the academic and industrial computational science community. The diverse computational science needs and user requirements, including the range of compute job shapes and sizes, needs to be met. In addition, we have a goal to enable researchers to future-proof their research in relation to new and emerging hardware architectures for the future.

Our goal is for T2 to encourage and widen participation from new users and those from different disciplines to access the service. We recognise that this cannot be achieved without building up support and expertise in software engineering skills and training for computational science. We will work towards a Tier-2 layer that is integrated with the HPC ecosystem across the UK, both vertically (into tier 1 and tier 3) and horizontally across to other tier 2 hubs.

Furthermore, the T2 layer should provide comprehensive national access for researchers within the UK which is driven by scientific need and location of expertise and is not defined by region. The evolving Tier-2 ecosystem will be enhanced by the sharing of expertise and collaboration between centres.

Key Features

- A landscape of diverse hardware architectures throughout the UK. This is in recognition of the need for a diverse range of hardware architectures to support the different requirements of the computational science community. These different architectures will also help to shape future Tier-1 systems for the UK.
- Encouraging skills and expertise in software engineering to support the range of T2 architectures which will be available in the UK.
- Investing in a number of individual Tier-2 hubs, which are located in the most appropriate area for a particular technical expertise or scientific need; this could be hosted by a consortium e.g. technical or a single institution.
- Encouraging easy access mechanisms to the whole Tier-2 layer, which allow access to researchers, both local and UK wide, and which encourages access by new users and disciplines.
- Encouraging industrial collaboration and use of T2 HPC where appropriate.
- Investing in Tier-2 Hubs that enable multidisciplinary computational science but with the centre of gravity in the engineering and physical sciences remit.
- Encouraging a community within the Tier-2 ecosystem that shares expertise.
• Encouraging future proofing and sustainability of codes by enabling access to new hardware architectures.
• Encouraging a Tier-2 layer that is integrated with the HPC ecosystem across the UK, both vertically (into Tier 1 and Tier 3) and horizontally across to other Tier 2 hubs.
• Encouraging sustainability of an agile, flexible and responsive Tier-2 provision which is able to meet the evolving needs of the computational science community.

**Case Study – Training at Regional Level**

The regional centres are adept at providing local training with international impact. An example is the ARCHIE-West consortium which has provided specialist training to software experts from industry and academia attracted to the specialist training.

Delegates have come from as far afield as the USA, France, Germany, Italy and Romania, providing a valuable additional income stream to support the research.

They study the highly dilute gas conditions which are encountered in a wide variety of technological applications including hypersonic spacecraft design, planetary and astrophysics problems and manufacturing processes in near-vacuum environments.

The dominant numerical technique for such rarefied gas flows is the direct simulation Monte Carlo (DSMC) method.

The image shows Oxfordshire company Reaction Engines’ Skylon spacecraft re-entering the Earth’s atmosphere at Mach 25 and 105 km altitude.

The contours are of linear kinetic energy and were calculated on Archie using the DSMC code *dsmcFoamStrath* developed at Strathclyde.

Although Regional HPC centres did not exist before 2012, the level of computing provision they offer is vital for the UK to achieve an efficient and effective e-infrastructure ecosystem in terms of investment and research outputs. Continued investment to exploit technology advances at all levels of the ecosystem is required to continue upskilling the whole pipeline and ensure researchers using the National Service are continuing to leading the world.
1.7 Continuity and Competitiveness

Since 2007, computational research has become ever more important to the research endeavour. The e-infrastructure ecosystem has developed and evolved and the UK ecosystem now gives researchers access to a wide range of hardware, software and training resources/support. All these resources are being exploited by computational researchers; and new user communities, who would not have used HPC 5 years ago, continue to develop and explore the potential that HPC can unlock.

Between 2007 and 2014, the national computing service ‘HECToR’ (High End Computing Tera-Scale Resource) provided the UK academic communities with computing speeds that initially placed the UK firmly in the top 20 fastest world systems in November 2007, while this £118m phased investment had a user base from over 250 organisations generating over 60 new innovations.

However, by 2013, HECToR had slipped to 50th place in the world’s top systems, coming under renewed pressure from the USA and China. Since 2013, the £23m national supercomputing service ‘ARCHER’ (Academic Research Computing High End Resource) has carried on the tradition of UK-based world-leading high performance computing when ARCHER entered the top 20 and maintained its position with a £10m upgrade in 2014 (as of the end of 2015, it is 41th).

The current ecosystem has enabled the UK to punch above its weight against global competition. For example, the science carried out on the previous national service HECToR was of very high quality with over 800 HECToR-enabled academic publications receiving 2.5 times more citations than the UK average, which is already higher than the world average.5

HECToR publications were also twice as likely as the UK average to be in the top 5% of papers in their fields. However, it takes some years before publications are produced and cited, so the impact of ARCHER cannot yet be quantified.

---

With such momentum behind HPC, the pipeline of research and software development is in full flow. We must consider, however, that the consequences of restricting funding for future investment will starve not only future research programmes, but jeopardise work done today.

This report underlines the case for future support of HPC and supplies incontrovertible evidence that the work of HPC is essential to science and a scientifically productive and prosperous nation.

In this new age of ‘Big Data’, HPC gives us the power to make sense of the avalanche of new information. Exploiting these advances will ensure that High Performance Computing can continue to have a direct and indirect impact on all aspects of our lives.

It is now the UK’s chance to recognise the importance of HPC nationally where an investment in HPC is an investment to secure the UK’s future. To realise the ambition of a healthy, connected, resilient and productive nation, we require long-term investment in HPC which includes technology refresh points to ensure the UK is internationally competitive and is a focus of global envy. We have a vision for a long-term and sustainable investment programme to support and maintain HPC for UK science and the following sections illustrate how this will enable new and ground-breaking science for the UK economy.

1.8 Technology Challenges and Opportunities

Many technological advances and benefits have been made possible through the use and application of HPC. Over the last 20 years, the computational power of the world’s fastest computers has increased by a factor of over a million, meaning that routine systems in use in industry and research far outstrip the power of the top machines of only a few years ago.

However, we are approaching a number of limiting factors in the technology and this means that future HPC provision will need to work smarter, as well as harder. For example, ever larger machines
require ever larger amounts of energy to power and cool them. This is often the limiting factor when planning and budgeting for new systems.

In addition, processor speeds are approaching the limits of current technology and are not expected to provide the predictable speed increases in future as they have done in the past. In order to make maximum use of the fastest processors, users will need to apply their codes in a different way on machines which are structured differently – the need for much greater parallelisation.

The future of high performance computing will not be a linear extension of the behaviours, technologies and performance we have seen over the last 20 years. We need to work with the users, vendors and software developers to prepare ourselves for future technologies and architectures.

While we are able to delve deeper into ever more complex problems, there are many issues to overcome in order to enable codes to scale effectively and thereby make most efficient and effective use of massive HPC resource.

While the major economies of USA, China and Japan scramble to lead the pack with the world’s fastest computer, of greater importance to the UK is to have an infrastructure that supports and enables the most valuable scientific results.

HPC has the power to make major impacts in industry and society. These are laid out in the second part of this document, where we explore the impacts of HPC in enabling a productive nation, a healthy nation, a connected nation, a resilient nation, a sustainable nation and a globally responsible nation.

---

**Case Study: Rolls-Royce and the National Service**

- Rolls-Royce took the opportunity of access to ARCHER to test the scaling of their codes for a variety of applications; fluid dynamics, noise, combustion and a structural model of a full engine test rig.
- Over the next 20 years air passenger traffic is forecast to increase by 5.2% p.a. and the world fleet is expected to grow by 3.6% p.a.
- Rolls-Royce is a major player in this market with an annual UK R&D spend over £800m and a total impact on UK GDP of over £10.2bn.
- Scaling is important for Rolls-Royce to ensure they can meet their design timescales and they were able to run at much longer time and larger scales on ARCHER.
- Access demonstrated the art of what was possible for Rolls-Royce and has set their computational science and engineering roadmap for the next 2-3 years.
Many HPC applications use so-called ‘legacy’ codes, which have been in use and in development over a period of many years. These are best used on particular HPC technologies, but are ill-prepared for disruptive HPC architectures. There is a considerable challenge in evolving these codes to take maximum advantage of new HPC.

In order to support the vision of a sustainable HPC infrastructure, we will need to invest in energy-efficient hardware and ensure that programming models, languages and methodologies are developed to increase productivity of those systems.
1.9 People and Productivity

The power of HPC does not just unlock academic potential but also transforms business. The UK HPC ecosystem contains the Hartree Centre which has an industry focus. However, the National Service can provide the tools to enable university-industry collaboration. This encourages knowledge transfer between universities and their industrial partners and the deepening of strategic research relationships. The work carried out on the National Service with industrial partners is precompetitive in nature and therefore fits within the wider UK e-infrastructure landscape.

Case Study: Research Software Engineers

- Research Software Engineers are the vital people who develop software for research.
- They form a fundamental part of the research endeavour but are rarely appropriately recognised, nor have a clearly defined career path.
- They ensure appropriate HPC resources are accessed and software isn’t developed that already exists.
- In 2015 EPSRC ran a pilot call for RSE Fellowships and invested over £3.5million in supporting 7 Fellows over 5 years.
- Support for an RSE Network has also been provided to help continue the fight in getting this important sector of the workforce recognised and retained where needed.
- The role of the RSE is key to enabling good science – they improve the software that enables better science.

The Research Councils have an established track-record of enabling partnership working between academia and industry. In 2014/15 EPSRC-sponsored researchers worked with over 2,200 organisations of which 60% were SMEs.

EPSRC also have 19 strategic partnerships with industry leaders such as BAE Systems, Dyson, GlaxoSmithKline, Jaguar Land Rover and Rolls-Royce who extensively use HPC internally.

Research and development carried out in partnership on the academic e-infrastructure is routinely transferred to industry and leads to increased productivity within the company. Technology transfer to industry is further supported by people transfer and an essential component of the UK’s e-infrastructure ecosystem is to provide a highly skilled workforce for the country. This increase in productivity is demonstrated at the European level where HPC investments are producing excellent returns-on-investment (ROI) for science and industry. In 2014, IDC captured detailed ROI information on 143 European HPC projects.

For projects that generated financial returns, each euro invested in HPC on average returned €867 in increased revenue/income and €69 in profits. It also found that where an HPC investment had been made, it generated on average, 29.8 new jobs at every site.

---

HPC is ubiquitous in science and evermore becoming an indispensable tool for today’s research programmes. It also delivers a highly skilled workforce who provides a competitive edge to their companies and thus an economic benefit from HPC for their companies and the wider economy. The importance of being at the cutting-edge of HPC has been recognised by the United States of America when President Obama announced his Executive Order of July 29th 2015 on “creating a National strategic computing initiative”.8 Through the Executive Order, the USA is preparing to exploit emerging technologies and build the foundation for U.S. leadership for decades to come, and ensure high-performance computing can meet the pressing challenges faced across many sectors.


Case Study: Women in HPC

- EPSRC supported the Women in HPC initiative and have been working with EPCC (current providers of the National Service) to improve the diversity in HPC.
- Events have been held at ‘Supercomputing’, the premier HPC conference in the world and UK researchers have played a key part in raising awareness across Europe.
- In 2015, the University of Edinburgh initiative won the Women in HPC: Readers’ Choice Award for Leadership in Workforce Diversity.
- “We are very honoured to receive this recognition from our peers within the HPC community and the editors of HPCWire. We started this organisation to bring awareness to the lack of diversity in the technical fields in the UK. We are thrilled that we are receiving international recognition for our efforts.” Alison Kennedy, Women In HPC Executive Director and EPCC Executive Director.

Case Study: Making High Performance Computing resources more accessible

- The development of the software package SPRINT (Simple Parallel R INTerface) has allowed bioinformatics researchers to exploit the power of High Performance Computing.
- The Software Sustainability Institute (funded by EPSRC, BBSRC and ESRC) helped achieve this by developing the programme in the preferred coding language of R and improving user engagement between the development team and users. This led to the development of better resources and support functions.
- Training courses were then held on the national supercomputer HECToR.
- The software is now producing so much data, so quickly that new filtering methods are needed to cope. Bioinformatics research has well and truly been supercharged.
Centres for Doctoral Training (CDTs) are one of the three main ways by which EPSRC provides support for Doctoral Training. EPSRC-funded Centres bring together diverse areas of expertise to train engineers and scientists with the skills, knowledge and confidence to tackle today’s evolving future challenges. They also provide a supportive and exciting environment for students, create new working cultures, build relationships between teams in universities and forge lasting links with industry.

Students are funded for four years and include technical and transferrable skills training, as well as a research element. Many Centres leverage additional studentships from other sources (eg university funding, EU funding, industrial funding, private funding etc).

Within these EPSRC Centres for Doctoral Training9, over half of the 117 Centres are involved with aspects of computational science, representing over 750 individual projects. Over 50% of the centres questioned said that computational science was ‘core’ or ‘important’ to their research.

NERC research using HPC is frequently used to support Government and the public sector. High resolution global and regional climate projections support DECC’s input to the Intergovernmental Panel on Climate Change. Severe weather and flash flooding models support the Natural Hazards Partnership, the Met Office, Environment Agency and DEFRA. Complex models of the chemistry of atmospheric pollutants support Defra in understanding and developing actions to mitigate against pollution levels in cities which threaten public health. Common to all these impacts is the critical role of HPC is enabling computational models to be run at resolutions which are beginning to capture the key physical processes and the scales of impact on human activity.

9 https://www.epsrc.ac.uk/skills/students/centres/

Case Study: Novel Coatings for Gas Turbine Power Generation

Gas turbine engines are widely used in industrial power generation. These engines require materials which can withstand high temperatures and aggressive operative environments. Nickel-based superalloys are employed for turbine blades, but increasingly rely on the performance of coating systems for high temperature degradation protection.

This project, involving over a dozen academic and industry partner organisations, simultaneously modelled and experimentally characterised the environmental degradation of selected coated turbine blade systems in order to improve life prediction and failure assessment methods.

The predictive techniques and data generated are already being used to aid design, quantify operational risks, and improve component inspection, repair and replacement in operational environments.

“With respect to industrial gas turbines, the rate of degradation of oxidation coatings on nickel-based superalloys reported by the Supergen project has already been incorporated into materials selection decisions.”

Jon Wells, RWE npower

---

9 https://www.epsrc.ac.uk/skills/students/centres/
Case Study: Global synthetic weather on PRACE HPC resources†

- Hurricanes evolve and grow from local sea and air conditions. Simulating hurricane climate (where, how strong, and how often) depends on being able to resolve small spatial scales over long periods of time.

- The UK National Centre for Atmospheric Science (NCAS) in partnership with the UK Met Office have investigated such high-impact weather by running global simulations at unprecedented spatial scales for many decades – building new understanding of hurricane and storm risk.

- With expertise garnered on UK HPC platforms, the team were able to build and run the relevant simulations on the HERMIT supercomputer in Stuttgart, Germany, via an allocation of time from PRACE, using - in one year, 2013 - the equivalent of over two months of full-time use of the more modern ARCHER.

- One year of simulations produced 0.4 petabytes of data, moved to, and analysed on JASMIN, the equivalent of a third of the output which the entire global modelling community contributed to the archive underpinning the fifth IPCC climate assessment report.

- These data are stored on JASMIN and will contribute to scientific and industrial impact for many years to come.

PART II - A PROSPEROUS NATION

2.1 EPSRC and NERC Science

EPSRC and NERC have identified inter-linked Outcomes which collectively underpin UK prosperity: Productivity, Connectedness, Resilience, Health, Natural Resources and Environmental Change. These Outcomes form the framework for EPSRC’s Delivery Plan (2016-2020) and NERC’s strategic direction *The Business of the Environment*, together reflecting the contribution of the whole portfolio of investments. High Performance Computing touches all parts of the portfolios of the two Research Councils and therefore these Outcomes form the backbone of the science case. We have a vision for one nation of science, but a number of different aspects to achieving that vision.

Investments made in HPC directly lead to impacts in the HEI sector and more widely.\(^{10}\)\(^ {11}\) The economic impacts leading from HPC investments have been extensively explored and, in all cases, it is concluded that the ability to invest in HPC leads to a greater return on that investment and significant savings on research costs.\(^ {12}\) The ability to model complex experimental possibilities in the processors of a computer means savings in consumables and experimental equipment. Added to this, there is a massive gain in efficiency by the ability to tweak a few variables in the software and run a whole new experiment.

This is particularly relevant in climate modelling. The ability to run a model many times and subtly change the operating parameters gives researchers new insights into how our climate behaves. Other examples are outlined in the following section to illustrate how HPC supports a prosperous nation. In each case, there is a momentum towards future research challenges that will require the greater computing power and efficient software of tomorrow.

The following sections give more detail on each of our ‘One Nation’ idea for High Performance Computing.

---

10 http://www.theregister.co.uk/2015/03/25/does_your_university_need_hpc_it_depends_on_disciplines/
12 “Creating Economic Models Showing the Relationship between Investments in HPC and the resulting Financial ROI and Innovation”, IDC, 2013
2.2 – One Nation, Many Views

A Productive Nation: A creative, innovative, competitive economy.

Understanding Products from Atoms to Application - Using HPC to enable science to delve deeper into the atomistic structures of matter and support industry develop new applications.

A Connected Nation: Surviving and Thriving in a Digital World.

Understanding Connections from Individual to Global – We’re reaping benefits from HPC codes that allow scientists to combine theory and experiment to make our world safe and secure for people and business.

A Resilient Nation: Adaptive, prepared, protected, secure, safe, sustainable.

Understanding Resilience from Systems to Society – We’re developing HPC codes to predict and prepare cost-effective and robust solutions to protect ourselves, our infrastructure, our society and our planet.

A Healthy Nation: Improved quality of life through better mental and physical health.

Understanding Health from Molecular to Population – We’re enabling scientists to use HPC to design and develop innovative healthcare technologies on a molecular level and apply the solutions to benefit the whole population.

A Sustainable Nation: Responsible use and management of our water, energy, minerals and ecosystems

Understanding Environmental Processes from Nature to Industry – We’re discovering how HPC can help us predict the consequences of exploitation and help us develop more sustainable use of our natural resources.

A Globally Responsible Nation: Managing Environmental Change

Understanding the Impact of Human Activities on our Planet – We’re using HPC to distinguish between natural variability and human induced change, so as to manage the environment responsibly and limit future adverse consequences of human activities.
2.3 NERC – Business of the Environment

The environment is everyone’s business. We depend on it for shelter, heat, light, food and water – all provided by globally interconnected trade, transport and communications. At present the world’s population is growing by around 1 billion people every 12 years. More than half of us live in cities and more than half the countryside is used for agriculture. The way we live has changed our relationship with the environment. People are no longer bystanders examining a natural world; we are the dominant source of change.

People aspire to escape poverty and improve their living standards. Achieving this whilst living within the Earth’s limits is the great challenge of the 21st century. NERC and the scientists we fund play a critical role in meeting this challenge.

NERC’s strategy, science and funding decisions will be built on partnership. We will work with business to support UK ambitions for growth, resilience in a changing world, and responsible management of the environment.

Managing our environment demands ever-increasing sophistication. NERC has been a custodian of the 20th-century environmental record. Now we will harness the rapid development of information technology to open the record to the wider world. With partners we will use our data and knowledge to develop products and services that directly address the needs of business, government and society.

Case Study: Safety at Sea - Oil and Gas Rigs

The safety of oil and gas platforms in the North Sea depends on knowledge of the risk from extreme wind and waves.

Platform operators have only two to three decades of observations with which to estimate their risk.

NCAS and University of Reading have together been exploiting massive ensembles of high-resolution HPC model simulations to provide over 1,200 years of simulated wind to assess the return period of high-risk extreme events. These risks are then used to provide operators with information to determine their platform design criteria.
2.3.1 Benefiting from Natural Resources.

Natural resources sustain life, wellbeing and economic activity. Yet growing UK and world populations make ever greater demands on food, water, energy, minerals and other essential services we get from nature. All natural resources are derived from physical, chemical and biological processes that interact in land, water and air. NERC science tells us how these environmental processes control resource availability, and how we can use resources responsibly. This knowledge will help us use and recycle resources safely and efficiently, live within the Earth’s limits, and steward natural resources for future generations.

Case Study – Oil and Gas Exploration

Each year the oil and gas industry is worth £30 billion for the UK economy, supporting 440,000 jobs.

The distribution of these natural resources depends on geological processes that create the ocean floor and the continents. NERC investment since the 1970s, now £12 million each year, supports the science that developed new geophysical imaging tools to understand how tectonic forces shape the Earth’s crust, how sedimentary rocks form in basins, and how fluids flow through underground faults and sediments. Now powerful HPC codes can show these forces at work and permit better modelling and prediction.

This science helps us find and extract energy and minerals ever more safely and efficiently. Over the last 50 years it has fuelled enormous growth in the energy industry – no other sector has created more prosperity for the UK.

NERC geological science is paving the way for geothermal energy and shale gas to reduce our dependence on coal and oil, and for storing our carbon emissions in empty oil and gas reservoirs.

2.3.2 Resilience to Environmental Hazards

Extreme weather, volcanoes, earthquakes, space weather, pollution, novel diseases and invasive species all have serious impacts on people, supply chains and essential infrastructure in the UK and internationally. Many such hazards are becoming more frequent and severe as our environment changes and as populations and cities grow.

NERC scientists are rapidly advancing our understanding of the processes that create natural and man-made hazards, so that we are better equipped to manage vulnerability, risk, response and recovery.
2.3.3 Managing Environmental Change

Some environmental variability is natural, but human activities are directly causing additional physical, chemical and biological changes – often at scales and speeds never before encountered. These changes provide huge opportunities and challenges for our economy and way of life.

NERC science tells us how the processes of natural variability and man-made change work – as a whole Earth system, from global to local scale, from millions of years past to the present and into the future. We will help our partners use this whole-system knowledge to inform responsible management of the environment for multiple benefits – for example to produce renewable energy and food while conserving wildlife, or to understand the consequences of engineering our environment and climate.

Case Study – Flood Prediction

NERC data and risk models are used by UK and local governments to predict flood events and to plan major infrastructure investments – saving lives and minimising disruption for people, business and the economy.

Rising sea levels and more frequent storms increase the risk of destructive coastal floods. NERC scientists have analysed UK sea level, tide and storm surges for more than 50 years, and used the data to build a computer model that predicts coastal flooding. In 2007 their model accurately forecast the worst storm surge in 20 years, enabling authorities to protect people and infrastructure at proportionate cost.

The same model feeds directly into the Thames Barrier control centre. Closing the Barrier protects thousands of lives, safeguards £4 billion of property and business, and avoids £94 million costs per flood day in London.

Predicting sea-level rise, storm surges and river flows over the coming decades now enables us to delay replacing the Thames Barrier until 2070 – avoiding billions of pounds in premature infrastructure costs.
2.3.4 Discovery Science

Many of the greatest advances in environmental science have been driven by curiosity. The quest for new knowledge about the planet we live on has fascinated and inspired generations of scientists, and it continues to do so. We call this ‘discovery science’ – asking fundamental questions about how the Earth works: past, present and future.

Curiosity-driven environmental science has, throughout its history, delivered benefits to society that were unforeseen when the research began. We will help our partners turn the outcomes of discovery science into lasting benefits for our economy and society.

**Case Study: Flash Flooding and Dam Over-Topping**

Flash flooding occurs in the UK when severe convective storms (e.g. thunderstorms) persist over areas where run-off is channelled by topography. This can lead to danger to life and severe damage to property (for example Boscastle flood 2004, Boltby spillway failure 2005, Ulley spillway failure 2007).

Better understanding of the processes leading to severe, stationary storms is necessary both for better assessment of risk and better forecasting of dangerous events.

The key to better process understanding and predictive capability is the development of very high resolution models incorporating the most significant turbulence, cloud and precipitation processes within the storm.

HPC has been used to analyse in detail past flash flooding events, leading to a deeper understanding of potential future risks and improved ability to forecast in the future.
PART III – ONE NATION

The following sections give more detail about the different aspects of a science-driven nation and how HPC is delivering real results and impacts across many aspects of 21st century UK.

From manufacturing to music, from data to diseases, HPC is enabling greater advances in science than ever before.

The Research Councils have a strong record of supporting HPC and computing infrastructure stretching back nearly 25 years. The current ARCHER service represents an investment of over £43m in capital alone. Its impacts on the whole of the engineering, physical sciences and environmental sciences national research programmes are huge – virtually all the sciences rely on the ability to compute, manipulate or analyse data.

A fracture in the investment programme jeopardises not only the UK’s world-beating research record, but also the careers of many trained people. In the same way that a fracture in the earth’s crust leads to earthquakes, a crack in the continuum of HPC funding will lead to seismic effects in the UK’s proudly held record as a leading nation in which to do research.

By recognising the impact of HPC on our modern world, we can show that HPC is a vital tool in enabling scientific advances and the impacts and outputs of that research.

Without a strategic programme of long-term investment, there is a real risk that the advances will be curtailed and the UK will be overtaken by nations with a strong high performance computing infrastructure.

Figure 7 - Developing State-of-the-art Desalination Processes using Molecular Dynamics, page 14.

Figure 8 (above) - HPC Midlands developing modelling capable of improving life predictions and reducing in-service failure for composite material parts.
3.1 A Productive Nation

High Performance Computing not only enables us to become a productive nation, but it can also help us to predict and model the future, protecting us from becoming unproductive. It gives us the ability to eliminate costly trial and error, through the development of tools such as virtual prototyping. To be without HPC would not only make us less competitive in the here and now but would cut us off from future discovery.

Materials

The descriptor of ‘materials’ covers a huge range of engineering and industrial substances, from nanowires to concrete; from smart plastics to engineered armour plating. This explains why much of ARCHER’s awesome power is given over to understanding and researching materials.

The research challenges we face are consequently equally broad. At one level, we begin by understanding how atoms join together to build molecules and how those molecules assemble to form materials on the macroscale. Once we have our material, we need to understand how it behaves and how its properties can be utilized in applications. For example, understanding how new polymers behave can have applications in developing safer vehicles, while understanding how novel photovoltaic films behave can lead us to the production of new, more efficient solar cells. By modelling these systems using HPC, we can tweak aspects of their characteristics in virtual space and optimise their properties. The ability to take these results and actually predict how as yet undiscovered materials will work saves uncounted hours of experimental trial and error and the associated experimental costs as well. The ability to design our materials also enables us to make more sustainable manufacturing decisions, as we can build in recyclability to the materials we design.

For example, HPC will help us to develop better materials for diverse applications such as bulk data storage, drug releasing materials, antibacterial materials, low wearing medical implants, energy storage, catalysts for industrial manufacturing processes and even make low-calorie chocolate retain the texture and taste of high-calorie chocolate.

The ability to predict how, when and why a material fails under stress is an important part of providing a safe and secure transport infrastructure and can have applications in aircraft to bicycles.
The question of ‘scale’ is often talked about in HPC circles with respect to size and time. In materials, we need to simulate and couple atomic behaviour to larger mechanical behaviour while also considering the timescales of these processes that cover ranges from less than a billionth of a second to potentially years. This is coupling across scale and time is one of the greatest current challenges within computational research.

**Case Study: Molecular level understanding of catalysis**

- Catalytic processes underpin the chemicals and pharmaceuticals industry and are responsible for the generation of products to the value of £50 billion per annum by UK industry and over £200 billion within the EU.
- The development and application by teams at UCL and Johnson Matthey of a powerful range of computational techniques has had a major impact on the understanding of catalysis at the molecular level.
- The use of this approach in industry has had impact on the development and optimisation of key catalytic systems used in energy, environmental and fine chemicals production.

**Case Study: Atomic modelling of new batteries**

- The use of a powerful range of computer modelling techniques on ARCHER by teams at Bath has had a major impact on our understanding of new battery materials at the atomic level.
- The use of this approach has had impact on the development and optimisation of key electrode systems used in rechargeable lithium- and sodium-ion batteries.
- The studies have been performed in collaboration with Sharp and Johnson Matthey, promoting a more science based approach to battery development.

**Computational Fluid Dynamics**

The science of CFD is applied to a plethora of difficult scientific challenges. It describes the flow and mixing of liquids or gases on a molecular or macro scale. It lets us better understand diverse problems like how air flows around buildings or cars and model how fuel combusts in a jet engine. It can tell us where to site wind or marine energy turbines or how an important chemical process can be made more efficient.
In today’s commercial world, a competitive advantage can be achieved by a small efficiency gain. With much of world trade carried by sea, the design of improved ships’ hulls and propellers can lead to lower emissions, faster ships and quicker deliveries. Even in the cutthroat world of Formula 1, HPC is being used to shave milliseconds off a lap time by modelling air flow around the car.

**Case Study: Improving chemical process efficiency**
- To mix effectively and economically is a big problem in many industrial settings ranging from the food industry to the petrochemical industry and pharmaceuticals industry.
- EPSRC funding through the UK Turbulence Consortium and HPC simulations are making it possible to design optimised energy-efficient mixers using fractal grids and blades.
- This work is now an essential part of a 3.8M Euro EU grant involving industrial partners such as Sulzer Chemtech.

**Case Study: Helping McLaren Racing take on the World**

*ARChER has boosted the international competitiveness of UK engineering via academic partnerships with McLaren and the supersonic Bloodhound car.*

In the world of Formula One a tenth of a second is everything. Key to fractional speed gains is an increase in aerodynamic downforce. Professor Spencer Sherwin, of Imperial College London, has worked with McLaren for the last decade. He used HECToR to develop a more precise tool for simulating the flow of air around a vehicle that will enable McLaren’s engineers to reduce turbulence and make their F1 car faster.

Sherwin said: “In Formula One competitive differentiation is measured in milliseconds. When you consider that only a two per cent performance gap exists between the top ten teams and a mere 0.3 per cent between the top three – you begin to appreciate the difference more accurate simulations make.”

“Here at the Royal Academy of Engineering we recognise the crucial importance of e-infrastructure to the high-impact engineering research we support, such as the Sherwin-McLaren collaboration. EPSRC provides access to state-of-the-art national computational facilities where the researchers we support can develop the next generation of software for future use by UK companies such as McLaren Racing.”

Robert Barrett, Royal Academy of Engineering
The benefits of CFD research is not limited to those building or operating machines, it can also predict how to make quieter, efficient jet turbine engines reducing noise levels in the community. HPC has been used to model a single turbine blade as it rotates in the compression chamber and advances in computing power now enable all the blades in an engine to be modelled. This permits a greater understanding of the air flow, combustion process and thus noise levels.

**Case Study: Designing environmentally friendly aircraft engines**

- By 2025 air travel will result in around a billion tonnes of annual CO₂ emissions. Urgent action is needed to reduce the impact of air travel.
- The low-pressure turbine is an important component in commercial aero engines. A better understanding of the flow physics is essential to make this key component more efficient and hence environmentally friendly.
- HPC has enabled eddy-resolving simulations to be carried out that are impacting on the design systems of Rolls-Royce.

In future, with sufficient computing power, we will be able to model the whole engine; its mechanical behaviours, the combustion process and flow of air and fuel. This is an example of scale; where the software can be utilised on more powerful HPC machines to model increasingly large and complex systems. Connected to data manipulation and visualisation, HPC provides an essential tool for industry – not only in modelling, but as a tool of discovery.

The petroleum industry is driven to increase its efficiencies in production and exploration. Scientific disciplines from geo-science to engineering, from fluid dynamics to plant design all contribute to this multi-billion dollar industry. Deep Casing Tools Ltd, an SME based in Aberdeen, has used HECToR to develop innovative products and be a leader in their sector.

**Case Study: Deep Casing Tools Ltd and HECToR**

- Focus on innovative design combined with precision engineering to develop the next generation of casing and completion tools for the oil and gas industry.
- The Turbocaser uses a motor powered by drilling-mud to ream oil wells prior to pipe installation.
- Important to optimise the performance of the advanced multi-stage motor. Have used HECToR to model the mud flow through various Turbocaser turbine designs.
- Allowed the company to validate the basic design and optimise the pressure drop versus torque across the multistage turbine.
3.2 A Connected Nation

In today’s data-driven and cyber-world, society depends on secure, safe and reliable connectivity. In many ways, HPC lies at the centre of this digital industry. It is estimated that the amount of data generated every day is 2.5 Quintillion bytes\(^{13}\) and by 2020 it is predicted to be 4300\% more than 2009 levels, reaching 35 Zettabytes by 2020 (1 zetabyte is a million million gigabytes)\(^{14}\). Increasingly, HPC allows science to make sense of this data and utilise its patterns to make us a more prosperous and effective society.

The exchange of data and using those connections can lead to new discoveries and insights into complex data and systems. Big data comes in many different forms and HPC can be used to analyse this data, such as the BBC’s music archive where HPC has been used to characterise the music by mood.

Case Study: In the Mood for Music

- The BBC plays over 200,000 different pieces of music every week.
- With so many to choose from they need to be able to quickly navigate the digital music archive over millions of songs.
- Working with Queen Mary University of London, I Like Music and N8 HPC, BBC Research & Development produced software that can classify tracks based on tempo, key and more than 36,000 keywords.
- The power of N8 HPC reduced the time taken for analysis from 1.5 years to just six hours.

Faced with complex data and scientific problems, there is much work to do to quantify uncertainty and ensure that the predictions made from the data are reliable and robust. HPC can crunch through the numbers and give science the assurance and confidence in its predictions. For example, combining data in real-time is needed for autonomous vehicles and HPC can give greater accuracy in processing of sensor data.

As technology advances, the HPC systems of today will be the standard laboratory tools of tomorrow. We have seen this occurring in present-day science.

---


\(^{14}\) [http://www.csc.com/insights/flxwd/78931-big_data_universe_beginning_to_explode]
programmes. Computer systems that previously were exclusive to big science are now routinely packed into ships and planes and used to study the oceans, atmosphere and the planet on which we live in greater detail than ever before. The supercomputers of tomorrow will one day be the mobile phones of the next generation but to enable these advances we need to invest in future supercomputer technology today.

Case Study: Modelling Buildings in their Environment

- Integrated Environmental Solutions (IES) is a Scottish SME benefitting from collaboration with EPCC.
- IES are the world’s leading provider of software and consultancy services which make the built environment more energy-efficient, reducing overheads and CO2 emissions.
- Buildings do not exist in isolation but are connected to their environment, therefore it is essential to model the environment the building sits in as well as the building itself.
- EPCC have helped IES to exploit the performance from parallel processing, reducing time-to-solution for a typical customer from several hours to less than one hour.
- One calculation that used to take 2 weeks can now be run on a small supercomputer and be complete in a matter of minutes.

As we are able to delve deeper and deeper into complexity, mathematics of topology and geometry are used in new ways and the software behind the models must continue to develop in order to address these more complex challenges. This is particularly true as the Internet of Things grows and more and more sensor networks are deployed and start to send data back for analysis. The city of the future may be a smart city but this will only happen if the sensor data can be analysed and actioned upon in a rapid manner.

Case Study: The Alan Turing Institute

- Supported with £42 million of government funding (via EPSRC) and £25 million from the five university partners the Alan Turing Institute will be a national focus for the development and use of advanced mathematics, computer science, algorithms and big data for human benefit.
- The ATI have already announced strategic partnerships with Lloyd’s Register Foundation (£10 million) and Intel.

- As the ATI develops their scientific agenda one area under consideration is the impact advanced mathematics and algorithms can have on the financial sector, including financial modelling, risk/insurance and trading.
- Finance is closely coupled with HPC and advances made by the ATI will have significant impacts on the world of Finance and HPC.
Many of the advances needed to produce a connected nation will come from fundamental developments in algorithms. The UK has a deep and rich heritage in algorithm research which continues to this day and which we need to capitalise on by continued support of these researchers.

**Case Study: UK leading the World in Algorithm Developments**

- Dr David Ham (NERC Independent Research Fellow and Lecturer at Imperial College London, left) and Dr Patrick Farrell (EPSRC Early Career Fellow at the University of Oxford, right) were part of the team that won the Wilkinson Prize for Numerical Software, 2015.

- The prize is awarded every four years to the entry that best addresses all phases of the preparation of numerical software; the recipients are authors of an outstanding piece of numerical software.

- The award winning work was for their dolphin-adjoint software which enables the study of the sensitivity and stability of physical systems and the optimisation of designs subject to constraints.

- It may be based on a high-level mathematical problem but it has applications across science.
3.3 A Resilient Nation

The capacity of HPC to take data and make predictions is one of the most powerful applications of the raw computing power. To become a truly resilient nation, we must ensure a reliable infrastructure which underpins the UK economy, develop solutions to threats, mitigate climate change and achieve energy security and efficiency.

HPC allows us to model and make assured predictions where no experiment is possible or just too dangerous. It is the raw power of HPC that allows scientists to model something as complex and large as the atmosphere on a scale never previously achieved.

Weather predictions are now as accurate at four days as they were at one day in 1980, and our confidence in the likelihood of future global climate change is underpinned by massive amounts of simulation.\(^{15}\)

As our understanding of climate change has increased, so has the need to pull through to advice and policy, but future policy needs require knowledge of regional climate change, and even more investment in HPC.

The ability to predict also allows industry to allocate resources in advance. The UK has a varied mix of energy generators and the ability to model and predict power consumption is key to ensuring a reliable supply to homes and industry. For example, HPC has been used to model large arrays of wave energy generators and the expected power generated from them.

---

\(^{15}\) http://www.metoffice.gov.uk/about-us/who/accuracy/forecasts
The broad range of energy challenges are being addressed by HPC. Research into new and cleaner fuels, the design of wind and tide turbines and materials all impact in the resilient nation. Only supercomputers are able to punch through the mathematics and make the accurate models that can be taken to production.

Defence is a key area where prediction and simulation on HPC means that, where experimentation is impossible, the UK can maintain and assure its nuclear capability, both for energy generation and defence. In energy generation, we can model nuclear reactions and the interior core of reactors while HPC is modelling the potential for fusion power.

---

**Case Study: Simulating Large-Scale Array of Interconnected Wave Energy Devices**

- Albatern is a company developing novel offshore marine devise: buoyant “Squid” modules that can be linked together to form a large “Wavenet” installation.

- Given the number of modules, prototypes of the “Wavenet” are expensive to produce, therefore HPC can help reduce the risk of design flaws.

- The company worked with the National Service, ARCHER, to develop the software algorithms and implement the calculation on an HPC platform.

- The computer visualisations and power generation data produced from large-scale array simulations will greatly improve investor confidence, increasing the chances of securing the vital continued investment required to proceed to utility-scale generation projects.

- This project has the potential to unlock the commercial exploitation of a global market valued at between £60bn and £190bn.

---

**Case Study: Blending biofuel into conventional fossil fuels**

- Blending of biofuel into conventional fossil fuel is an important step towards a low-carbon economy.

- If the boiling points of the two fuels are considerably different it can lead to microexplosions due to superheating of the embedded sub-droplet.

- Through the UK Turbulent Reacting Flows Consortium, researchers from Brunel University London have used the power of ARCHER to investigate microexplosion dynamics for the first time.

- The results will be used to guide the development of accurate droplet breakup models to be incorporated in advanced simulations of spray combustion of complex fuels.
As the world becomes more connected through e-infrastructure it is ever more important that security aspects of these connections are considered and the infrastructure and interactions enabled are secure and resilient. In 2013 EPSRC invested in two cyber security Centres for Doctoral Training at the University of Oxford and Royal Holloway, University of London. These two centres will train over 50 of the next generation of cyber security experts. These students will cover themes ranging from; security of “Big Data”, effective systems verification and assurance and real-time security. These aspects are vital to provide a fully connected and integrated e-infrastructure ecosystem.

**Case Study: Tokamak Fusion Modelling**

- Through the Plasma Physics High-End Computing Consortia, researchers from the University of York have used ARCHER to model how hot plasma behaves at the edge of tokamak fusion devices.
- This is important because the edge region determines where heat and particles are deposited onto the walls of the machine.
- By better understanding this region, this research contributes towards improving the design and operation of future fusion power plants.

**Case Study: Understanding and predicting the characteristics of volcanic plumes**

- The eruption of Eyjafjallajökull in 2010 demonstrated just how devastating volcanic eruptions can be for the European aviation industry.

- Developments in airspace management since 2010 now facilitate considerably more scope for safe aviation operations if high ash concentrations can be predicted, detected and avoided.

- Safe aviation operations require trustworthy predictions of the long range dispersion of volcanic ash plumes and these forecasts in turn require reliable characterisation of plume structure close to the volcano.

- HPC has been used to enable the Weather Research and Forecasting (WRF) model to be adapted to incorporate all the key physical processes associated with ash plumes and thereby to investigate in unprecedented details and flow, dispersion and physical processes within volcanic plumes.
3.4 A Healthy Nation

A healthy nation ensures a productive and effective society. There are five key objectives in ensuring a healthy nation:

- Transform community health and care;
- Improve prevention and public health;
- Optimise diagnosis and treatment;
- Develop future therapeutic technologies;
- Advance non-medicinal interventions.

HPC is already addressing the whole range of challenges to ensure a healthy nation, but greater complexity of problems will require access to more powerful resources.

On a molecular level, the interaction between drugs and the human body receptors requires enormous amounts of computing resource. HPC has helped scientists to design and create new nano-scale molecules which can deliver drugs to targeted sites in the body. This area of research is still in its infancy, yet offers enormous promise for more effective therapies.

Case Study: Theory Inspired Insights into Anti-Cancer Treatments

- UCL, Tufts and Perkin-Elmer combined forces to perform modelling that has provided critical supporting data to prove radioactive decay had been imaged for the first time, leading to an understanding of how nanoparticles might be tailored to reduce cancer treatment side-effects.

- High-quality electronic structure calculations provided crucial evidence confirming real-time imaging of radioactive decay of I to Te. The work is of particular importance since the observation has potential to be exploitable in anti-cancer therapeutics.

- Work is currently underway to design gold-nanoparticles containing I-125 which would target tumours directly yet be emitted from the body, without the hazard of thyroid accumulation.

- HPC resources were pivotal in enabling the resolution of the detailed electronic fingerprint of Te-125 and explaining the enhanced stability of I-loaded films.

Modelling drug transport in the human body and the relationship between drug structure and drug function at targeted cell sites are areas of key importance in the fight against disease. Through
studies in protein folding, receptor site reactions and drug interactions, HPC is able to model these relationships with accuracy but it requires vast amounts of computing power and data management. By eliminating non-productive drug candidates at an early stage, the outcome will be a faster route to market for successful therapies and drugs, short-circuiting years of trials and testing.

**Case Study: Computing Drug Molecule Affinity**

- Researchers from the University of Oxford have worked with international and industrial partners to predict how tightly a drug molecule interacts with a protein target.
- They have combined molecular dynamics with statistical mechanics principles to obtain an estimate of the affinity.
- The large amount of configurational space that must be sampled requires the strength of a supercomputer.
- Previously it has not been apparent if computational analysis could give the required level of accuracy but the team have shown that it gives comparable accuracy to experiment.
- The ability to compute accurate binding affinities holds tremendous value to the pharmaceutical sector as the number of complex physical experiments is vastly reduced.

Similarly, the ability to model genome data and chemical pathways in the body and brain will lead to improved therapies and targeted solutions for particular health problems. The lack of access to the correct compute resource will cause the termination of projects or whole lines of enquiry.

In many ways, the human body is a mechanical system and we have made significant advances in prosthetics, replacement joints and body parts. HPC has a part to play in modelling these solutions, but also how the human body interacts with artificial replacements.

**Case Study: Bone Development and Response to Disease**

- Scientists at the University of Hull have developed their simulation software to utilise ARCHER to model complete bones or large sections of bones.
- This offers the exciting opportunity to model skeletal development and adaptation.
- The potential benefits are enormous, ranging from a better understanding of both the fundamental biomechanics of bone and the cause and effects of musculoskeletal conditions, to better implant design.

Expanding therapeutic solutions to the wider population requires careful planning and HPC is already being used with statistical analysis to understand epidemiological data and biosocial pharmacogenomic traits in understanding the determinants of health. This will help science to understand health risks in the wider population and the ability to predict disease patterns in society.
Coupled to environmental risk factors, such as air and water quality, HPC can help understand how populations around the world may be at risk from disease.

**Case Study: Detecting Protein Pockets**

- Researchers from the University of Manchester have worked with colleagues from Johnson and Johnson to improve the computational modelling of protein surfaces.

- Accurate prediction of protein plasticity has the potential to reveal druggable pockets on the surface of the protein which are not apparent from experimental techniques.

- Targeting these pockets provides new directions in the design of therapeutics e.g. small molecular inhibitors.

- Dr Berthold Wroblowski from Johnson and Johnson has said; “The expertise and flexibility of the team from the University of Manchester, as well as the computational resources from N8 HPC were key in defining new opportunities for drug design”.


3.5 A Sustainable Nation

The growth in world population is putting unprecedented pressure on our resources. Sustainable use and management of our natural resources is essential for the well-being of current and future generations. HPC is already addressing a wide range of scientific challenges to underpin the sustainable use of water, minerals, energy and the ecosystem, and to provide the evidence needed for sensible choices.

Discovering and exploiting resources efficiently and cleanly is being aided by HPC simulations to predict the geological processes and history of potential mineral reservoirs. This offers the potential of discovering ore deposits in sites previously thought unsuitable, and to avoid exploration in sensitive environments.

Case Study: Long time scale development of dynamic topography

- Dynamic topography is generated by vertical flow in the Earth's mantle. Elevation differences from dynamic topography can be kilometres or more in magnitude and control, for instance, the long term sea level of low lying cratonic regions, and influence short-term estimates of sea-level rise due to climate change.

- ARCHER is allowing researchers at UCL to model dynamic topography and to predict the thermal history of possible hydrocarbon reservoirs, including those in developing countries in South America.

- This work is being conducted as part of a collaboration between UCL and Neftex with the predictions supporting hydrocarbon exploration.

Mineral extraction often comes at a cost to local water supplies and research at the atomic scale on our HPC machines is providing the science to understand chemical reactions between pollutants, water and minerals in order to develop effective re-mediation strategies. Using HPC to model flow in the subsurface is essential for evaluating non-traditional extraction of deep gas reservoirs and its
effect on the environment. Flow modelling is also required to assess the impact of over-abstraction of water supplies.

Complex modelling on the largest computers can provide predictions of how biodiversity and ecosystems react under threats from global change and human interactions. Such modelling is needed to prevent land degradation, assess the benefits of ecological restoration management, and provide decision-making tools for sustainable management strategies.

**Case Study: Nucleation and growth of Iron Sulphides**

- Iron sulphides are widespread in the environment and regulate and control the global geochemical iron and sulphur cycles.
- As well as being indicators for seawater anoxia, a catalysis for early life, and recorders of palaeomagnetic signals, their dissolution leads to the problems of acid mine drainage.
- Despite their importance in the environment, they have been relatively poorly studied.
- Modelling on ARCHER has enabled researchers at Cardiff University to understand the nucleation and growth of iron sulphides as this controls their stability and reactivity in the environment.

Bringing these simulations and data into complex high volume new datasets requires dedicated data analysis facilities such as JASMIN: one example is the development of a 1km spatial resolution dataset at the Centre for Ecology and Hydrology to drive a land surface model to understand crop growth, hydrology and biogeochemistry. This is managed alongside multiple runs from simulations so that downstream users can exploit the data on a machine where complex data analysis is possible. Similarly, JASMIN is also used to host websites that allow users to run medium-complexity models of the land surface on JASMIN itself and analyse their data without learning how to use HPC.

Earth observation data also generates a requirement for HPC data analysis facilities such as JASMIN. One example is a global observation of lake water temperature from space, where data from the ENVISAT satellite is processed to produce maps of lake water surface temperature for over 1000 lakes. This process exploits the JASMIN HPC to managed and exploit the relevant data, including voluminous intermediate products. This work is expected to transition into a climate service with UK and European Space Agency involvement.
3.6 A Globally Responsible Nation

As one of the world’s major economies, the UK plays leading role in tackling global challenges including:

- Strengthening global peace, security and governance;
- Strengthening resilience and response to crises;
- Promoting global prosperity;
- Tackling extreme poverty and helping the world’s most vulnerable.

**Case Study: The future of African climate**

Understanding how rainfall will change over Africa in the future is critical for informing adaptation to climate change, and has major implications for agriculture, water resource management, disaster risk reduction and sustainable development.

Very high resolution simulations of African climate on ARCHER are explicitly modelling convective clouds and rainfall over Africa, leading to dramatic improvements in simulating the daily cycle of rainfall.

This pioneering research was initially undertaken through the NERC Cascade project on the HECToR and ARCHER HPC platforms, with each month of simulation requiring 36 million CPU hours. This research is now being taken forward in the Future Climate for Africa, IMPALA and project funded by Newton Fund.

Addressing these global challenges allows the UK to the UN’s 2030 Agenda for Sustainable Development (which builds on the UN’s Millennium Development Goals). HPC is already embedded
within global challenges, encouraging economic growth and wealth creation in developing countries, helping to mitigate climate change and informing adaptation and low-carbon growth.

Examples include using HPC to further our understanding of the climate system within developing countries to improve seasonal forecasts and climate change projections. Improved seasonal forecasts allow for better planning e.g. in the agriculture and water resource sectors, while improved climate change projections can better inform strategies for sustainable development and adaptation to climate change.

**Case study: UK regional climate**

The UK High Resolution Global Climate Modelling programme (a partnership between the NERC National Centre for Atmospheric Science, NCAS, and the Met Office) aims to predict climate change over the coming decades on a sub-national scale, allowing informed planning and mitigation measures to be undertaken.

Over the last fifteen years it has exploited all the national HPC platforms (HPCx, HECToR and ARCHER) and Met Office computing, as well as the Japanese Earth Simulator and a European PRACE supercomputer (HERMIT).

Each of these systems has contributed to different aspects of the programme; from code development and optimisation (the highest resolution models are initially developed on leading HPC and later in life can be maintained on smaller systems), to routine science runs and then, at intervals, massive campaigns such as UJCC which exploited the then largest computer in the world.