The impact of HECToR

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EPSRC

Pioneering research and skills

Acknowledgments

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Abbreviations

ARCHER	Advanced Research Computing High End Resource
BBSRC	Biotechnology and Biological Sciences Research Council
DEISA	Distributed European Infrastructure for Supercomputing Applications
EPSRC	Engineering and Physical Sciences Research Council
EPCC	Edinburgh Parallel Computing Centre
NERC	Natural Environment Research Council
HECToR	High-End Computing Terascale Resource
HPC	High Performance Computing
HEC	High End Computing
NAG	Numerical Algorithms Group
PRACE	Partnership for Advanced Computing in Europe
RCUK	Research Councils UK
STFC	Science and Technology Facilities Council

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Executive summary

High performance computing is now a crucial part of the UK's scientific infrastructure, underpinning its position as a leading research nation. This study has been commissioned by the Engineering and Physical Sciences Research Council to evaluate the impact of HECToR, the UK's high end computing resource from 2007 to 2014. It has been prepared by specialists in research evaluation and communication from four organisations: Research Consulting Limited, Research in Focus Limited, Bulletin and Elsevier.

Our work found that HECToR's impact was broad and wide-ranging:

- **A truly national resource** – HECToR was used by nearly 2,500 researchers across the length and breadth of the UK. Due in large part to the strength of its consortia model, users from 272 different organisations, across academia, government and industry were able to harness its power.

- **An enabler of world-leading research** – HECToR had a significant impact on the scientific community. 92% of HECToR users believe access to the facility improved the quality of their research, and publications arising from HECToR are cited nearly twice as often as other UK publications in the same field. The benefits of HECToR extend across multiple discipline areas, and HECToR publications frequently appear amongst the most highly cited in their fields.

- **A focal point for international collaboration** – Through HECToR and its consortia, the UK was able to access the pan-European HPC infrastructure, and collaborate with the best researchers across the globe. The overseas experts consulted as part of our review confirmed HECToR's crucial role in keeping UK researchers at the forefront of international computational research.

- **A training ground for future leaders in HPC** – Well over 100 PhD students were trained in high performance computing through HECToR. Safeguarding this pipeline of skilled people is of paramount importance both to the health of UK computational research, and to industrial users of HPC in the UK.

- **A centre of expertise in code development and optimisation** – The UK is a world leader in the development and optimisation of HPC software. Code improvements delivered through HECToR's computational science and engineering (CSE) support service delivered efficiency savings for academic and industrial HPC users that run into many millions of pounds.

- **A proven innovation accelerator** – Studies in the UK and overseas have repeatedly demonstrated the importance of HPC facilities in delivering innovation. Our work uncovered more than 60 innovations that had been supported by HECToR, a high proportion of which were considered to be 'major discoveries and pioneering breakthroughs'.

Research enabled by HECToR has had a far-reaching impact on the UK economy and society. Key achievements include:

- **Boosting the international competiveness of UK engineering** – HECToR has underpinned numerous industry-academic partnerships in engineering, including Rolls Royce, McLaren and the supersonic Bloodhound car.

- **Developing innovative ways to diagnose, treat and prevent disease** – HECToR has been used by academics and clinicians to model flows of blood in the human body, bringing the goal of personalised medicine closer to reality.

- **Improving our understanding of climate change** – Work on HECToR has informed weather and climate models used by the Met Office, the World Meteorological Organisation and the Intergovernmental Panel on Climate Change.

- **Capturing the public imagination** – The results of HECToR research are reaching the public in a multitude of ways, from modelling dinosaurs' movement to understanding the causes of falls in the elderly.

Much of the fundamental research undertaken on HECToR will only bear fruit years or even decades into the future. Nevertheless, there remains untapped potential to leverage the national HPC service for the benefit of UK industry and society through:

- **Strengthening links with industry** – HECToR's socioeconomic impact primarily occurred indirectly rather than as part of a top-down strategy. We therefore welcome the increased emphasis on industrial engagement now being pursued by the EPSRC for HECToR's successor facility, ARCHER.

- **Securing the service's status as a strategic asset** – Sustained investment in service provision and support should be married with a more flexible and responsive approach to hardware procurement.

- **Enhancing evaluation and monitoring** – Information to support evaluation of the service's impact should be collected on an ongoing basis, with clear linkages between HECToR usage and research outcomes.

What is not in doubt is the continued importance to the UK of retaining a national HPC facility. The UK's strength in computational research is an indispensable tool in meeting the major economic and societal challenges we face as a nation. If the capability on which these strengths are built is allowed to erode, the long-term damage to the UK's knowledge and skills base could prove irreparable.

HECToR in numbers

HECToR could perform
800 million million
calculations per second

1,000 million million million million
bytes of data could be stored by HECToR

of its users believe HECToR improved the quality of their research

Utilisation of HECToR rose from **59%** to **81%** over the course of its life

At least **13** different industry sectors benefited from research performed on HECToR

32%
of HECToR users were involved in direct or indirect collaborations with industry

8%
of HECToR users identified impacts on public policy as a result of their research

It had nearly **2,500 users** from more than **250 organisations**

HECToR led to **60** different innovations

45%
of HECToR users are involved in international collaborations

£66m
Total value of follow on funding for research performed on HECToR

>800
HECToR-enabled academic publications, which received **2.5** times more citations than average

HECToR publications are **twice** as likely as the UK average to be in the **top 5%** of papers in their field

Total cost of HECToR funded by 3 different Research Councils **£118m**

46%
of HECToR users developed codes that benefited the wider HPC community

At least **130** PhD students were trained on HECToR, with virtually **100%** finding employment on graduation

88%
of major research projects on HECToR progressed onto its successor, ARCHER

1.0

Introduction

1.1 Background and context

High performance computing (HPC) is a crucial part of the UK's scientific infrastructure, underpinning its position as a leading research nation. HECToR provided UK researchers with a world-class supercomputer from 2007 to 2014, at a cost of £118m, but other countries increased their investment in HPC at a faster rate than the UK over the same period. This report provides an independent evaluation of the impact HECToR delivered for UK science, the economy and society.

The United Kingdom is a highly productive research nation that acts as a focal point for global research collaboration and researcher mobility[1].

Maintaining this position of leadership in the global research landscape relies on access to internationally competitive scientific infrastructure, of which high performance computing and e-infrastructure are now essential components. Computational research has taken its place alongside theory and experimentation as the third mode of scientific discovery, and underpins many of the 'Eight Great Technologies' that support UK science strengths and business capabilities[2].

Dominic Tildesley, Co-Chair of the e-Infrastructure Leadership Council, observed that one of these technologies, big data, 'is so significant that it will transform all areas of business, government and research. Sustained investment in our HPC and e-infrastructure is therefore essential if the UK is to remain globally competitive in science and business'[3].

The purpose of the UK's national high performance computing facility is to provide researchers with a world-class supercomputer, powerful enough to run simulations and calculations at the very frontiers of scientific knowledge. Users also receive access to computational science and engineering (CSE) support, enabling them to develop and refine software codes to make the best possible use of the hardware.

HECToR, or High-End Computing Terascale Resource, was the UK's high-end computing resource from 2007 to early 2014. Costing £118m over the course of its life, HECToR was funded by three UK Research Councils, and run under a partnership arrangement between the Engineering and Physical Sciences Research Council, higher education and industry.

In early 2014, HECToR was replaced by its even faster successor, ARCHER, reflecting the perpetual need for the UK to reinvest in the latest technology to retain its competitive advantage. The enormous investment being made in HPC by countries, including the US, China, Japan and Russia, meant that even between HECToR's introduction in late 2007 and its retirement in 2014 the UK's share of global high-end HPC capacity had dropped from 7.4% to 5%[4].

The UK currently faces a period of austerity, which itself follows what has been described as a 'sustained, long-term pattern of under-investment in public and private research and development (R&D) and publicly funded innovation'[5].

Increasing the UK's ability to exploit cutting-edge global research is considered a key driver of economic development[6], ensuring that its scientific infrastructure contributes to tackling the challenges facing businesses and public services, and that its graduates are equipped with the skills needed to thrive in the modern world.

Further investment in HPC must therefore be based on sound evidence of its value, and considered in the light of the rapid growth in cloud-computing services, and the development of pan-European HPC infrastructure.

This report provides an evidence-based, independent assessment of the value HECToR has delivered for the scientific community, the UK economy and society at large.

It was commissioned by the Engineering and Physical Sciences Research Council (EPSRC) and has been prepared by specialists in research evaluation and communication from four organisations: Research Consulting Limited, Research in Focus Limited, Bulletin and Elsevier.

1.2 Scope of work

The overall purpose of this study was to assess the impacts of the HECToR service on scientific research and discovery, the UK economy and society. The following objectives were agreed with the EPSRC:

1. To demonstrate the socio-economic and scientific impact of a publicly funded state-of-the-art High-Performance Computing facility for computational research in the UK
2. To assess the impacts of the service in accordance with an agreed framework of economic, societal and academic impacts
3. To consider cost-benefit analyses of HECToR, based on the above impacts
4. To demonstrate how the "HECToR model" of running a facility provides value for money as well as a successful and efficient service to the user base
5. To demonstrate how this joint investment by three research councils (EPSRC, NERC, BBSRC) has enhanced the benefit for the science community.

1.3 Report structure

The remainder of this report is structured as follows:

- Section 2 provides an overview of who used HECToR, across the UK and beyond
- Section 3 outlines our approach and methodology
- Section 4 summarises the impact HECToR has had on academic disciplines and the international standing of UK science
- Section 5 explores HECToR's wide-ranging impact on the UK economy and society
- Section 6 addresses the role of the HECToR model in delivering impact
- Section 7 sets out our conclusions and recommendations.

2.0

How HECToR was used

2.0 How HECToR was used

HECToR was used by researchers across the length and breadth of the UK, from Inverness to Plymouth, East Anglia to Ulster. The establishment of consortia in key areas of computational science allowed users from 272 different organisations to harness its power, across academia, government and industry. Meanwhile, the partnerships it enabled with European and U.S. HPC facilities allowed UK researchers to collaborate with leading scientists across the globe.

HECToR was based at the University of Edinburgh's Advanced Computing Facility (ACF), designed to house large-scale computers in a secure, purpose-built environment. However, its 2,500 users came from 272 different organisations from across the UK and beyond, encompassing academic and research institutions, government departments and industry.

HECToR's primary role was to support UK academic research, and this is reflected in the breakdown of its user base. The map in figure 2 shows how usage of HECToR was distributed across the UK. The 12 EPSRC framework universities[7] accounted for 58% of HECToR's usage, but in total, users at 58 different UK universities gained access to the facility. HECToR also supported research in a wide range of discipline areas, most notably in the physical sciences, but also in engineering, the life sciences and social sciences. Users drew on HECToR to publish findings in fields as diverse as immunology, the arts and humanities, decision science and agriculture.

The majority of time on HECToR was allocated through its consortia model, allowing scientists from multiple institutions and countries to collaborate and draw on flexible allocations of time on the machine. Through European initiatives such as the Partnership for Advanced Computing in Europe (PRACE), a proportion of HECToR's capability was made available to scientists from across the continent, and in turn UK researchers gained access to Europe's most powerful HPC facilities. More than 80 commercial users representing 39 different organisations were registered on the facility, with many more industry partners benefiting indirectly from collaborations with members of HECToR's academic user community.

Allocation of time on HECToR – 2008 -2014

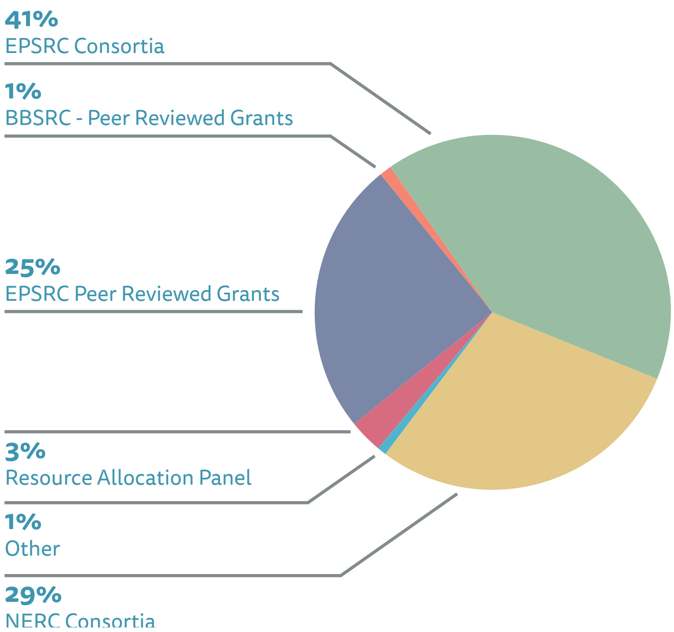


Figure 1

Utilisation of HECToR by organisation

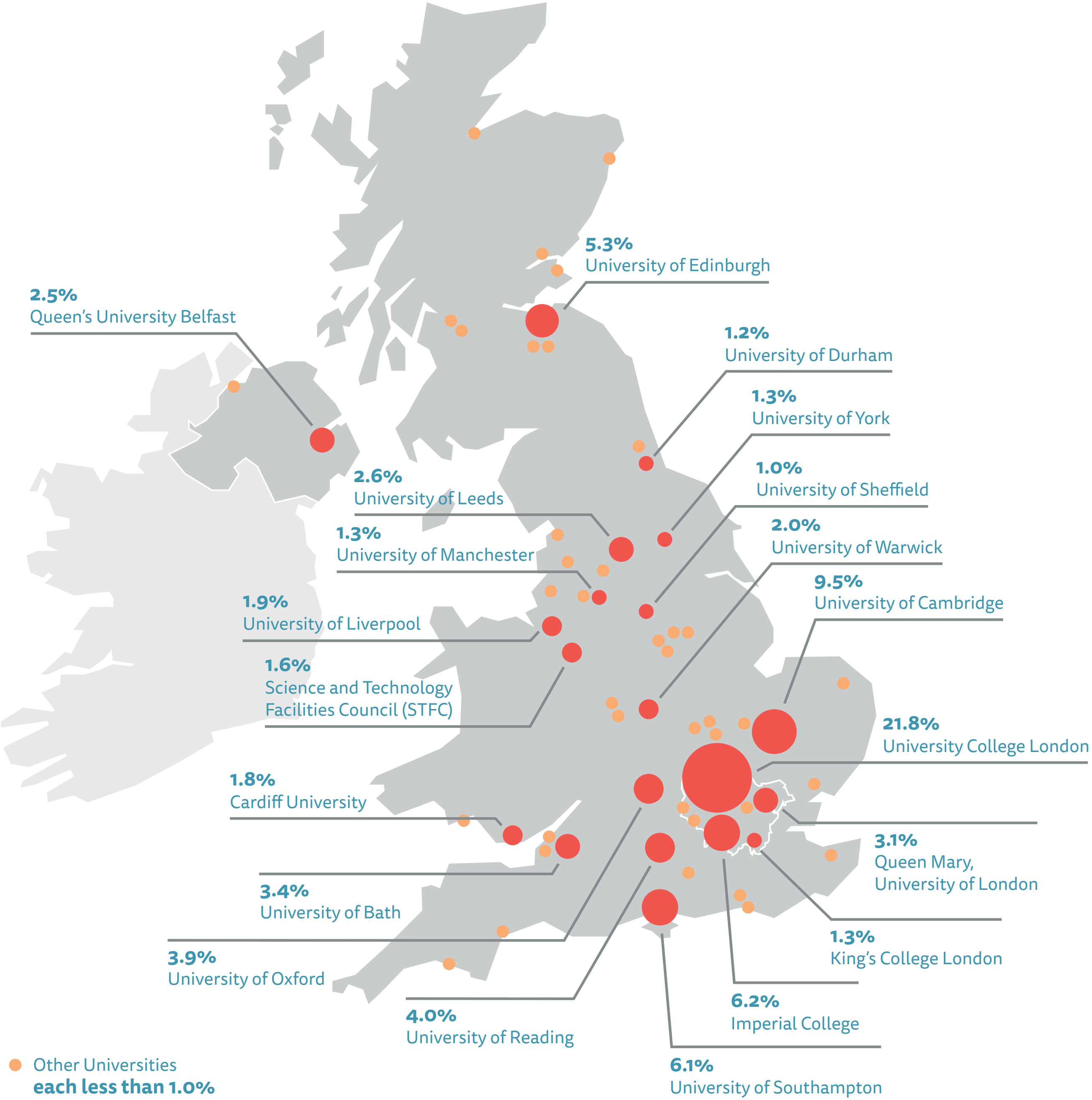


Figure 2

Highest number of user accounts by organisation (top five)

Organisation	Number of users
University of Edinburgh (includes 149 students on the MSc in HPC)	511
University College London	248
University of Cambridge	155
University of Reading	106
Imperial College	103

Figure 3

Distribution of HECToR user accounts by organisations

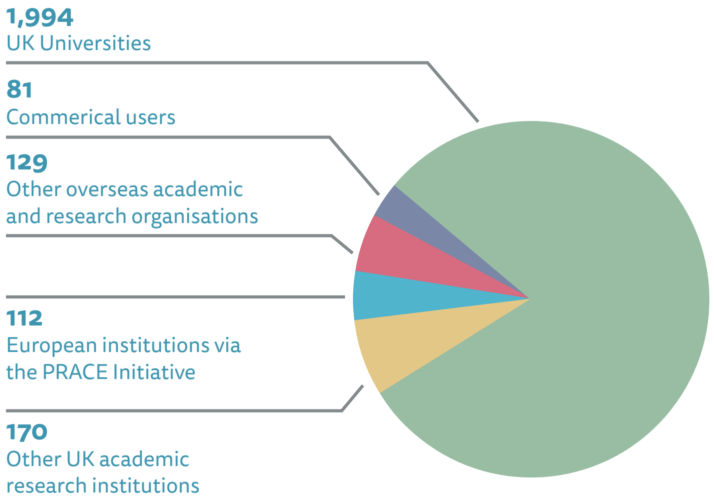


Figure 4

Case study

The race for speed

HECToR 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. And to achieve this, racing car designers use computational fluid dynamics (CFD) to model the flow of air around a vehicle and identify optimum configurations that reduce drag.

Demand for more accurate CFD simulations – without the prohibitive cost – is on the rise. Professor Spencer Sherwin, of Imperial College London, has worked with McLaren for the last decade. He used HECToR to develop a code called Nektar++, which is integral to the development of new techniques to model fluid dynamics.

In 2012 Sherwin was appointed as McLaren/ Royal Academy of Engineering Research Chair in Computational Fluid Mechanics. The aim of the partnership is to create a more precise tool that will enable McLaren engineers to manage turbulence flow structures better. In other words: make the McLaren F1 car faster.

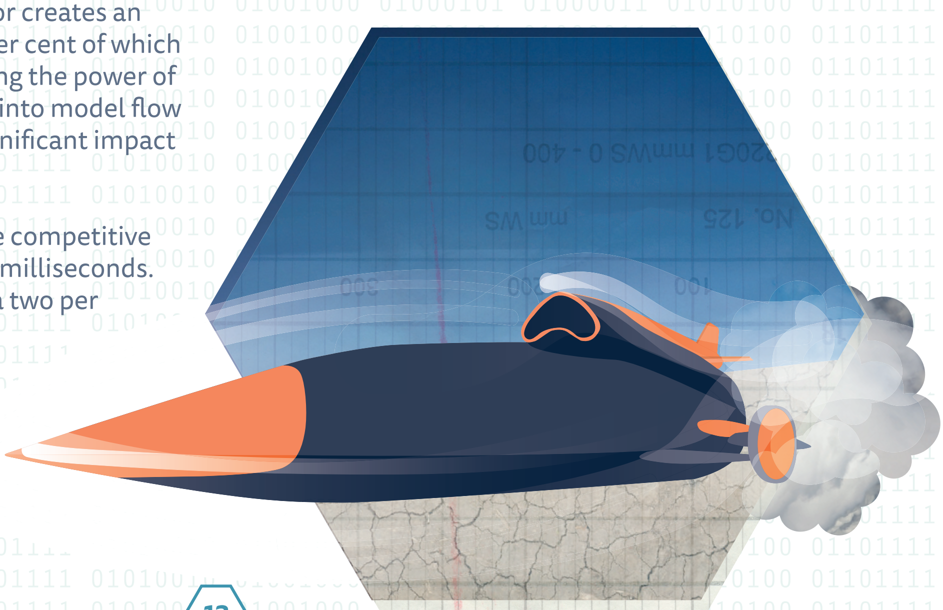
Around 4,500 companies are involved in the UK's motorsport and performance engineering sector, employing 40,000 people (25,000 are qualified engineers). The sector creates an annual turnover of £6bn, 30 per cent of which is poured into R&D. Channelling the power of high performance computing into model flow mechanics is set to make a significant impact on the industry.

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 CFD simulations make."

Sherwin is continuing his work with McLaren on ARCHER, the successor to HECToR. The partnership is also training the next generation of potential F1 engineers. McLaren has funded two PhD students to work on the HECToR project. One went on to work for the company; the other is now principal aerodynamicist at Lotus F1.

HECToR has also been employed in the design of the Bloodhound SSC, a supersonic car that will attempt to set a new world land speed record of 1,000mph. The Bloodhound team called on the supercomputer to solve its airbrake design conundrum: how to reduce the turbulence created by the airbrake airflow.

One of the key aims of the Bloodhound team is to inspire the British public to take a greater interest in science and engineering. It is running a series of educational programmes around the science behind the supersonic car across thousands of UK schools.



3.0

Study methodology

3.1 Our approach

There is little consensus on the optimal methodology for evaluating the impact of large-scale scientific facilities, and the full impact of much of the research performed on HECToR will only become apparent many years or even decades into the future. Our approach to evaluating HECToR's impact was based on bibliometric analysis and a wide-ranging user survey, supplemented by illustrative case studies of the emerging benefits to the UK economy and society.

In developing our methodology it was apparent to us that no single measure or group of measures could effectively capture the impact of HECToR.

Existing studies of the impact of HPC have typically focussed on facilities of a much smaller size than HECToR[8], and do not address the added value of a national facility over local or regional HPCs.

Large-scale scientific facilities such as HECToR are just one of many inputs to the programmes of research being carried out in UK academia, and there is little consensus on the scope, depth of coverage, analytical frameworks and data collection strategies to be used in evaluating them[9].

Furthermore, with so much of the facility's capacity dedicated to fundamental research, the majority of the downstream economic and social benefits of this research will occur some years in the future[10].

A mixed method approach was thus adopted for our study, broken down into five stages, as follows:

Stage 1 – Review of existing evidence

Desk-based review of relevant literature, original HECToR business case and annual reports; site visit to the University of Edinburgh; review of existing data associated with the HECToR facility from RCUK's Research Outcomes System and EPCC's own systems.

Stage 2 – User survey

Online survey issued to the HECToR user community and all Principal Investigators on RCUK grants which included time on HECToR.

This survey sought evidence from users on national and international academic impact, general economic benefits, commercialisation and job creation, as well as social, environmental and cultural impact.

Survey responses were received from 100 users, and provided coverage over 82% of HECToR's total utilisation in the period 2007-2014.

Stage 3 – Bibliometric analysis

A bibliometric analysis of research outputs identified as supported by the HECToR facility was completed by Elsevier, using the following metrics:

- Publications
- Citations
- Field-Weighted Citation Impact (FWCI)
- The number of publications by top citation percentiles (1%, 5%,10%)

- The number, percentage and Field-Weighted Citation Impact of internationally co-authored publications
- Academic-corporate collaborations.

Stage 4 – Expert interviews and case studies

Interviews were conducted with a wide range of stakeholders, including:

- Research Councils UK staff
- EPCC management, as the facilities provider for HECToR
- NAG management, as the provider of computational science and engineering support for HECToR
- Chairs of the HECToR consortia
- Industrial collaborators
- International collaborators
- A sample of users, in order to follow up and validate findings from the user survey.

Stage 5 – Analysis and evaluation

All findings were collated and used to inform our overall evaluation of the HECToR facility as presented here.

Our impact model and the analysis arising from it were based upon RCUK's typology of research impacts[11], modified to take account of best practice in the evaluation of HPC and to allow comparability with international benchmarks where available.

4.0

HECToR's scientific impact

4.1 Underpinning high quality research

HECToR underpinned high quality research which had a significant impact on the scientific community. 92% of HECToR users believe access to the facility improved the quality of their research, and publications arising from HECToR are cited nearly twice as often as other UK publications in the same field. The benefits extend across multiple discipline areas, and when benchmarked internationally HECToR publications are far more likely than average to be amongst the most highly cited in a given field.

Our assessment of HECToR's scientific impact is based on opinion data gathered via the online survey and interviews with consortia chairs/ members and supported by bibliometric analysis of more than 800 papers arising from research performed on HECToR.

Based on the results of our survey, 92% of users believe that access to HECToR increased the quality of their scientific publications. Other benefits HECToR brought to users' research included:

- Increasing publication rates
- Enhancing approaches to modelling the performance of scientific codes
- Increasing researchers' ability to publish in high impact journals
- Lifting the quality of the underlying science
- Increasing the impact of UK work on the international scientific community.

HPC facilities are a prerequisite for much of the surveyed research to be conducted in the first place. For example, 7% of respondents stated that HPC was essential to their research, but not whether this need could also have been met through local or regional facilities, or whether it was dependent on the additional processing power of HECToR.

"HECToR opened up research problems and publishing opportunities that would not have been possible otherwise"

HECToR academic user

In order to gauge the importance of HECToR to its users, survey respondents were asked what proportion of their research was conducted using HECToR; 11% relied on HECToR for the entirety of their scientific output over the period of HECToR's life, while a further 47% relied on it for at least half of their output. This suggests that HECToR was an indispensable tool for the majority of its users, while the remainder combined its use with research enabled by other facilities or not using HPC.

Bibliometric analysis was carried out on a set of publications gathered through the Research Councils' Research Outcomes System (and predecessors) and the online survey. This provided a core of 800 papers on which Elsevier's Research Intelligence Analytical services team were able to undertake a suite of analyses (see Annex 1 for guidance on bibliometric indicator definitions and analysis methods).

As expected the number of publications associated with HECToR increased steadily in the years after "switch-on", reaching over 150 papers per year in the period 2011-2013. Figures for 2014 are for a part-year only, but publications associated with HECToR can be expected to further decline as researchers migrate to the ARCHER facility, which came online in November 2013.

In addition to an analysis of volume of outputs, citations are often used as a proxy for quality. The Field-Weighted Citation Impact (FWCI) is an indicator of mean citation impact, comparing the actual citations received by an output with the expected number of citations for similar outputs.

The indicator controls for the type of output, the subject field and the year of publication and is always defined with reference to a global baseline of 1.00. For this dataset the FWCI for a

Publications underpinned by HECToR

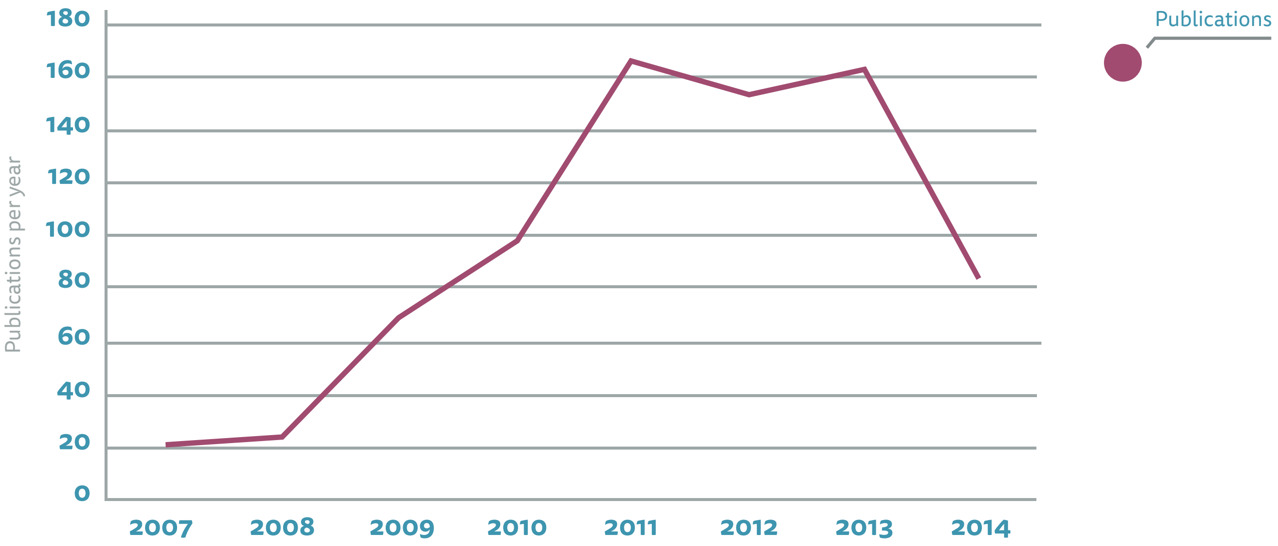


Figure 5

Field-Weighted Citation Impact – HECToR vs UK and World Averages

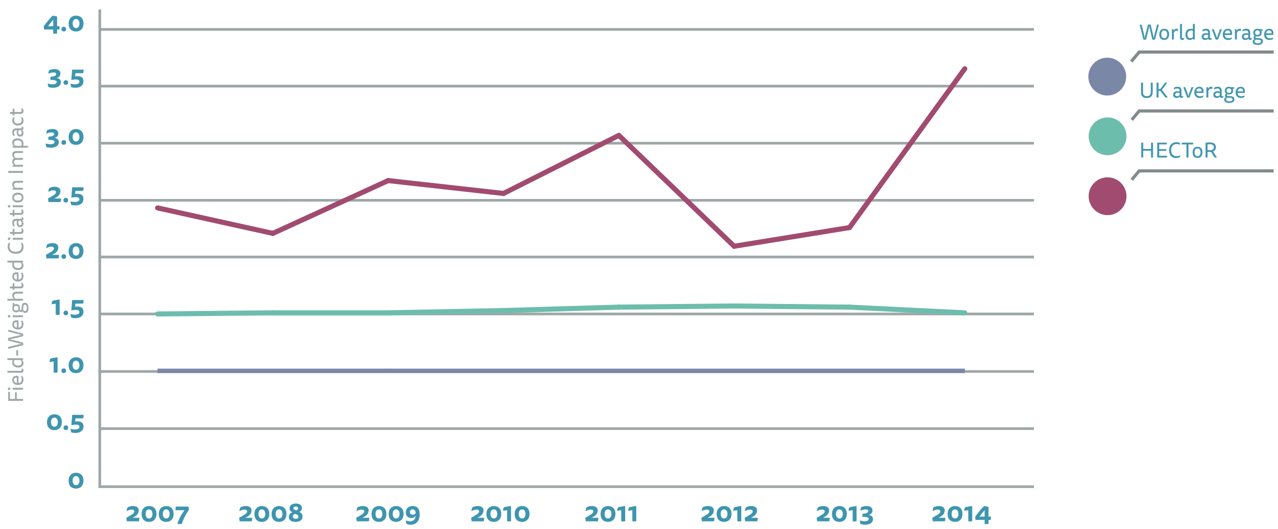


Figure 6

given year varies between 2 and 3.65, meaning the outputs in this dataset were cited between 2 and 3.65 times more than the world average for similar publications. In addition, the FWCI for the UK during this period varied between 1.50 and 1.57 meaning that the papers in this dataset were cited between 0.5 and 2.1 times more than the UK average for similar outputs (figure 6).

This is a striking result and can be further explored via examination of the number of papers within this dataset found in the top 10%, 5% and 1% of the most highly cited papers; as shown in figure 7.

During this period the UK had an average of 19.6% of its publications in the world top 10%, 10.1% in the top 5% and 2.5% in the top 1%. This is impressive as a measure of national output, but perhaps more impressive is that during this period 39% of all HECToR publications were in the world top 10%, 20.3% in the top 5% and 3.2% in the top 1%.

In other words, the UK punches far above its weight in terms of citations and publications supported by HECToR punch even further above the level of the UK as indicated by these measures. The proportion of HECToR publications in the most highly cited categories is more than twice the UK norm in all but the top 1%, where there are only 30% more HECToR papers than the UK norm.

HECToR supported research across a wide range of discipline areas, as illustrated in figure 8.

In almost all cases, publications supported by HECToR saw higher levels of citation than the world and UK average for the discipline in question. The graph in figure 9 shows the Field-Weighted Citation Impact for the ten fields in which the largest number of HECToR publications were produced.

The greatest benefit from use of HECToR accrued to publications in Engineering (UK FWCI = 1.45, HECToR papers = 3.81), Computer Science (UK FWCI = 1.48, HECToR papers = 3.24) and Physics and Astronomy (UK FWCI = 1.53, HECToR papers = 2.57).

In these disciplines, plus Materials Science, Earth and Planetary sciences, Chemical Engineering and Chemistry, publications supported by HECToR were cited more than twice as frequently as the world average. HECToR usage appears to have made very

Highest cited papers

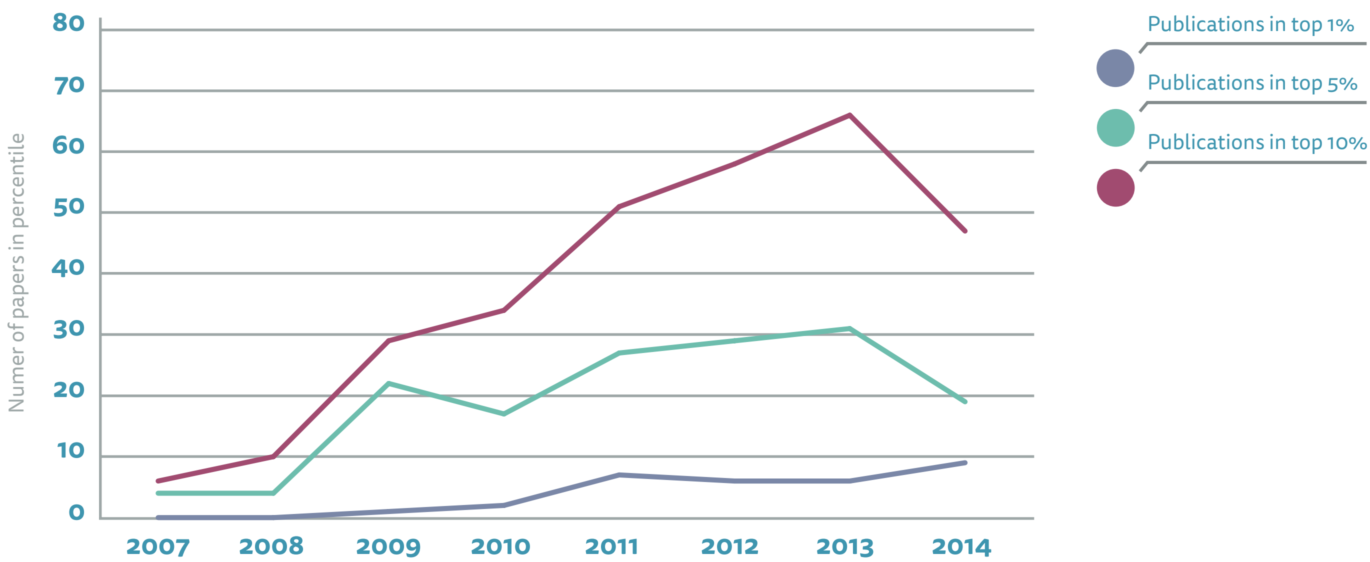


Figure 7

HECToR utilisation by discipline area (2008-2014)

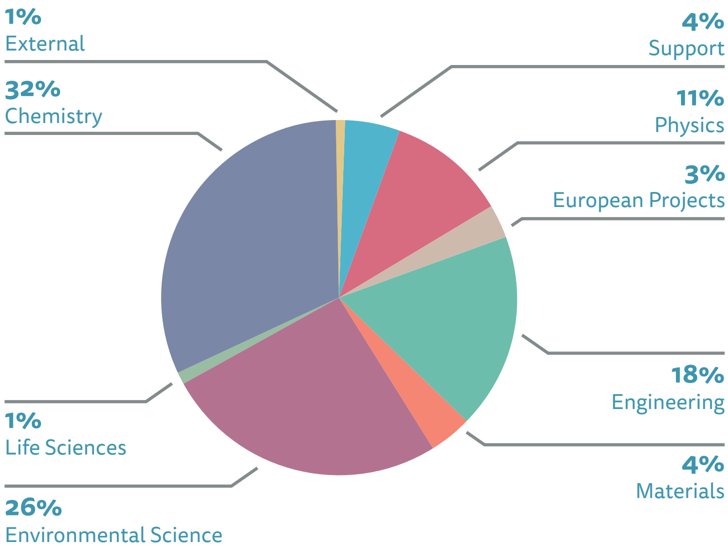


Figure 8

little difference to the citation impact of publications in Energy where the UK FWCI for the 2008 – 2014 period is 1.56 and the HECToR papers in this study's dataset have an FWCI of 1.57.

Another frequently used indicator of quality is the number of publications in 'general science' journals such as Nature and Science, in which papers receive a particularly high number of average citations, as measured by their impact factor.

Only a small number of HECToR publications were published in this category, but these achieved a particularly high level of impact, with an FWCI of over 4, representing four times more citations than expected compared to the world average in the 'general science' category.

Field-Weighted Citation Impact by discipline area (2008-2014)

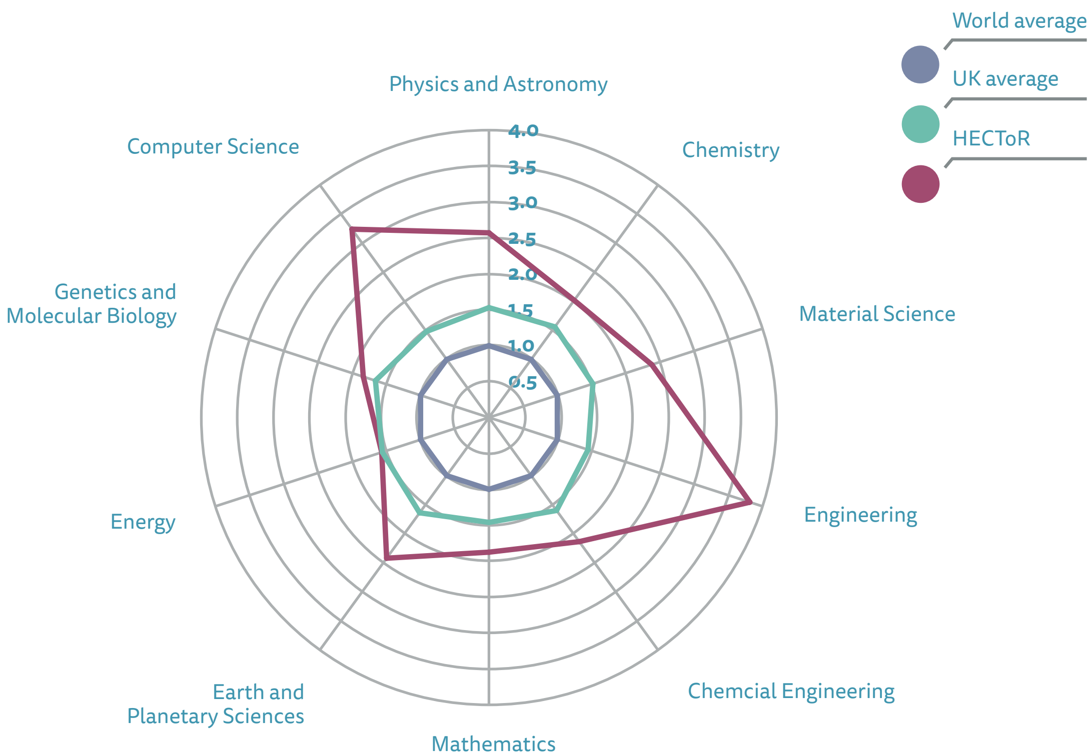


Figure 9

Case study

Body modelling

HECToR has accelerated the development of innovative ways to diagnose, treat and prevent disease more accurately at a lower cost.

By modelling blood flows around the brain and electrical activity in the heart, scientists have made significant progress towards providing clinicians with powerful new technology to detect and treat disease. Researchers say doctors will be able to run computer simulations in real time to guide life-saving surgical interventions for patients who have suffered severe strokes and heart attacks.

While this scenario is likely decades away, the use of blood flow modelling to make earlier diagnoses could be possible much sooner, according to Dr Derek Groen, a researcher at UCL's Centre for Computational Science (CCS). Groen is part of a team that relied on HECToR's processing power to develop the *HemeLB* simulation code to understand how blood moves through cerebral vessels.

Using a model of a patient's blood vessels generated by a rotational angiography scan, the code can help predict where aneurysms are most likely to occur. He said: "With this work, we aim to help clinicians decide whether patients require surgery, and whether patients could make lifestyle adjustments to reduce the risk of fatal strokes."

The UCL group has used HECToR's successor, ARCHER to increase the scalability of the code. Reliable, long term access to the national supercomputing resource has enabled the researchers to develop a fruitful collaboration with clinicians at University College Hospital (UCH), Groen said. The academics have been allowed to run simulations using the anonymised data of five UCH patients, with further larger-scale studies planned.

The research conducted through HECToR led to the publication in 2014 of *Computational Biomedicine: Modelling the Human Body*, co-authored by CCS director Professor Peter Coveney. The first textbook of its kind, it promises to demonstrate how the field can "revolutionise our understanding of the human body, and the therapeutic strategies available to maintain and protect it."

This vision of personalised medicine is driving scientists to develop cardiac simulators for use in clinical settings. A team led by the University of Oxford's Dr Gernot Plank used HECToR to make its heart modelling software 20 times faster, allowing them to simulate one cardiac cycle in less than five minutes.

Dr Sanjay Kharche, a senior research fellow at the Universities of Exeter and Manchester, was part of a team that developed a cardiac simulator (BeatBox) that models electrical impulses to identify arrhythmia. He said: "HECToR has enabled the pursuit of our ultimate goal: to personalise medicine. Cardiac modelling can be used to quickly identify the most effective drug interventions, which will ultimately improve patients' quality of life and cut healthcare costs."

4.2 Training the next generation of HPC-aware researchers

HECToR served as a training ground in high performance computing for well over 100 PhD students, who went on to follow careers in academia, industry and public service, both in the UK and overseas. The high employment rate for these students reflects the continuing demand for highly-skilled users of HPC. Safeguarding the pipeline of skilled people is of paramount importance both to the health of UK computational research, and to industrial users of HPC in the UK.

A key issue in the sustainability of research disciplines and their continued impact is whether there is an in-flow of new researchers matched to national and international needs and whether there is an appropriate balance of those moving from PhDs to permanent positions in industry, academia or the public sector. This study was asked to examine HECToR's role in training highly skilled people and comment on the status quo but not to examine the balance of supply and demand in the area.

Whilst HECToR was in service, the EPSRC and more recently other UK Research Councils, changed their approach to doctoral training. The EPSRC now supports PhD students via its model of Doctoral Training Grants and Centres for Doctoral Training, with these forms seen as the most effective way of supporting students. Project students are no longer permitted on research grants.

One relevant EPSRC Centre for Doctoral Training was identified during this study; the Centre for Molecular Modelling and Materials Science[12] at University College London which has trained a steadily increasing number of PhD students since 2004 and dedicates part of its activity to HPC training and usage.

No longitudinal career data exists as to the paths of those specifically involved in HPC research as part of their PhDs, so no data is available about long-term career trajectories. This study set out to discover how many students had been involved with HECToR and where those students had found employment directly after completing their studies. The evidence gathered shows that a total of 130 graduated students were supervised by 42 academics. Of the 125 with known locations of first permanent employment after their PhD, approximately 60% went into academia and 33% to a role within industry.

> "The UK belongs to a group of internationally leading nations, with world leadership in certain areas such as the simulation of inorganic materials. Between 2007 and 2014, UK researchers continued to be leaders in their fields with new generations of scientists emerging, UK leadership could not have been sustained without the computing resources of HECToR "
>
> Prof. Dr. Joachim Sauer of the University of Humboldt, Berlin

Bibliometric evidence gathered as part of this study demonstrated that HECToR use is associated with an extremely internationally diverse and well connected community and this is further evidenced by 40% of those PhD graduates who took up an academic post doing

Destination of PhD students who used HECToR

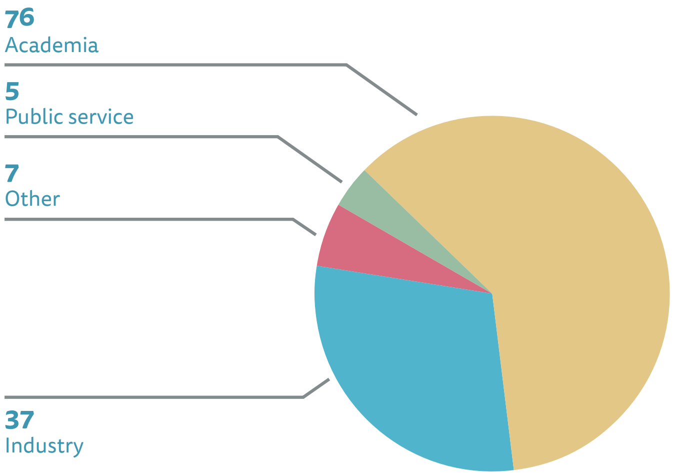


Figure 10

> "...Modelling is used more and more within Johnson Matthey, as a consequence JM recruits from across the world, including the UK. Without projects like HECToR, the ability to recruit within the UK will be diminished."
>
> Rob Potter, Scientific Consultant at *Johnson Matthey PLC*

so outside of the UK; popular locations included Germany, Spain, Japan, Canada and the US.

It was not within the scope of the study to investigate whether there was a reverse flow of overseas academics into the UK, although it is notable that many of the leading UK academics interviewed as part of our study were either born or experienced part of their training overseas.

Anecdotally, there would appear to be a flow of highly skilled researchers both into and out of the UK, but further work in this area is needed before any firm conclusions can be drawn. For the 33% of students who moved to a role within industry the majority appear to have stayed within their specialism and within the UK. Large, multinational businesses were cited as the first permanent role for over 60% of these individuals.

> "This kind of capability does not just help the privileged few. It opens research opportunities to a host of investigators that might otherwise not be able to do research."
>
> Prof William K. George, Distinguished Teaching Professor (Prof. Emeritus), *Princeton University*

Arrangements for PhD training and development of the next generation of HPC researchers were explored with consortia chairs and relevant industrial contacts. Without exception, students were seen as a central part of consortium activities, through full inclusion in workshops and networking activities.

However there appeared to be little specific focus on generic skills, which might be more commonly found within a collaborative doctoral training (CDT) environment e.g. entrepreneurship, strategy and networking. No evidence was found of groups of students sharing their experiences and learning via a cohort style of management within the consortia. The study did not examine the impact of the change in doctoral funding and whether the withdrawal of project students associated with grants has changed the number of students engaged in HPC in the UK.

Given the relatively small number of PhD students trained in HPC methods over the seven years of HECToR's operation and the apparent high employment rate, there remains a question as to whether an appropriate number of students are being trained in a world where simulation appears to be increasingly important. It was not possible for this study to conduct a thorough demand analysis but comments such as those received from Johnson Matthey suggest that this question warrants further exploration.

4.3 Software efficiency and optimisation

The delivery of computational science and engineering (CSE) support was an integral part of the HECToR service, with 20 full-time equivalent staff members dedicated to this per annum. As a result, 46% of HECToR users developed or optimised codes that benefited the wider HPC community, delivering efficiency savings for academic and industrial HPC users that run into many millions of pounds.

Many of our interviewees commented that the UK research community was internationally renowned for its efficient code authoring and optimisation.

The UK's strength in this area was attributed in part to the limited availability of high end computing resource, which incentivised users to find ways of making the most of the available facilities.

Their ability to do so, however, was greatly enhanced by the provision of computational science and engineering support as part of the HECToR service. Delivered by the Numerical Algorithms Group (NAG), 20 full-time equivalent members of staff were dedicated to CSE support in each year of HECToR's life.

A critical feature of the CSE Support Service was the distributed CSE (dCSE) programme which, through lightweight peer review, delivered performance and scalability projects on specific codes in response to proposals from users.

46% of HECToR users who responded to our call for evidence had developed, refined, optimised and shared codes that are of benefit to the wider HPC community. Examples included:

- ONETEP (Order-N Electronic Total Energy Package), which was developed jointly at Imperial College and the Universities of Cambridge and Southampton, is a linear-scaling code for quantum-mechanical simulations based on density functional theory.

  Development work using HECToR and Imperial's CX1 machine greatly improved the code's parallel efficiency, especially when studying systems of solids. By the time that HECToR closed, calculations involving systems of up to 32,768 atoms of crystalline silicon had been demonstrated, scaling efficiently up to 256 cores.

  ONETEP is used for a wide variety of applications by several UK and international research groups, including studies of protein-ligand interactions and self-assembly in semiconductor nanorods and is available under an Academic License/ marketed by Accelrys as part of the Materials Studio package.

- CASINO is the world's most widely used diffusion quantum Monte Carlo code for simulating the properties of molecules and solids.

  Before development work, CASINO ran efficiently on, at most, tens of thousands of cores; as a result of a HECToR dCSE project,

"[The CSE support service] is a partner in tool development and has been instrumental in progressing codes so that they run efficiently and are ready for next generation machines"

HECToR Consortia Chair

it now scales with essentially perfect parallel efficiency on up to 0.5 million cores, resulting in a performance increase of a factor of four.

Unable to test this scaling on HECToR, the team turned to the Japanese K computer (a machine with 0.5M cores). The savings in HPC time now achievable run into many millions of pounds, and the advances benefit the entire global community of scientists who use quantum Monte Carlo to study chemistry and physics.

- CASTEP is a commercial and academic software package which uses density functional theory with a plane wave basis set to calculate electronic properties of solids from first principles.

  A HECToR dCSE project resulted in a performed increase of between two and four times and the code now scales to over 1000 cores against 256 previously.

  The time savings achievable as a result of the increased code efficiency were estimated to be worth £2m on HECToR alone.

"This research and the resulting software is considered by our company to contribute significantly to materials science innovation for our customer companies in the UK, Europe and around the world.

The quantum mechanics expertise and software provided to us by the CASTEP Developers Group enable us to provide more complete and valuable software solutions to our customers.

Globally, we have 830 unique customers who use this software, and sales revenue for the CASTEP software now exceeds $30,000,000. These statistics provide clear evidence of the importance of CASTEP to materials related product innovation."

Ted Pawela, Senior Director, Materials Science Product Marketing at high-tech software company *Accelrys, Inc.*

Case study

Jurassic impact

How modelling dinosaur movement with HECToR has inspired the animation industry, engaged the public in science – and addressed falls in the elderly.

HECToR helped Dr Bill Sellers solve the mystery of how exactly the plant-eating hadrosaur evaded its carnivorous predators: it reached speeds of 50km per hour by running on its back legs.

Sellers, a researcher at the University of Manchester's Faculty of Life Sciences, used the supercomputer to model the skeleton of the duck-billed dinosaur and produced 3D animations to simulate how it used to move. As Sellers puts it, HECToR's sheer speed shrunk a year's work into a month.

But the research was driven by more than just curiosity in how extinct species once roamed the earth. Sellers said: "We modelled dinosaurs because they are fun and because the animations capture the public imagination. But there is a very serious aim here. Dinosaurs' musculoskeletal systems are similar to our own so the biomechanical principles can be applied directly to humans."

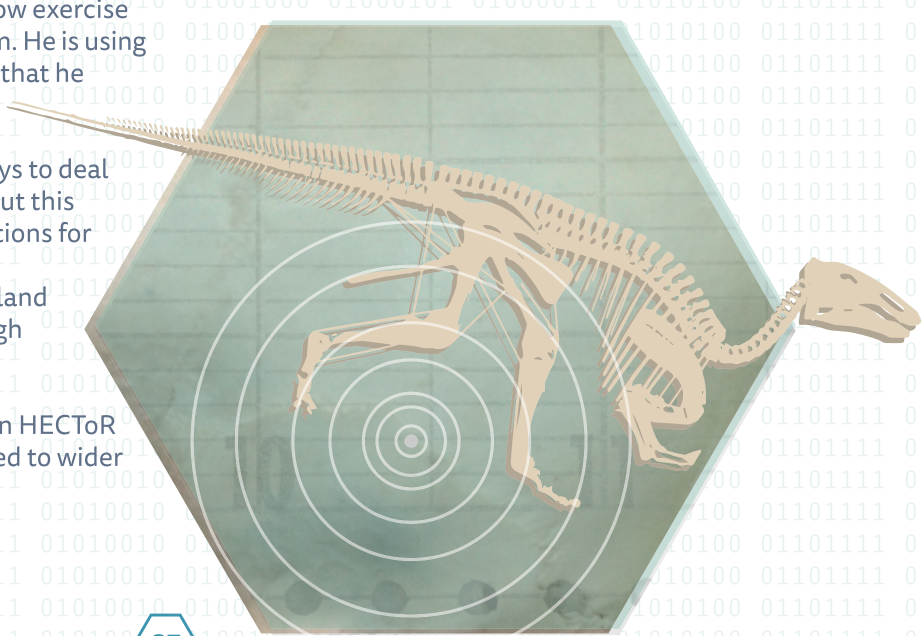
Using HECToR's successor ARCHER, Sellers is one year into a project that is running simulations of human locomotion to better understand the causes of falls in the elderly and how exercise programmes can help prevent them. He is using the open source software *GaitSym* that he developed on HECToR.

"This is about establishing new ways to deal with a major public health issue. But this kind of modelling also has applications for robotics – we are working with the Institute for Field Robotics in Thailand for example – and in the field of high performance sport," he said.

Much of the research conducted on HECToR was basic science. And this often led to wider economic and social impact in unexpected places. Animation and special effects companies already use physical modelling techniques and Sellers and his team are in discussions with digital studios specialising in motion capture technology for film and video games to exploit this work.

Sellers said: "Animation companies are really starting to see the benefits of the kind of computational methods we developed using HECToR. It's obviously a lot cheaper and less time-consuming than say, capturing the movements of a chimp in a lab."

The modelling has also been a hit with the general public. At the Royal Society Summer Science Exhibition 2014, Sellers linked up the software to a Wii Fit balance board to appeal to a younger audience. Children – and their parents – were able to use the balance board controller to march a dinosaur across a large screen. It was also on display in The Manchester Museum.



4.4 HECToR's role in enabling collaboration

HECToR opened up a range of collaborative opportunities for UK researchers. The HECToR consortia served as focal points for their research fields in the UK, and facilitated connections with international researchers and non-academic collaborators. Through HECToR the UK was able to access the pan-European HPC infrastructure, and its researchers are recognised internationally as amongst the leaders in their fields.

HECTOR usage was found to be highly associated with collaboration within the UK as well as internationally.

The High End Computing (HEC) consortia act as a focal point for their research fields, playing a vital role in coordinating researchers' efforts, enabling networking, new science and facilitating connections with international researchers and non-academic research users.

For example, the Materials Chemistry Consortium has worked directly with publishers to coordinate a number of journal special editions, including a special issue of the Proceedings of the Royal Society A in 2011 and more recently, a special issue of Physical Chemistry and Chemical Physics.

This study uncovered much high quality activity happening outside of the consortia, but their critical mass enabled interaction with the international research scene and non-academics to occur in a far more streamlined way.

Membership of the HEC consortia was particularly evident from the online survey; 68% of respondees said they had gained access to HECToR via one or more of these consortia, with 21% of respondees having gained access through both a consortia and either a peer reviewed grant or other means.

The evidence gathered to underpin this study also shows that there is a significant volume of mutually supportive collaborations between experiment and simulation as demonstrated by some of the comments received in the survey:

" We were able to complement experimental data taken by collaborators at ELETTRA in Trieste... most of my research would not have been possible without HECToR."

" We were able to run massive multiple replica simulations and get fully converged free energy simulations that were in good agreement with experimental data."

" An example could be the determination of the structure of a complex MgO grain boundary in collaboration with Yuichi Ikuhara, Univ. Tokyo, Japan. Without the atomistic models made possible with HECToR electron microscopy alone was insufficient to determine the complex atomic structure which led to a publication in Nature."

" The collaborator needed computational insights into the problem we were studying. Another computational chemist in a different country could possibly have used their own national supercomputer to do this project, but as a UK theorist, the calculations were only possible on HECToR."

In terms of international collaboration, 45% of users surveyed stated that they had international collaborators and in many cases it was having access to HECToR that had enabled these. The allocation of a small amount of time on HECToR to the Partnership for Advanced Computing in Europe (PRACE) initiative was particularly beneficial in this regard.

Participation in PRACE allowed UK researchers to access high-end HPC infrastructure across Europe while retaining the benefits of a dedicated national facility. The level of international collaboration enabled is reflected in the fact that just under half of the publications arising from HECToR included an international co-author, as shown in the graph in figure 11.

Two themes emerged as to the relationship between international collaboration and access to HECToR:

1. that a nation must have access to a high-end HPC resource as an entry ticket to major international consortia; or

2. that HECToR is attractive to international collaborators for its own qualities and thus UK academics are actively sought out as a route to gaining access to this resource, albeit indirectly.

"..UK researchers have for a long time been amongst the leaders in the fields of fluid mechanics and turbulence... High performance computing is a key tool for tackling these problems and leading resources such as HECToR have allowed these leading researchers to stay at the forefront of the field."

Professor Ivan Marusic, *University of Melbourne*

In each case international collaboration was felt to raise the overall quality of the science achieved and thus represented a gain for UK research. Three quarters of the researchers who had worked with an international collaborator further stated that HECToR had enabled the collaborator to do something new or different which would not have otherwise been possible.

Internationally co-authored publications

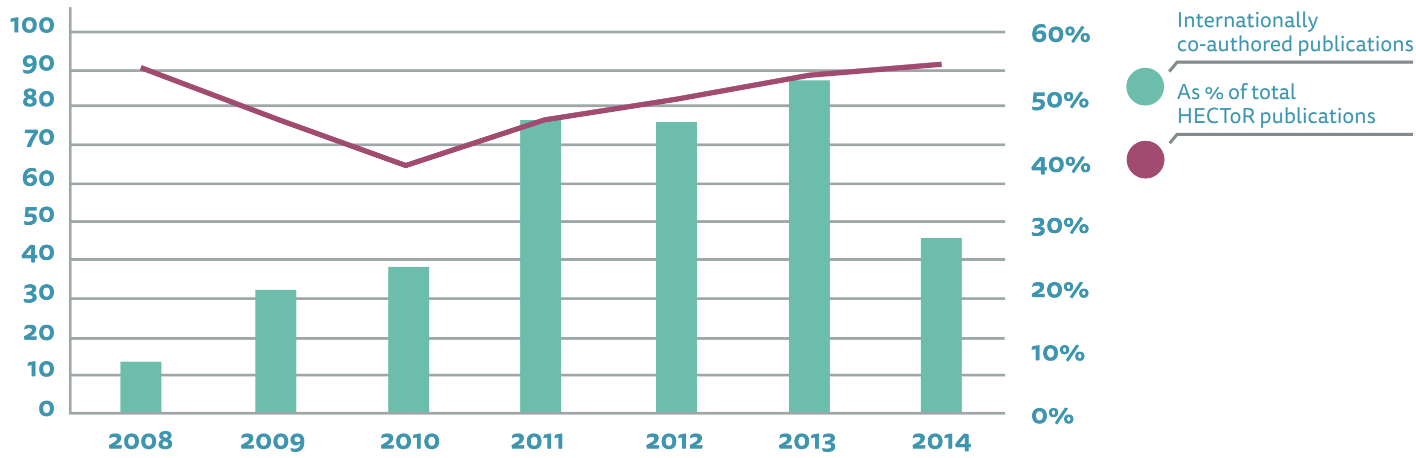


Figure 11

Case study

The fusion future

HECToR has underpinned UK contributions to the development of nuclear fusion and informed the design of a multi-billion-pound scientific collaboration.

ITER is one of the world's most ambitious endeavours: scientists from all corners of the globe working together to harness nuclear fusion for an unlimited supply of clean energy.

Construction of the world's largest experimental tokamak nuclear fusion reactor – a magnetic confinement system that produces energy through the fusion of light nuclei – is underway in France. Comprising one million parts, it will be 30 metres high and 23,000 tonnes. Research made possible by HECToR is informing key elements of its hugely complex design.

A leading issue for ITER and future fusion plants is Edge Localised Modes (ELMs). These are plasma eruptions that often occur at the edge of a tokamak plasma. They erode the surface of the machine, rendering the reactor economically unviable. By fully understanding why they occur, scientists can bring them under control.

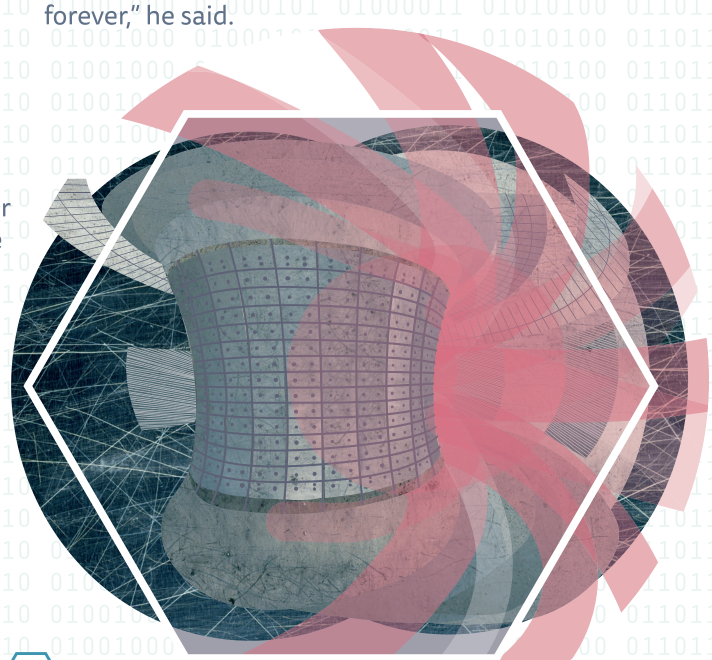
Dr Ben Dudson, a physicist at the University of York, used HECToR to test and modify a code called BOUT++ to study ELMs, which has led to new developments in the modelling of tokamak edge plasmas. International organisations, including the Lawrence Livermore National Laboratory in the US, are using BOUT++. Crucially, it has informed late changes to the design of ITER.

Dudson said: "Having a national supercomputer resource is vital – it gives us the independence we need to carry out research efficiently."

Dr Colin Roach, Leader of the Plasma Confinement Group at the Culham Centre for Fusion Energy, needed access to HECToR to work on state-of-the-art plasma turbulence simulations aimed at improving the efficiency of magnetic confinement fusion devices. Heat and particles leak from devices at a rate predominantly determined by plasma turbulence. Reducing this turbulence and its associated losses is key to making nuclear fusion possible. Calculations on HECToR have unveiled new ways to improve plasma performance, including in the Joint European Torus (JET), currently the world's largest and most powerful tokamak experiment.

He said: "Access to HECToR has enabled the UK plasma turbulence modelling community to grow from a small base. The UK now ranks as a world leader alongside the US and Germany. More than 16 PhD students from my own group of collaborators have benefitted, receiving excellent training in high performance computing and in plasma physics. Seven have since moved on to post-doctoral positions in the field, while others have taken their highly transferable skills into the broader economy."

A full understanding of plasma turbulence is essential if the world is to maximise its return on investment in projects like ITER, Roach says. "Successfully running a burning plasma device to produce energy would have a huge impact on our lives. There is only so much climate change we can bear. We simply cannot burn carbon forever," he said.



4.5 HECToR's role in underpinning innovation

Studies in the UK and overseas have repeatedly demonstrated the importance of HPC facilities in delivering innovation, and users of campus-based HPC facilities in the UK remain convinced of the added value offered by a leadership class system such as HECToR. Our work uncovered more than 60 innovations that had been supported by HECToR, a high proportion of which were considered to be 'major discoveries and pioneering breakthroughs'.

In 2008, the U.S. Council on Competitiveness described HPC as 'a proven innovation accelerator, shrinking time to insight and time to discovery'[13], based on the findings of a series of studies of its impact on private sector competitiveness.

A small number of academic studies have also explored the correlation between the use of HPC and research productivity.

In 2006, Tichenor and Reuther analysed the time and costs saved by the use of HPC in order to demonstrate the significant savings available in both academic and industrial contexts[14].

In 2010, Apon et al[15] used correlation and regression analysis to evaluate the research-related returns on investment in HPC for US universities, concluding that consistent investments in HPC at even modest levels are strongly correlated to research competitiveness.

A further study by Apon et al in 2014 found that locally-available HPC resources enhanced the technical efficiency of research output in certain disciplines such as Chemistry, Civil Engineering, Physics and History, but not in others such as Computer Science, Economics, and English[16].

In the UK, the UK High Performance Computing Special Interest Group undertook a 2010 study to measure the range and evaluate the impact of mid-range HPC facilities in UK universities[17]. This highlighted the breadth and depth of research being undertaken on HPC across the UK, and its associated impact, but noted the 'very strong support amongst the community of campus HPC service providers for a UK leadership-class system' – the role filled by HECToR.

In order to assess HECToR's contribution to innovation against that of other HPC facilities around the world, we compared the findings of our user survey with those of a 2013 IDC international study of HPC[18].

Representing the most comprehensive evaluation to date of the benefits of investment in HPC, the IDC study indicated that investment generated substantial financial returns for industrial users, with $356.5 on average in revenue per dollar of HPC invested, and $38.7 on average of profits (or cost savings) per dollar of HPC invested.

For academic and government facilities such as HECToR, IDC developed an innovation index, allowing the significance of innovations arising from the use of HPC to be evaluated.

Utilising the innovation index developed by IDC, we found the following:

- 60 innovations were found to have originated from research underpinned by HECToR.
- The average cost per innovation from HECToR was approximately £2m, or $3m. This is comparable to the results of IDC's international study which found an average cost per HPC-supported innovation of $3.1m.
- HECToR delivered a higher proportion of 'major discoveries and pioneering breakthroughs' than average, and those discoveries were also more significant, scoring 5.2 on IDC's innovation index versus a worldwide average of 4.4.
- HECToR delivered a smaller number of 'incremental innovations or process improvements', and these were typically less significant than the worldwide average (scoring 3.8 versus an average score of 5.5).

These findings are subject to a number of caveats, and are reliant on users' own assessment of the significance of innovations. IDC's study showed the consistency of this assessments was highly variable, and that UK respondents tended to rate innovations lower than sites in other countries did, on average.

The results should therefore be treated with caution, but do provide a further perspective on HECToR's important role in underpinning basic research both in the UK and internationally.

Significance of innovations enabled by HECToR (basic and applied research)

Significance to relevant field	Basic	Applied	Total
10 = One of the top 2–3 innovations in the past decade	0	0	0
9 = One of the top 5 innovations in the past decade	3	0	3
8 = One of the top 10 innovations in the past decade	1	0	1
7 = One of the top 25 innovations in the past decade	1	0	1
6 = One of the top 50 innovations in the past decade	4	0	4
5 = It had a major impact and is useful to many organisations	11	12	23
4 = A minor innovation that is useful to many organisations	5	11	16
3 = A minor innovation or only useful to 2–3 organisations	2	3	5
2 = A minor innovation or only useful to one organisation	0	1	1
1 = An innovation that is recognized ONLY by experts in the field	2	4	6
Total	**29**	**31**	**60**

5.0

Socio-economic impact

5.1 HECToR's contribution to socio-economic impact

HECToR forms part of the UK's research infrastructure, and work supported by the service contributes to a wide range of industry sectors. HECToR was established primarily to support fundamental research, but the research it enabled has in turn resulted in applications and innovations that deliver benefit to the UK economy and society.

Direct commercial usage of HECToR accounts for less than 1% of the systems utilisation, and only 11% of users worked directly with a commercial collaborator. However, our study found that the indirect benefits of HECToR to industry and society are much greater than these figures would suggest.

HECToR is part of a rich research infrastructure, an innovation ecosystem, where infrastructure, participants and organisations interact, in an often complex manner, to transform knowledge and funding into innovations in the commercial and public sectors and society as a whole.

HECToR was established with the purpose of supporting the highest quality fundamental academic research, which feeds applied research, other fundamental research and indeed directly into application and innovation. Whilst it has been in operation the impact agenda has gathered pace to a point where considering one's own most effective role on the pathway to impact is now routine for UK researchers.

In assessing HECToR's contribution to impact, consideration was given to RCUK's typology of socio-economic impact[19], expectations of societal impact[20] and the 2012 'Software as an Infrastructure' strategy[21]. Relevant highlights from these documents are provided in Annex 3. RCUK defines impact very widely to include positive change in areas such as society, the economy, the environment, policy and public services.

HECToR, of course, has not only underpinned impact arising from research but has delivered direct benefits from its presence as part of the national research infrastructure i.e. economic benefits to the Edinburgh area, impact on suppliers, staff and the usual knock-on effects of such facilities[22].

Additionally, many of the students trained on HECToR will have gone on to make significant impacts in their own fields. However, assessing the impact due to these factors was not within the scope of this study and therefore the impacts presented here concentrate solely on those due to the research itself enabled by HECToR.

This study found that only 1% of the total utilisation of HECToR was by commercial users and a total of only 11 impacts were captured against HECToR grants in the RCUK Research Outcomes System. Past studies of major research facilities have shown that low levels of commercial usage are not unusual (typically less than ten per cent[23]), and that indirect industrial access through collaboration with academics often yields greater benefits.

Additionally, trends in the number of papers

Publications co-authored with industry

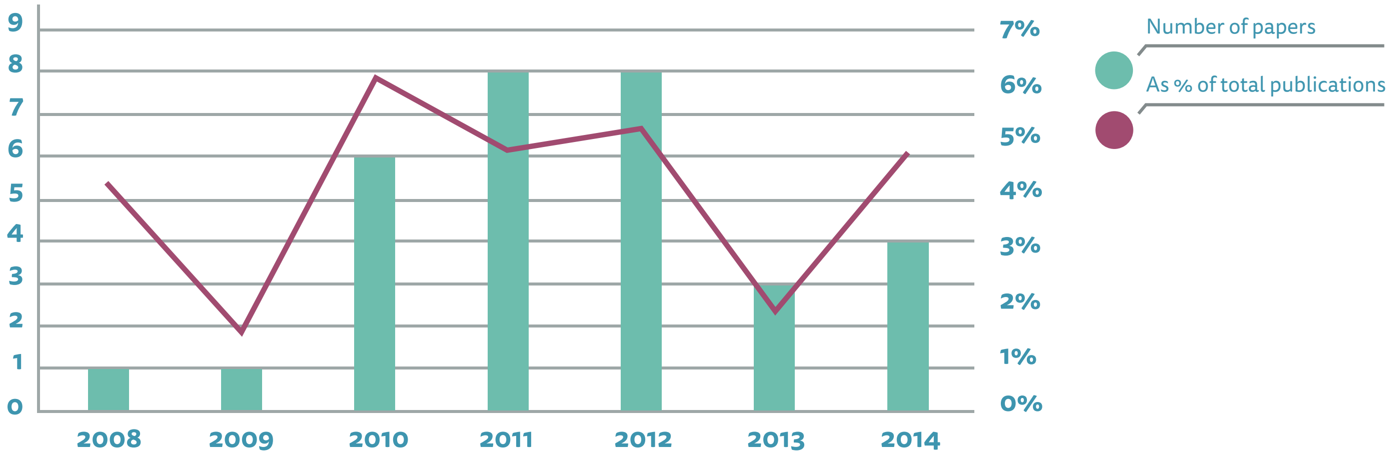


Figure 12

co-authored with industrial collaborators were examined as part of the bibliometrics exercise. This revealed that only a small proportion of papers within the dataset (between 2 and 6%) had industrial co-authors, although this is broadly consistent with the UK average of 3%[24] in the period. This contextual data pointed to a low culture of impact surrounding HECToR. However as further evidence was collected the picture changed markedly.

Evidence gathered through the online survey found the following:

- 11% of respondees had directly collaborated with a commercial partner on a HECToR project;
- A further 21% stated that a commercial partner had benefited from their HECToR-enabled work even if that partner had, themselves, not taken a direct role in the relevant projects;
- 18% of respondees stated that they had collaborated with the public sector or that policies had been informed by their HECToR enabled research; and
- 11% of respondees stated that their research on HECToR had a direct or indirect impact on the environment.
- A total of 86 examples of impact were gathered from the 100 survey responses received, ROS/ROD data and the HEC consortia.

The further the interactions between the HECToR research community and those outside of academia were examined, the more examples of impacts arose. Following on from the online study a series of semi structured interviews were held with representatives of commercial organisations who had been involved with HECToR projects.

A consistent theme of these conversations was the long term nature of the evolving partnership between academics and their industrial counterparts. Furthermore, the nature of impacts found was such that many build capacity and capability in the commercial, public and third sectors, but do not lend themselves to standard financial analysis.

The findings of this study suggest that, contrary to the minimal commercial use of the facility and low levels of industrial co-authorship, industrial collaboration and impact are more

Count of sectors benefiting from HECToR research

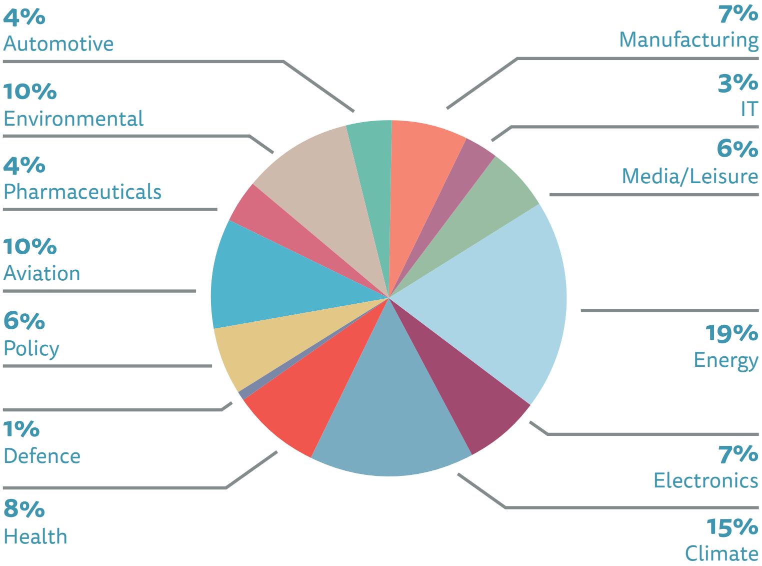


Figure 13

extensive than first thought, especially within the HEC consortia.

As can be seen in figure 13, despite HECToR being an investment in fundamental research infrastructure, impact has occurred in a wide variety of sectors. This data is indicative only, representing a simple count of the various sectors mentioned by HECToR users, and the magnitude of impact within each sector is likely to be significantly different.

A large volume and variety of impact is being underpinned by HECToR, but the usual challenges of attributing particular impact to particular bodies of research are accentuated here. The evidence uncovered in this study suggests that HECToR is a classic example of the importance of fundamental research infrastructure playing its part in underpinning the innovation ecosystem.

It is not possible to fully quantify these impacts, and thus the limited data presented here is likely to vastly underestimate the true value that HECToR and its users have delivered to the UK and more broadly.

In consequence, much of the evidence of socio-economic impact presented in the following sections is narrative in nature, with illustrative case studies grouped as follows:

- Industry partnerships to inform code base development (section 5.2)
- Industry collaborations for product design/development (section 5.3)
- Support for small and medium-sized enterprises (SMEs) (section 5.4)
- Public policy, health and environmental impact (section 5.5).

Impacts have been quantified and mapped against the goals set out in RCUK's 'Software as an Infrastructure' strategy wherever possible.

5.2 Industry partnerships to inform code base development

HECToR supported partnerships between academics and companies including AWE, Rolls Royce and SEMATECH to inform code base development. This activity is closely aligned to the goals of 'Shaping Capability', 'Ensuring Trust' and 'Developing Leaders and Skills People' within RCUK's 'Software as an Infrastructure' strategy.

A number of large, multinational businesses benefit from the presence of HECToR to inform their own code development.

These codes may be products themselves, may aid design of products or may be used as test cases in large value procurements of in-house HPC facilities, which run proprietary, highly protected commercial codes unsuitable for use on national facilities.

SEMATECH (SMT)

Dr Alexander Shlugar and colleagues from UCL's Department of Physics & Astronomy used HECToR and other techniques to investigate the properties of new materials for the electronics industry.

Their industrial partner, SEMATECH (SMT), is a specialist industrial research and technology organisation funded by member companies such as Intel and IBM, who have used these results to improve the quality and reliability of high-performance microelectronic devices based on transistors. Recommendations made by SMT have been implemented by industrial partners in their currently manufactured devices, such as the 22nm process technology released by Intel in 2011.

AWE

The Centre for Computational Plasma Physics (CCPP) is an AWE-funded initiative at the University of Warwick to support the development of software relevant for High Energy Density Physics research and the characterisation and optimisation of that software across all current and planned HPC platforms.

The CCPP grew out of many years of collaboration between AWE and the Physics and Computer Science departments at Warwick covering code development and optimisations, and consolidates all funding under a single coherent organisation. CCPP is initially funded for three years and supports 50% of 4 PhD studentships, 25% of 2 Post-Doctoral Research Assistants and the time of two Professors.

Central to all of the work of CCPP is optimised physics codes on HPC systems and thus having access to the HECToR system was essential for

> "The collaboration has allowed us to consolidate some parts of our required code structure across the company, improving output and reducing our costs, allowing us to concentrate further investment into application areas that expand our current contracts and customer base. We have a long history of common interests and aspirations and it is a pleasure to be able to formally acknowledge this."
>
> Dr Alec Milne, Director, *Fluid Gravity Engineering Limited*

setting up this Centre and optimising the first major release of the relevant code.

Accelrys

The Nanotechnology Consortium (advised by Professor Richard Catlow, UCL), collaborated with the STFC Daresbury lab to develop a QM/MM module (QMERA) for Accelrys' Materials Studio® modelling and simulation environment software. Materials Studio enables investigators to relate product performance with material properties and behaviour at the molecular, atomic and meso scales.

Since the launch of Materials Studio®, modules influenced by Professor Catlow, of which there are at least three, have generated significant revenue and have been sold to hundreds of companies and academic institutions worldwide who utilise the software for product and process optimisation. These developments have been underpinned by a wide range of computers from desktop PCs right up to HPC facilities including HECToR and its predecessors.

Rolls Royce PLC

Dr Leigh Lapworth, Chief Design Systems Architect at Rolls Royce, described the significant impact that working with UK HEC academics has had on Rolls Royce's capability to undertake extremely complex calculations.

Rolls Royce works with a number of academics through its University Technology Centres, many of which use the national e-infrastructure, and has also collaborated closely with the HEC consortia. The benefits of these collaborations have included:

- A significant amount of Rolls Royce's simulation code base has been influenced by tools and techniques originally developed in collaborative academic projects utilising HECToR and its predecessor HPC(x).

"Simulation is now the third leg of science, together with theory and experiment. As such we need to be sure that results are driven by the science itself rather than a bug or artefact in the code. The 'Software as an Infrastructure' programme is absolutely the right way to ensure that the UK has the skills to take this increasingly important way of doing science forward. If ARCHER were to be taken away the UK would be hugely disadvantaged in both the leading edge science it can perform and the economic benefits that are derived."

Leigh Lapworth, Chief Design Systems Architect, *Rolls Royce*

- The collaboration showed that, by increasing core counts, calculation times could be reduced by a factor of 30. Specific CSE developments within the UTCs showed like-for-like improvements of over a factor of 3 in some cases.

- The establishment of a dedicated in-house CSE team was prompted by evidence of the benefits delivered from HECToR's own CSE support.

- A flexible approach to intellectual property (IP) arrangements has allowed Rolls Royce to derive greater value from CSE developments.

Many of the impacts on Rolls Royce from UK HPC researchers would not have been possible for the company to deliver in-house. Rolls Royce and EPSRC are now working to develop a model for industrial access to ARCHER, HECToR's successor, with a pilot already showing, in its first three months, that calculations 10 times larger than previously possible can be run and with further increases to come. The model builds directly on the experience of HECToR and Dr Lapworth sees this as a natural maturation of the collaboration it enabled.

5.3 Industrial collaboration for product design/development

Research undertaken on HECToR helped to inform product development by Johnson Matthey and General Electric Global Research, in line with the goal of 'Delivering Impact' in the 'Software as an Infrastructure' strategy.

Other examples of impact (often indirect) arose where businesses drew on the scientific results emerging from HECToR projects.

Johnson Matthey (JM), the British multinational chemicals and sustainable technologies company, has partnered with academics around the country to use HECToR to model their chemical catalysts. One example is in the development of new catalysts for use in catalytic convertors.

JM is looking to study complex metal oxide materials to understand how these function, but needs access to vast computing power to do this successfully. JM has partnered with UCL to enable access to ARCHER in order to tackle these computationally challenging problems.

Misbah Sarwar, Principal Scientist at JM, said: "The work on HECToR and now ARCHER has helped give us a fundamental insight into how catalysis works so we can bring our catalysts swiftly to market." Over the last six years JM has funded several PhD studentships that involve the use of HECToR and ARCHER at institutions including UCL, Cardiff University and the University of Southampton.

This material will soon go into plant trials. Overall, this collaborative approach has substantially shortened JM's development path to inorganic oxide catalysts by providing a faster route to invention and optimisation.

It is difficult to provide an exact quantification of the value of product and process optimisation summarised above, but the annual value to JM of products referred to is £70 million and the processes in which they are used lead to products with an annual value of £25 billion.

The impacts used here as examples are extremely broad and as such affect many parts of the partner's businesses. It is for this reason that the overall economic value is extremely difficult to calculate – it could be argued that much of what has been achieved did not involve HECToR, but likewise, without HECToR the impacts are unlikely to have occurred.

Furthermore, to calculate the total extent of economic value related to HECToR would require detailed individual calculations to be carried out on each individual organisation and its customers. Many companies would be unable to disclose the information needed to inform these calculations on grounds of commercial confidentiality.

"..we were able to tackle industrial relevant problems that required a very fundamental approach, and massive computational resources, in order to advance understanding and, ultimately, improve design performance. The cooperation was and still is very productive, and it is expected to further improve performance excellence in the wide range of aerodynamics design challenges."

Professor Vittorio Michelassi, GE Global Research.

5.4 Support for small and medium-sized enterprises (SMEs)

HECToR has been used by SMEs to evaluate the benefits available from HPC, to analyse an innovative new marine device, and even to help brew the perfect cup of coffee.

Examples of partnerships and impacts involving SMEs were relatively few in number, reflecting the nature of the research enabled by HECToR and SMEs' limited capacity to engage in long-term partnerships to inform their code base or product development.

Small companies that need HPC can rarely afford the levels of investment needed to acquire systems that will make a difference to their business – most have to make do with modest systems that do not allow HPC to show its full potential. Access to systems such as HECToR on a pay-per-use basis can however give SMEs the opportunity to evaluate high capability HPC without major capital investment.

HECToR was an important factor in helping EPCC, the HECToR service provider, in its mission to transfer technology to industry, and in particular to SMEs, through the Supercomputing Scotland initiative (see www.supercomputingscotland.org).

SMEs that benefited from this include Prospect, an Aberdeen-based engineering company specialising in renewable energy; Fios Genomics, a biotechnology company in Edinburgh; and Glasgow-based Partrac who used HECToR to analyse an innovative new marine device.

HECToR was also used in the early stages of the European Commission-funded Fortissimo project, which offers an HPC simulation service aimed at SMEs with similar properties to cloud computing (on demand and pay-per-use).

Mark Sawyer, Business Development Manager at EPCC explained: 'The existence of systems such as HECToR enables SMEs to make a sound business case either to invest in HPC infrastructure, or to use the system as an on-demand production service. However SMEs also face an expertise gap, so it is the combination of HPC hardware, operational and in-depth support teams and software developers that helps them overcome this barrier. In this sense it was the HECToR service, together with our model of carrying out consultancy projects with industry that has been successful; hardware by itself is not enough.'

"The project and collaboration has been fruitful for our business. The atmosphere of creativity and science has inspired myself and staff, and this transfers into the approach they have at work."

Maxwell Colonna-Dashwood, 2012 & 2014 UK Barista Champion and 2012 & 2014 World Finalist.

HPC has also found application in the food and drink industry. Dr Christopher H. Hendon from the University of Bath has published on the application of HPC tools to the perhaps surprisingly complex chemical extraction required to produce the perfect cup of coffee.

He used this knowledge to help a Bath coffee shop owner to become the 2014 UK Barista Champion and number 5 in the world. His work has also featured in Chemistry World and in the popular media (including Business Insider and various BBC regional radio stations) and was one of four projects nominated by HPC Wire (Magazine) for the best application of HPC in the entertainment industry.

5.5 Public policy, health and environmental impacts

HECToR played a significant role in delivering broader societal impact. It was used to improve climate modelling and energy conservation, to undertake research on health and well-being and to support work in the aviation and automotive sectors to reduce pollution and increase engine efficiency.

Of the 100 survey respondents 18% noted impacts on the public sector including a small number of policies informed, mainly in the climate/sustainability/energy fields but also in terms of EU HPC infrastructure.

There were a significant number of impacts noted on forecasting, particularly in terms of long term weather patterns but also for climate change and adaption.

HECToR has been used extensively in producing codes and results which have informed various Met Office models, one such example being highlighted in more detail in the case study "A more certain climate", shown on page 43.

Energy conversation, efficiency, sustainability and new forms of energy production/storage were common themes, including a new materials for energy storage theme within the Materials Chemistry Consortium. An example of HECToR enabling new energy paradigms is described in more detail on page 30 in the case study "The fusion future".

Aside from energy conservation the environment featured heavily in the impacts described. For example, over 10% of impacts referred to modelling the environmental impact of particular interventions.

This includes a project led by Dr Len Shaffrey on increasing understanding of climate change and variability. It originally examined how El Nino affects tropical cyclones and how increasing the resolution of climate models improves the representation of a wide range of climate phenomena. It has since gone on to be supported via a Knowledge Transfer Partnership (KTP) with BP whereby the environmental risk to offshore infrastructure in the North Sea is being examined.

Likewise, impacts on the aviation and automotive sectors were identified in terms of reducing pollution by the use of new materials and/or increasing the efficiency of engines for the same purpose.

Furthermore, a small number of impacts on health and well-being have been produced, one of which is described in more detail in the case study "Body modelling", shown on page 22.

The "Jurassic impact" case study on page 27 details how health related impacts have been produced alongside impacts on public engagement with science and the media.

These examples of HECToR's impact on public policy, health and the environment illustrate the growing societal value of computational research in the twenty-first century. The models and forecasts enabled by facilities such as HECToR are fast becoming an indispensable tool for effective policy development, and can help science enter the public consciousness as never before.

Further examples of HECToR's environmental impact are summarised on the next page.

Examples of environmental impacts underpinned by HECToR:

Underpinning the global climate change debate

Professor David Stevenson was a contributing author on the Fifth Assessment Report (AR5) of the Intergovernmental Panel on Climate Change (IPCC). His research results feature prominently, including in the Summary for Policymakers (Figure SPM5 – ozone and Methane). This report aims to inform climate change policies worldwide.

Assessing ozone levels

John Plane, Professor of Atmospheric Chemistry at the University of Leeds was involved in the international World Meteorological Organization's (WMO) ozone assessment (2011), which included his research results from HECToR.

Communicating the impact of climate change to the public and financial services sector

Professor Pier Luigi Vidale, a HECToR user, is a senior scientist at the National Centre for Atmospheric Science and Willis Chair of Climate System Science and Climate Hazards at the University of Reading. He has had a significant impact on government policy via IPCC participation and on industry via coordination of the Willis Research Network, the world's largest collaboration between public science and the financial sector. Members of this network have brought this research to the attention of the public via interviews for the Today programme, Newsnight, BBC News, BBC Breakfast, BBC Radio, Sky News, print media and an NCAS Climate initiative for the general public.

Improved forecasting of weather phenomena

Dr Nicolas Klingaman from the National Centre for Atmospheric Science/University of Reading improved the ability of the Met Office Unified Model to simulate the Madden-Julian oscillation, the leading driver of weekly and monthly variations in tropical rainfall, including the Asian and Australian monsoons. An improved simulation of this phenomenon has allowed the Met Office to produce better forecasts of tropical rainfall, with benefits to users of forecast information throughout the tropics, including farmers who can delay the planting of delicate crops or store water in drought periods.

Protecting the ozone layer

HECToR results produced by Professor John Pyle of the Department of Chemistry at the University of Cambridge fed into the Montreal Protocol (on substances that deplete the ozone layer) discussions, of particular relevance to DEFRA and the EU.

Protecting the marine environment

Dr Dmrtiy Aleynik of the Scottish Marine Institute aided development of offshore renewable energy extraction and the aquatic farming industry by producing a better understanding the hydrodynamics around Scotland via increased understanding of sea lice and Harmful Algal Bloom (HAB) dispersal.

Case study

A more certain climate

HECToR has helped the UK and the rest of the world to better understand the impacts of climate change in order to adapt more effectively.

High-resolution models of the world's oceans are an integral component of future climate change predictions. They allow scientists to investigate hugely complex scenarios such as how global warming may influence ocean currents and the implications of an ice-free Arctic.

By exploiting the calculation speed of HECToR to magnify the resolution of its models, the National Oceanography Centre (NOC) has identified new ocean circulation phenomena.

The NOC has worked closely with the Met Office to combine these models with atmosphere and sea-ice models. This work has been influential in the decision by the Intergovernmental Panel on Climate Change to run its next set of climate change scenarios with the highest resolution models yet. They will be operational in 2016.

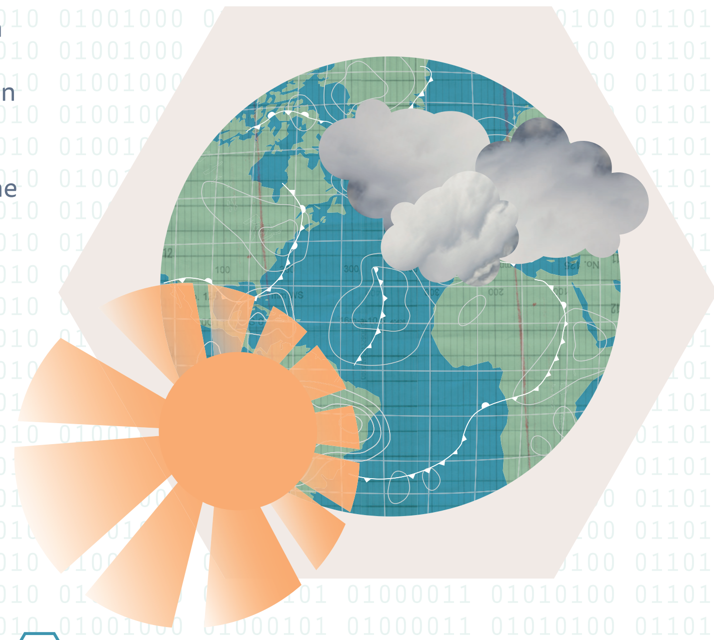
Modelling at very high resolutions allows researchers to study precise details that could have a significant impact on the climate. For example they can explore how different light scenarios could affect plant growth in oceans, which in turn changes the carbon flux.

Dr Andrew Coward, a specialist in large ocean scale modelling at the NOC, said: "We could never do this kind of higher resolution work on a global scale without a supercomputer like HECToR. As soon as you lower the resolution you begin to lose crucial data and decrease the reliability of the models."

Coward's ocean models, which have been featured in documentaries for National Geographic and Channel 4, allow the Met Office a glimpse of the future. HECToR produced models at a resolution of one quarter of a degree at a time when the Met Office's own supercomputer was running them at one degree. Now it is using its new machine to perform one-quarter degree resolutions; Coward is using HECToR's successor ARCHER to run models at one twelfth of a degree.

The Met Office is continually developing its weather and climate models – and HECToR has played its part in their design. In July 2014 the Met Office adopted its new ENDGame dynamical core, which allowed it to increase the resolution of its global weather forecasts and improve their accuracy. Research has already begun on the next-generation dynamical core, which is expected to come into operation within the next 10 years.

Professor Rob Scheichl and Dr Eike Mueller, of the University of Bath, are part of a group of academics that, under the GungHo! project, is developing the new model which the Met Office believes will deliver a "step change in scalability required to continue to exploit future generations of computers".



5.6 Indicators of future impact

Much of the work done on HECToR was at a fundamental level, and has not yet translated into direct socio-economic impact. The award of £66m of follow on funding for projects supported by HECToR and the progression of 88% of major projects on HECToR onto its successor, ARCHER, provide important indicators that the original research was valuable, and is thus more likely to yield impact in the future.

In addition to the consideration of examples of impact this study also examined follow on funding as a proxy for perceived success. A total of £66m in follow on funding was identified from the HECToR related grants awarded by the EPSRC.

As expected a large proportion of subsequent projects were funded by the Research Councils but there are also significant proportions being supported by other UK funders, including charities, the European Commission and industry.

This indicates that HECToR-enabled research led to valuable findings, which are now being drawn on in subsequent studies. Further evidence of this can be found in the high rate of continuation from the HECToR service to ARCHER. A total of 151 out of 253 (60%) projects have progressed from HECToR to ARCHER, representing more than 95% of the usage on HECToR. Forty-four out of the 50 (88%) largest projects have already moved from HECToR to ARCHER.

Proportion of follow on grants by number of grants

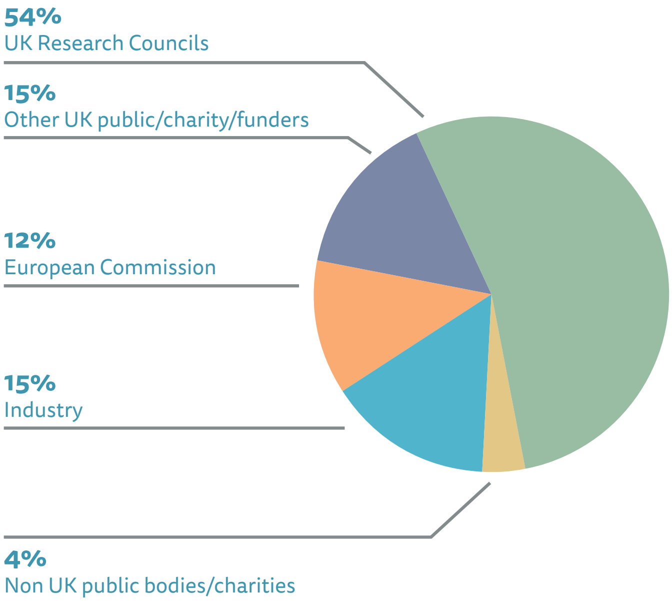


Figure 14

	Value of follow on projects	Number of follow on projects
UK Research Councils	£46m	42
Industry	£2m	12
European Commission	£15m	9
Other UK public/charity funders	£2m	12
Non UK public bodies/charities	£1m	3
Total	**~£66m**	**78**

6.0

Evaluating the HECToR model

6.1 How HECToR was run and funded

The model used to procure and manage HECToR is heavily geared towards the requirements of the service's users, and designed to promote competition and value for money in the procurement process. The relatively short-term nature of contracts for service provision and computational science and engineering support is however at odds with the service's status as a strategic asset of the UK.

As the primary funding agency for HECToR, EPSRC procured the hardware, facilities management and computational science and engineering support through three separate contracts. Following award of the facilities management contract to EPCC, the hardware contract with Cray was novated to them. A more typical model, commonly deployed in the US and Europe, is for a dedicated supercomputing centre to handle hardware procurement on behalf of the relevant funding agency.

HECToR cost a total of £118m over the course of its life, comprising £60m in capital expenditure and a further £58m on resource spend. Resource costs were split between the three partner Research Councils, with NERC and BBSRC contributing 22% and 5% of the total running costs respectively.

The House of Lords Select Committee's 2013 report *Scientific Infrastructure* notes that failure to make adequate provision for operating costs is a common issue in large infrastructure projects of this nature. In the case of HECToR, operating costs proved to be more than 50% higher than originally budgeted, due largely to tenders for facilities management and CSE support being higher than the initial estimates and a 10 month delay in the planned start date.

In our view, strengths of the approach taken to HECToR's procurement and management included the following:

- An emphasis on meeting the needs of end users through their close engagement in

£118m
Total cost of HECToR over the course of its life

This comprises:

£60m capital expenditure

£58m resources

Figure 15

the system's procurement and management. This was rightly prioritised over maximising the theoretical performance of the system or placement on the top 500 list of supercomputing sites[26].

- Additional investment made in the delivery of computational science and engineering support. This proved extremely beneficial to academic and industrial users, helping them to make more efficient use of HECToR's capabilities.

- Flexibility from the EPSRC and the other Research Councils in adapting resource allocation and other processes in response to evolving requirements, and in balancing the requirements of different disciplinary areas.

- The promotion of competition in all elements of the procurement, which mitigates the risk of centres and hardware suppliers becoming too closely associated and helps to ensure value for money.

Weaknesses of the HECToR model included:

- Due to the rapid development of HPC technology, hardware suppliers were unlikely to commit to providing the best available solution in the latter phases of the contract period. This risk was only partially mitigated through the use of a 'Four plus Two' contract structure, where EPSRC retained the option to extend the contract by two years with the same provider or to let a new two year contract to a new provider.

- The relatively short nature of the contracts for facilities management and CSE support meant only a handful of tenders were received, and providers found it difficult to plan and invest over the longer term. For example, a combined heat and power plant would offer increased energy efficiency and reduced operating costs for the Advanced Computing Facility, but requires a planning horizon of some ten years, while development and retention of staff with relevant expertise is heavily compromised in the latter stages of a CSE contract of only six years' duration.

- Parallel procurement of the hardware and facilities management services meant EPSRC were unable to draw on the technical expertise within facilities management providers such as EPCC at the hardware procurement stage.

- The close alignment of CSE support to use of the HECToR facility restricted the wider benefits of this service. We note that initiatives introduced late in HECToR's life to extend the distributed CSE service to universities were substantially oversubscribed, and considered to be highly beneficial by the user community.

The cost of moving data to and from a remote HPC service means cloud infrastructure is unlikely to offer a viable alternative to a national facility in the foreseeable future, and so the case for such a facility remains strong.

Nevertheless, the challenges of managing big data and the opportunities presented by cloud services and cluster computing mean a more flexible and heterogeneous approach to hardware procurement may become appropriate as the service continues to evolve.

The UK Government has recently affirmed its commitment to a long-term, strategic approach to investment in scientific infrastructure[27]. In view of this, we believe the national facility should increasingly be treated as a strategic asset. Consideration should be given to decoupling short-term, two or three year, contracts for hardware procurement from long-term strategic contracts for CSE and facilities management services in future procurements of this nature.

6.2 Service utilisation and resource allocation

Benchmarking suggests HECToR's utilisation fell slightly below the average for European Tier-O facilities, and there remains scope to introduce greater flexibility in resource allocation in order to maximise usage of the national service.

The proportion of HECToR's theoretical capacity that was used in each year of its life is shown in figure 16. Two pan-European studies of Tier-O HPC availability and utilisation, completed in 2008 and 2011, found average utilisations of 71% and 79% respectively, compared with 65% and 69% for HECToR.

Our work suggested the below average levels of utilisation achieved on HECToR reflected the following factors:

- Machines dedicated to narrow disciplinary areas were able to achieve higher levels of utilisation than HECToR
- The allocation of time on HECToR for 3-5 year periods led to users 'stockpiling' time
- The initial arrangements for resource allocation, based on peer reviewed grants and fixed consortia allocations, were insufficiently flexible to maximise utilisation.

These weaknesses were partially addressed over the system's life, leading to higher levels of utilisation in later years. The dedicated resource allocation panel (RAP) introduced in 2010 allowed users to apply for time on HECToR outside of the standard grant application process, and several other initiatives were introduced to encourage greater utilisation. Nevertheless, we were informed that a number of sound scientific proposals were rejected on grounds that they did not fit the narrow remit of the RAP. We are pleased to note that the panel's remit has subsequently been expanded, and that time allocations on HECToR's successor, ARCHER, are made over much shorter time periods, typically two years.

HECToR utilisation by funding source

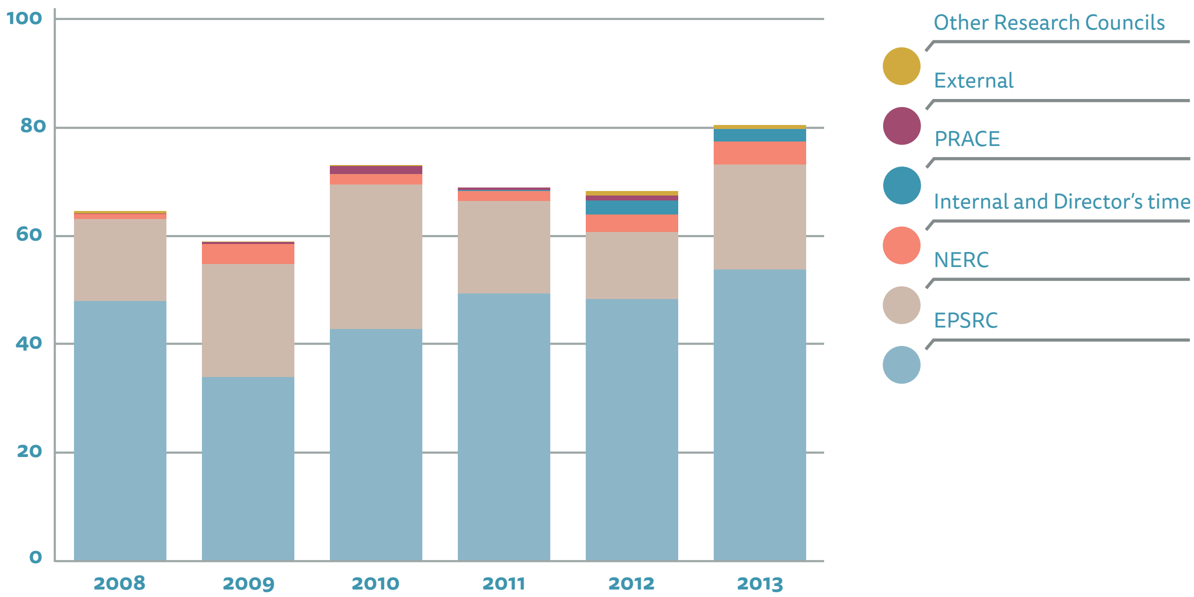


Figure 16

6.3 Performance against critical success factors

HECToR successfully delivered the majority of critical success factors identified within the service's original business case, including a major expansion of CSE support and strengthened partnerships with US and European HPC facilities. Areas of under-performance were levels of industrial partnering on the system, which fell below target, and failure to fully implement planned arrangements for evaluation and monitoring.

A number of critical success factors and an associated benefits realisation plan were put in place at the outset of HECToR's life. We reviewed the service's delivery against each of the identified targets, and noted a number of significant achievements:

- Development of a benchmarking process for the purposes of hardware procurement, based on user codes.
- A high level of technical reliability was achieved, despite some issues in the early stages of HECToR's life and following a major upgrade in 2010.
- Successful establishment of a Resource Allocation Panel in 2010, whose role was to control over-utilisation and encourage greater capability usage.
- Delivery of Computational Science and Engineering Support equivalent to 20 FTEs per annum, twice the level of effort provided by the previous HPCx service.
- Establishment of the Cray Centre of Excellence for HECToR, whose role was to work closely with the service and CSE providers to maximise usage of the computational resource.
- Successful completion of joint simulations in conjunction with US National Science Foundation facilities, and participation in the Distributed European Infrastructure for Supercomputing Applications (DEISA) and Partnership for Advanced Computing in Europe (PRACE) initiatives.

However, we noted a small number of areas where the service fell short of expectations, or planned activities were not followed through. The most significant of these were:

- **Industrial partnering on the system** – A minimum target was set for 20% of grants with time on HECToR to include an industrial collaborator. Our work found that only 11% of survey respondents had worked directly with an industrial collaborator in practice, although a further 21% were involved in indirect collaborations with industry.
- **Evaluation and monitoring** – Bi-annual citation analysis of papers supported by HECToR and an international review of the service in its third year of operation were anticipated as part of the benefits realisation plan. We note that these did not take place in practice, and the collation of output data for the purposes of our review required extensive consultation with the user community, with only a limited evidence base being available from existing EPCC and RCUK systems.

7.0

Conclusion

7.0 Conclusion

HECToR has delivered world-leading research, enabled collaborations that span the globe, benefited international corporations and SMEs alike, and informed evidence-based public policy. In a rapidly changing technological environment and in the context of constrained public finances the need for a national HPC facility remains a constant. If this capability were to be lost the long-term damage to the UK's knowledge and skills base could prove irreparable.

HECToR was set up to enable fundamental research leading to new scientific discoveries and knowledge. It has done so with tremendous success, resulting in research that has been of enormous importance to the scientific community around the world.

Since HECToR's inception, the emphasis on enabling impact from the scientific research base has changed markedly. We have shown in this report that not only has HECToR enabled some highly significant advances in our fundamental understanding of the world around us but also that researchers associated with HECToR have considered the most relevant pathway to impact for that knowledge.

Many have formed partnerships in order that those most effectively equipped to apply that knowledge have access to it sooner and with a greater depth of understanding. In turn this means that some of the fundamental knowledge produced with the aid of HECToR has already started to find application in small and large businesses and public sector organisations across the UK and internationally.

We have further shown that HECToR has enabled some very significant international partnerships where the UK's reputation for excellence in particular research fields has been enhanced.

The UK's e-infrastructure has evolved rapidly since 2007. Big data, cloud computing and the growing number of regional HPC facilities all open up new opportunities for researchers.

> "There is a clear and ongoing need for provision of a HPC national service to provide the capability to tackle leading edge computational science and simulation"
>
> Report of the e-Infrastructure Advisory Group, 2011

Nevertheless, our findings echo those of the UK HPC Special Interest Group in 2010[28] and the e-Infrastructure Advisory Group in 2011[29], which both found a compelling case for a national facility such as HECToR.

It is recognised that investment in HPC infrastructure is fraught with challenge. Such investments are extremely costly and difficult to justify in times of economic austerity. It is also true that the research findings, software codes and skilled researchers developed through HECToR will continue to deliver benefits that far outlive the hardware itself.

However, the nature of research, and in particular HEC-based research, means that if funders were to "pull the plug" for a year or two it is unlikely that the UK would recover, at least during the tenure of the current research leaders.

With the growing rate of investment being made by other countries in HPC, to regain the UK's current strong position in the field thereafter would require a far more significant investment to "kick start" an ailing research community.

In considering the case for future investment in national HPC facilities, we believe EPSRC should address the following priorities:

- **Securing the facility's position as a strategic asset** – The national HPC facility is a strategic asset of the UK, and its enduring value lies in the capability of its service providers and the skill-sets of its staff. Securing this value for the long-term requires strategic planning and investment that is not unduly tied to the short useful economic life of HPC hardware.

- **Maximising flexibility in hardware procurement** – Consideration should be given to a more flexible and heterogeneous approach to hardware procurement in future, based on a formal needs analysis, which could offer greater value to the facility's broad community of users.

- **Developing responsiveness to end-users of research** – HECToR's economic and societal impact occurred largely through the efforts of its academic user community. The national facility's impact could be further increased through improving connectivity with local and regional HPC facilities, and actively promoting both direct and indirect collaborations with non-academic partners.

- **Ongoing impact evaluation** – Ongoing collation and analysis of the facility's impact (as envisaged in the original Benefits Realisation Plan for HECToR) and improved data capture of associated research outputs would ensure a robust evidence base is available to support future evaluation exercises.

HECToR was the jewel in the crown of the UK's e-Infrastructure, and played a fundamental role in supporting world-leading UK computational research, and in translating this research into wider economic and societal benefits.

The UK must continue to build on this position of strength, securing the knowledge and skills-base HECToR has enabled for the benefit of future generations of researchers and society at large.

Notes

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2 See www.gov.uk/government/publications/eight-great-technologies-infographics

3 Department for Business Innovation and Skills (2014) Creating the Future: A 2020 Vision for Science and Research available at: www.gov.uk/government/consultations/science-and-research-proposals-for-long-term-capital-investment

4 www.top500.org

5 Department for Business, Innovation and Skills (2014) Insights from international benchmarking of the UK science and innovation system, available at: www.gov.uk/government/publications/science-and-innovation-system-international-benchmarking

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9 Technopolis Group (2013) Big Science and Innovation, available at: www.gov.uk/government/uploads/system/uploads/attachment_data/file/249715/bis-13-861-big-science-and-innovation.pdf

10 A 2010 study of the economic impact of Russell Group universities found that the timescale from basic, curiosity driven research to first realising a commercial return averaged over 17 years. See The economic impact of research conducted in Russell Group universities, available at: www.russellgroup.ac.uk/uploads/RG_ImpactOfResearch2.pdf

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13 U.S. Council on Competitiveness (2008) Advance: Benchmarking Industrial Use of High Performance Computing for Innovation, available at: www.compete.org/publications/detail/486/advance

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18 Joseph, E., Conway, S. And Dekate, C., (2013). Creating Economic Models Showing the relationship between investments in HPC and the resulting financial ROI and Innovation and how it can impact a nation's competitiveness and innovation. IDC #243296, Framingham: IDC.

19 See: www.rcuk.ac.uk/RCUK-prod/assets/documents/impacts/TypologyofResearchImpacts.pdf

20 See www.epsrc.ac.uk/research/ourportfolio/themes/researchinfrastructure/subthemes/einfrastructure/strategy/roadmap

21 See: www.epsrc.ac.uk/research/ourportfolio/themes/researchinfrastructure/subthemes/einfrastructure/software

22 For a more in-depth exploration of these issues please refer to the 2013 Big Science Facilities and Innovation report by Technopolis (www.technopolis-group.com/?report=big-science-facilities-innovation).

23 Commissariat à l'Energie Atomique (CEA) et al (2009) European Research Infrastructures, Development Watch (ERID-Watch) available at: http://cordis.europa.eu/documents/documentlibrary/125670151EN6.pdf

24 Elsevier SciVal data for all UK publications 2008 – 2014, in all subject areas.

25 www.publications.parliament.uk/pa/ld201314/ldselect/ldsctech/76/7604.htm

26 www.top500.org

27 Department for Business Innovation and Skills (2014) Creating the Future: A 2020 Vision for Science and Research available at: www.gov.uk/government/uploads/system/uploads/attachment_data/file/321522/bis-14-757-consultation-on-proposals-for-long-term-capital-investment-in-science-and-research-v2.pdf

28 See: http://hpc-sig.org/publications

29 See: www.rcuk.ac.uk/RCUK-prod/assets/documents/documents/e-IAGreport.pdf

30 See: www.rcuk.ac.uk/RCUK-prod/assets/documents/impacts/TypologyofResearchImpacts.pdf

31 See: www.rcuk.ac.uk/RCUK-prod/assets/documents/innovation/expectationssei.pdf

32 See www.epsrc.ac.uk/research/ourportfolio/themes/researchinfrastructure/subthemes/einfrastructure/software

Annex 1
Bibliometric measures and analysis methodology

Methodology

The Elsevier bibliometric methodology is based on the theoretical principles and best practices developed in the field of quantitative science and technology studies, particularly in science and technology indicators research.

The Handbook of Quantitative Science and Technology Research: The Use of Publication and Patent Statistics in Studies of S&T Systems (Moed, Glänzel and Schmoch, 2004) provides a good overview of this field and is based on the pioneering work of Derek de Solla Price (1978), Eugene Garfield (1979) and Francis Narin (1976) in the USA, and Christopher Freeman, Ben Martin and John Irvine in the UK (1981, 1987), and several European institutions including the Centre for Science and Technology Studies at Leiden University, the Netherlands, and the Library of the Academy of Sciences in Budapest, Hungary.

The analyses of research output data in this report are based on recognised advanced indicators (e.g., the concept of relative citation impact rates). Our base assumption is that such indicators are useful and valid, though imperfect and partial measures, in the sense that their numerical values are determined by research performance and related concepts, but also by other influencing factors that may cause systematic biases.

In the past decade, the field of indicators research has developed best practices that state how indicator results should be interpreted and which influencing factors should be taken into account. The Elsevier methodology builds on these practices.

Bibliometric Indicators – Definitions

Citation is a formal reference to earlier work made in an article or patent, frequently to other journal articles.

A citation is used to credit the originator of an idea or finding and is usually used to indicate that the earlier work supports the claims of the work citing it. The number of citations received by an article from subsequently published articles is a proxy of the quality or importance of the reported research.

Field-Weighted Citation Impact (FWCI) is an indicator of mean citation impact, and compares the actual number of citations received by an article with the expected number of citations for articles of the same document type (article, review, or conference proceeding paper), publication year, and subject field.

Where the article is classified in two or more subject fields, the harmonic mean of the actual and expected citation rates is used. The indicator is therefore always defined with reference to a global baseline of 1.00 and intrinsically accounts for differences in citation accrual over time, differences in citation rates for different document types (reviews typically attract more citations than research articles, for example) as well as subject-specific differences in citation frequencies overall and over time and document types.

It is one of the most sophisticated indicators in the modern bibliometric toolkit. When FWCI is used as a snapshot, an unweighted variable window is applied.

The FWCI value for “2008,” for example, comprises of articles published in 2008 and their FWCI in the period 2008 to 2014, while for “2014,” it comprises of articles published in 2014 and their FWCI in 2014 alone.

When FWCI is used in trend analysis, a weighted moving window is applied. The FWCI value for “2010,” for example, comprises of the weighted average of the unweighted variable FWCI values for 2008 and 2012 (weighted 13.3% each), 2009 and 2011 (weighted 20% each), and 2010 (weighted 33.3%).

The weighting applies in the same ratios for previous years also. However, for the most recent years, it is not possible to extend the weighted average by two years on either side, so weightings are readjusted across the remaining available values.

Highly cited articles (unless otherwise indicated) are those in the top-cited X% of all articles published and cited in a given period.

Annex 2
HECToR HEC Consortia

Consortium
Materials Chemistry Consortium
UK Turbulence Consortium
Plasma Physics HEC
Bimolecular Simulation HEC
Car-Parrinello
Mesoscale Engineering Science (COMES)
Ocean Modelling
NERC Centres for Atmospheric Research (NCAS)
Computational Mineral Physics
The Sea Shelf Consortium (now merged with the Ocean Modelling consortium)

Annex 3
RCUK Impact Typology, Expectations and Software as Infrastructure Strategy

RCUK Impact Typology[30]

- Changing organisational culture and practices
- Enhancing the research capacity, knowledge and skills of public, private and third sector organisations
- Wealth creation, economic prosperity and regeneration
- Improving health and well-being
- Enhancing cultural enrichment and quality of life
- Commercialisation and exploitation
- Improving social welfare, social cohesion and/or national security
- Attracting R&D investment
- Enhancing the effectiveness and sustainability of organisations including public services and businesses
- Environmental sustainability, protection and impact
- Evidence based policy-making and influencing public policies
- Increasing public engagement with research and related societal issues.

RCUK Expectations for Societal and Economic Impact[31]

The Research Councils give their funding recipients considerable flexibility and autonomy in the delivery of their research, postgraduate training and knowledge transfer activities. This flexibility and autonomy encompasses project definition, management, collaboration, participation, promotion and the dissemination of research outputs; this approach enables excellence with impact.

In return, the Research Councils expect those who receive funding to:

- demonstrate an awareness of the wider environment and context in which their research takes place
- demonstrate an awareness of the social and ethical implications of their research, beyond usual research conduct considerations, and take account of public attitudes towards those issues
- engage actively with the public at both the local and national levels about their research and its broader implications
- identify potential benefits and beneficiaries from the outset, and through the full life cycle of the project(s)
- maintain professional networks that extend

beyond their own discipline and research community

- publish results widely – considering the academics, user and public audiences for research outcomes
- exploit results where appropriate, in order to secure social and economic return to the UK
- manage collaborations professionally, in order to secure maximum impact without restricting the future progression of research
- ensure that research staff and students develop research, vocational and entrepreneurial skills that are matched to the demands of their future career paths
- take responsibility for the curation, management and exploitation of data for future use
- work in partnership with the Research Councils for the benefit of the UK.

Software as an Infrastructure Strategic Goals[32]

- Shaping Capability
- Developing Leaders and Skilled People
- Delivering Impact
- Ensuring Trust
- Planning for the Future.

EPSRC
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